Engineering and Scientific Subroutine Library for AIX



# Guide and Reference

Engineering and Scientific Subroutine Library for AIX



# Guide and Reference

#### Notes!

- Before using this information and the product it supports, be sure to read the general information under "Special Notices" on page xix.
- For a summary of changes for ESSL Version 3 Release 1.1, see page xxxiii.

#### Second Edition (October 1998)

This edition applies to Version 3 Release 1.1 of the IBM\* Engineering and Scientific Subroutine Library (ESSL) for Advanced Interactive Executive (AIX)\* licensed program, program number 5765-C42 and to all subsequent releases and modifications until otherwise indicated by new editions. Significant changes or additions to the text and illustrations are indicated by a vertical line (|) to the left of the change.

In this document, ESSL refers to the above version of ESSL for AIX. Changes are periodically made to the information herein.

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IBM 3838 Array Processor							 					

# **Looking for a Subroutine?**

CGEADD 381         CTBMW 358         DGER 307         DPTNG 923         DTPMW 352           CGEF 466         CTBSW 578         DGER1 307         DPTS 576         DTPSW 526           CGEMM 411         CTPSW 526         DGES 469         DQINT 870         DTREC 867           CGEMMS 405         CTRMM 428         DGESUB 388         DRCFT2 792         DTRMM 428           CGEMVI 395         CTRMM 352         DGESVF 674         DRCFT3 813         DTRWV 352           CGEMV 296         CTRSM 532         DGESVF 674         DRCFT3 813         DTRMV 352           CGERC 307         CTRSW 526         DGETMI 460         DROTG 242         DTRSW 526           CGERC 307         CVEA 259         DGETMO 450         DSCMTG 253         DURXOR 953           CGESM 469         CVEM 267         DGETRS 483         DSCTR 253         DURXOR 953           CGESUB 388         CWLEV 874         DGHMQ 942         DSDCG 661         DVEM 259           CGESUB 388         CWLEV 874         DGHMQ 942         DSDCG 666         DVES 263           CGETTMI 450         CYAX 271         DGKFS 595         DSDGCG 666         DVES 263      <	CAXPY 216 CAXPYI 288 CCOPY 219 CDOTC 222 CDOTCI 291 CDOTU 222 CDOTUI 291 CGBMV 340	CSCTR 279 CSROT 249 CSSCAL 253 CSWAP 256 CSYAX 271 CSYMM 420 CSYR2K 442 CSYRK 435	DGEICD 514 DGELLS 687 DGEMM 411 DGEMMS 405 DGEMTX 296 DGEMUL 395 DGEMV 296 DGEMX 296	DPOICD 519 DPOLY 861 DPOSM 503 DPPF 492 DPPFCD 508 DPPICD 519 DPPS 500 DPTF 574	DSYR 323 DSYR2 331 DSYR2K 442 DSYRK 435 DTBMV 358 DTBSV 578 DTPI 540 DTPINT 906
CGEF 466         CTPMV 352         DGES 469         DQINT 870         DTREC 867           CGEMMM 411         CTPSV 526         DGESM 473         DRCFT 755         DTRI 540           CGEMMS 405         CTRMM 428         DGESUB 388         DRCFT2 792         DTRMM 428           CGEMUL 395         CTRMV 352         DGESVF 674         DRCFT3 813         DTRMV 352           CGEWC 307         CTRSV 526         DGETMI 450         DROTG 249         DTRSM 532           CGERC 307         CVEA 259         DGETMO 453         DSBMV 347         DURAND 946           CGES 469         CVEM 267         DGETRF 479         DSCAL 253         DURXOR 953           CGESM 473         CVES 263         DGETRS 483         DSCTR 279         DVEA 259           CGESMB 388         CWLEV 874         DGHMQ 942         DSDCG 661         DVEM 267           CGETIMI 450         CYAX 271         DGKFRS 595         DSDGCG 666         DVES 263           CGETIMI 450         CYAX 271         DGKTRN 983         DSDMX 372         DWLEV 874           CGETIMI 450         CYAX 271         DGKTRS 983         DSINF 778         DYAX 271 <t< td=""><td>CGEADD 381</td><td>CTBCV 578</td><td>DGER 307</td><td>DPTNQ 923</td><td>DTPMV 352</td></t<>	CGEADD 381	CTBCV 578	DGER 307	DPTNQ 923	DTPMV 352
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CGEMMS 405         CTRMM 428         DGESUB 388         DRCFT2 792         DTRMM 428           CGEMWL 296         CTRSM 532         DGESVF 674         DRCFT3 813         DTRSM 552           CGERC 307         CTRSW 526         DGESVS 682         DROT 249         DTRSM 552           CGERC 307         CVEA 259         DGETMI 450         DROTG 242         DTRSW 526           CGES 469         CVEM 267         DGETRF 479         DSCAL 253         DURAND 945           CGESM 473         CVES 263         DGETRS 483         DSCTR 279         DVEA 259           CGESUB 388         CWLEV 874         DGHMQ 942         DSDCG 661         DVEM 267           CGETMI 450         CYAX 271         DGKFS 595         DSDGGG 666         DVES 263           CGETRM 453         CZAXPY 274         DGKTRN 983         DSDMX 372         DWLEV 874           CGETRS 479         DASUM 213         DGLQQ 935         DSINF 778         DYAX 271           CGETRS 483         DAXPYI 288         DGLNQ 926         DSKFS 613         DZAXPY 274           CGTHR 282         DAXPYII 288         DGLNQ 929         DSKTRN 989         DZAXPY 274					
CGEMV 296         CTRSM 532         DGESVS 682         DROT 249         DTRSM 532           CGERC 307         CTRSV 526         DGETMI 450         DROTG 242         DTRSV 526           CGERU 307         CVEA 259         DGETMO 453         DSBMV 347         DURAND 946           CGES 469         CVEM 267         DGETRF 479         DSCAL 253         DURXOR 953           CGESSM 473         CVES 263         DGETRS 483         DSCTR 279         DVEA 259           CGESUB 388         CWLEV 874         DGHMQ 942         DSDCG 661         DVEM 259           CGETMI 450         CYAX 271         DGKFS 595         DSDGCG 666         DVES 263           CGETMO 453         CZAXPY 274         DGKTRN 983         DSDMX 372         DWLEV 874           CGETRS 479         DASUM 213         DGLOQ 935         DSINF 778         DYAX 271           CGETRS 483         DAXPY 216         DGLNQ 926         DSKFS 613         DZAXDM 213           CGTHR 282         DAXPYI 288         DGLNQ2 929         DSKTRN 989         DZAXPY 274           CGTNP 565         DCFT 747         DGSS 555         DSLMX 315         EINFO 960 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
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CGESUB 388         CWLEV 874         DGHMQ 942         DSDCG 651         DVEM 267           CGETMI 450         CYAX 271         DGKFS 595         DSDGCG 666         DVES 263           CGETMO 453         CZAXPY 274         DGKTRN 983         DSDMX 372         DWLEV 874           CGETRS 479         DASUM 213         DGLGQ 935         DSINF 778         DYAX 271           CGETRS 483         DAXPY 216         DGLNQ 926         DSKFS 613         DZASUM 213           CGTRS 282         DAXPYI 288         DGLNQ2 929         DSKTRN 989         DZAXPY 274           CGTNP 565         DCFT 747         DGSS 585         DSLMX 315         EINFO 960           CGTNPS 565         DCFT 747         DGSS 591         DSLR1 323         ERRSAV 963           CGTNPS 571         DCFT2 785         DGTF 560         DSLR2 331         ERRSET 964           CHBMV 347         DCFT3 807         DGTHR 282         DSMCG 659         IBSRCH 890           CHEMM 420         DCOPY 219         DGTHR 285         DSMMCG 659         IBSRCH 890           CHEMW 315         DCRFT 763         DGTNP 565         DSMMCG 659         IBSRCH 890	CGES 469	CVEM 267	DGETRF 479	DSCAL 253	DURXOR 953
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CGETRF 479         DASUM 213         DGLGQ 935         DSINF 778         DYAX 271           CGETRS 483         DAXPY 216         DGLNQ 926         DSKFS 613         DZASUM 213           CGTHR 282         DAXPYI 288         DGLNQ2 929         DSKTRN 989         DZAXPY 274           CGTNPS 565         DESR 890         DGRAQ 938         DSLEV 707         DZNRM2 236           CGTNP 565         DCFT 747         DGSF 585         DSLMX 315         EINFO 960           CGTNPF 568         DCOSF 771         DGSS 591         DSLR1 323         ERRSAV 963           CGTNPS 571         DCFT2 785         DGTF 560         DSLR2 331         ERRSET 964           CHBMV 347         DCFT3 807         DGTHR 282         DSMCG 643         ERRSTR 966           CHEMM 420         DCOPY 219         DGTHR 285         DSMGG 659         IBSRCH 890           CHEMV 315         DCRFT 763         DGTNP 565         DSMMTM 365         ICAMAX 201           CHER 323         DCRFT2 799         DGTNPF 568         DSMTM 368         IDAMAX 201           CHER2K 442         DCSIN2 915         DGTS 563         DSORT 882         IDAMIN 204					
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CGTHR 282         DAXPYI 288         DGLNQ2 929         DSKTRN 989         DZAXPY 274           CGTHRZ 285         DBSRCH 890         DGRAQ 938         DSLEV 707         DZNRM2 236           CGTNP 565         DCFT 747         DGSF 585         DSLMX 315         EINFO 960           CGTNPF 568         DCOSF 771         DGSS 591         DSLR2 323         ERRSAV 963           CGTNPS 571         DCFT2 785         DGTF 560         DSLR2 331         ERRSET 964           CHBMV 347         DCFT3 807         DGTHR 282         DSMCG 643         ERRSTR 966           CHEMW 420         DCOPY 219         DGTHRZ 285         DSMMCG 659         IBSRCH 890           CHEMV 315         DCRFT 763         DGTNP 565         DSMMX 365         ICAMAX 201           CHER 323         DCRFT2 799         DGTNPF 568         DSMTM 368         IDAMAX 201           CHER2 331         DCRFT3 819         DGTNPS 571         DSORT 882         IDAMIN 204           CHER2K 442         DCSINZ 915         DGTS 563         DSORTS 887         IDMAX 207           CHEK 435         DCSINT 909         DIZC 864         DSORTX 884         IDMIN 210 <td></td> <td></td> <td></td> <td></td> <td></td>					
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CGTNPF 568         DCOSF 771         DGSS 591         DSLR1 323         ERRSAV 963           CGTNPS 571         DCFT2 785         DGTF 560         DSLR2 331         ERRSET 964           CHBMV 347         DCFT3 807         DGTHR 282         DSMCG 643         ERRSTR 966           CHEMM 420         DCOPY 219         DGTHRZ 285         DSMGCG 659         IBSRCH 890           CHEMV 315         DCRFT 763         DGTNP 565         DSMMX 365         ICAMAX 201           CHER 323         DCRFT2 799         DGTNPF 568         DSMTM 368         IDAMAX 201           CHER2 331         DCRFT3 819         DGTNPS 571         DSORT 882         IDAMIN 204           CHER2K 442         DCSIN2 915         DGTS 563         DSORTS 887         IDMAX 207           CHERK 435         DCSINT 909         DIZC 864         DSORTX 884         IDMIN 210           CHLEV 707         DDCON 847         DNAXPY 226         DSPEV 707         IESSL 967           CHPEV 707         DDCOR 847         DNORM2 239         DSPR 323         ISAMIN 201           CHPRV 315         DDOT 222         DNORM2 239         DSPRV 316         ISMIN 210					
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	CSCAL 253	DGEGV 724	DPOFCD 508	DSYMV 315	

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# **Programming Interfaces**

This Engineering and Scientific Subroutine Library (ESSL) Version 3 Guide and Reference manual is intended to help the customer to do application programming. This ESSL Version 3 Guide and Reference manual documents General-use Programming Interface and Associated Guidance Information provided by ESSL Version 3.

General-use programming interfaces allow the customer to write programs that obtain the services of ESSL Version 3.

## **About This Book**

The Engineering and Scientific Subroutine Library (ESSL) for AIX is a set of high-performance mathematical subroutines. ESSL is provided as five run-time libraries, running on RS/6000\* POWER, PowerPC, POWER2, and POWER3 processors. ESSL can be used with Fortran, C, C++, and Programming Language/I (PL/I) programs operating under the AIX operating system.

This book is a guide and reference manual for using ESSL in doing application programming. It includes:

- An overview of ESSL and guidance information for designing, coding, and processing your program, as well as migrating existing programs, and diagnosing problems
- Reference information for coding each ESSL calling sequence

This book is written for a wide class of ESSL users: scientists, mathematicians, engineers, statisticians, computer scientists, and system programmers. It assumes a basic knowledge of mathematics in the areas of ESSL computation. It also assumes that users are familiar with Fortran, C, C++, and PL/I programming.

#### **How to Use This Book**

**Front Matter** consists of the Table of Contents, Special Notices, and Preface. Use these to find or interpret information in the book.

**Part 1. "Guide Information"** provides guidance information for using ESSL. It covers the user-oriented tasks of learning, designing, coding, migrating, processing, and diagnosing. Use the following chapters when performing any of these tasks:

- Chapter 1, "Learning about ESSL" gives an introduction to ESSL, providing highlights and general information. Read this chapter first to determine the aspects of ESSL you want to use.
- Chapter 2, "Designing Your Program" provides ESSL-specific information that helps you design your program. Read this chapter before designing your program.
- Chapter 3, "Setting Up Your Data Structures" describes all types of data structures, such as vectors, matrices, and sequences. Use this information when designing and coding your program.
- Chapter 4, "Coding Your Program" tells you how to code your scalar and array data, how to code calls to ESSL in Fortran, C, C++, and PL/I programs, and how to do the coding necessary to handle errors. Use this information when coding your program.
- Chapter 5, "Processing Your Program" describes how to process your program under your particular operating system on your hardware. Use this information after you have coded your program and are ready to run it.
- Chapter 6, "Migrating Your Programs" explains all aspects of migration to ESSL, to this version of ESSL, to different processors, and to future releases and future processors. Read this chapter before starting to design your program.

 Chapter 7, "Handling Problems" provides diagnostic procedures for analyzing all ESSL problems. When you encounter a problem, use the symptom indexes at the beginning of this chapter to guide you to the appropriate diagnostic procedure.

Part 2. "Reference Information" provides reference information you need to code the ESSL calling sequences. It covers each of the mathematical areas of ESSL, and the utility subroutines. Each chapter begins with an introduction, followed by the subroutine descriptions. Each introduction applies to all the subroutines in that chapter and is especially important in planning your use of the subroutines and avoiding problems. To understand the information in the subroutine descriptions, see "How to Interpret the Subroutine Descriptions" on page xxx. Use the appropriate chapter when coding your program:

- Chapter 8, "Linear Algebra Subprograms"
- · Chapter 9, "Matrix Operations"
- Chapter 10, "Linear Algebraic Equations"
- · Chapter 11, "Eigensystem Analysis"
- Chapter 12, "Fourier Transforms, Convolutions and Correlations, and **Related Computations**"
- Chapter 13, "Sorting and Searching"
- Chapter 14, "Interpolation"
- Chapter 15, "Numerical Quadrature"
- Chapter 16, "Random Number Generation"
- · Chapter 17, "Utilities"

Appendix A. Basic Linear Algebra Subprograms provides a list of the Level 1, 2, and 3 Basic Linear Algebra Subprograms (BLAS) included in ESSL.

Appendix B. LAPACK provides a list of the LAPACK subroutines included in ESSL.

**Glossary** contains definitions of terms used in this book.

Bibliography provides information about publications related to ESSL. Use it when you need more information than this book provides.

# How to Find a Subroutine Description

If you want to locate a subroutine description and you know the subroutine name, you can use the "Looking for a Subroutine?" on page xvii, following the Table of Contents. You can also find them listed individually or under the entry "subroutines, ESSL" in the Index.

### Where to Find Related Publications

If you have a question about the SP, PSSP, or a related product, the following online information resources make it easy to find the information you are looking

 If you have installed the RS/6000 SP Resource Center available with Parallel System Support Programs (PSSP) Version 3 Release 1 or later, you can access the SP Resource Center by issuing the command:

#### /usr/lpp/ssp/bin/resource\_center

If you have the SP Resource Center on CD ROM, see the readme.txt file for information on how to run it.

Access the RS/6000 Web site at:

http://www.rs6000.ibm.com

A list of all ESSL publications, as well as related programming and hardware publications, are listed in the bibliography. Also included is a list of math background publications you may find helpful, along with the necessary information for ordering them from independent sources. See "Bibliography" on page BIB-1.

## How to Look Up a Bibliography Reference

Special references are made throughout this book to mathematical background publications and software libraries, available through IBM, publishers, or other companies. All of these are described in detail in the bibliography. A reference to one of these is made by using a bracketed number. The number refers to the item listed under that number in the bibliography. For example, reference [1] cites the first item listed in the bibliography.

# **Special Terms**

Standard data processing and mathematical terms are used in this book. Terminology is generally consistent with that used for Fortran. See the Glossary for definitions of terms used in this book.

# **Short and Long Precision**

Because ESSL can be used with more than one programming language, the terms short precision and long precision are used in place of the Fortran terms single precision and double precision.

# **Subroutines and Subprograms**

An ESSL subroutine is a named sequence of instructions within the ESSL product library whose execution is invoked by a call. A subroutine can be called in one or more user programs and at one or more times within each program. The ESSL subroutines are referred to as subprograms in the area of linear algebra subprograms. The term subprograms is used because it is consistent with the BLAS. Many of the linear algebra subprograms correspond to the BLAS; these are listed in Appendix A on page APA-1.

## How to Interpret the Subroutine Names with a Prefix Underscore

A name specified in this book with an underscore (\_) prefix, such as \_GEMUL, refers to all the versions of the subroutine with that name. To get the entire list of subroutines that name refers to, substitute the first letter for each version of the subroutine. For example, \_GEMUL, refers to all versions of the matrix multiplication subroutine: SGEMUL, DGEMUL, CGEMUL, and ZGEMUL. You do not use the underscore in coding the names of the ESSL subroutines in your program. You code a complete name, such as SGEMUL. For details about these names, see "The Variety of Mathematical Functions" on page 4.

## **Abbreviated Names**

The abbreviated names used in this book are defined below.

Short Name	Full Name
AIX	Advanced Interactive Executive
BLAS	Basic Linear Algebra Subprograms
ESSL	IBM Engineering and Scientific Subroutine Library
HTML	Hypertext Markup Language
LAPACK	Linear Algebra Package
PL/I	Programming Language/I
POWER, POWER2, POWER3, and PowerPC processors	RS/6000 processors
SL MATH	Subroutine Library—Mathematics
SMP	Symmetric Multi-Processing
SSP	Scientific Subroutine Package

#### **Fonts**

This book uses a variety of special fonts to distinguish between many mathematical and programming items. These are defined below.

Special Font	Example	Description
Italic with no subscripts	m, inc1x, aux, iopt	Calling sequence argument or mathematical variable
Italic with subscripts	$x_1, a_{mn}, x_{j1,j2}$	Element of a vector, matrix, or sequence
Bold italic lowercase	x, y, z	Vector or sequence
Bold italic uppercase	A, B, C	Matrix
Gothic uppercase	A, B, C, AGB	Array
	IM=ISMAX(4,X,2)	Fortran statement

# **Special Notations and Conventions**

This section explains the special notations and conventions used in this book to describe various types of data.

#### Scalar Data

Following are the special notations used in the examples in this book for scalar data items. These notations are used to simplify the examples, and they do not imply usage of any precision. For a definition of scalar data in Fortran, C, C++, and PL/I, see Chapter 4 on page 111.

Data Item	Example	Description
Character item	'T'	Character(s) in single quotation marks
Hexadecimal string	X'97FA00C1'	String of 4-bit hexadecimal characters
Logical item	.TRUE. .FALSE.	True or false logical value, as indicated
Integer data	1	Number with no decimal point
Real data	1.6	Number with a decimal point
Complex data	(1.0,-2.9)	Real part followed by the imaginary part
Continuation	1.6666	Continue the last digit (1.66666666 and so forth)

#### **Vectors**

A vector is represented as a single row or column of subscripted elements enclosed in square brackets. The subscripts refer to the element positions within the vector:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

$$\begin{bmatrix} x_1 & x_2 & x_3 & \dots & x_n \end{bmatrix}$$

For a definition of vector, see "Vectors" on page 55.

#### **Matrices**

A matrix is represented as a block of elements enclosed in square brackets. Subscripts refer to the row and column positions, respectively:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \ddots \\ \vdots & & \ddots \\ \vdots & & \ddots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

For a definition of matrix, see "Matrices" on page 62.

## Sequences

Sequences are used in the areas of sorting, searching, Fourier transforms, convolutions, and correlations. For a definition of sequences, see "Sequences" on page 105.

## **One-Dimensional Sequences**

A one-dimensional sequence is represented as a series of elements enclosed in parentheses. Subscripts refer to the element position within the sequence:

$$(x_1, x_2, x_3, ..., x_n)$$

## **Two-Dimensional Sequences**

A two-dimensional sequence is represented as a series of columns of elements. (They are represented in the same way as a matrix without the square brackets.) Subscripts refer to the element positions within the first and second dimensions, respectively:

## Three-Dimensional Sequences

A three-dimensional sequence is represented as a series of blocks of elements. Subscripts refer to the elements positions within the first, second, and third dimensions, respectively:

$a_{111}$	$a_{121}$ .	$a_{1n1}$	$a_{112}$	$a_{122}$ .	$a_{1n2}$		$a_{11p}$	$a_{12p}$ .	$ a_{1np}$
$a_{211}$	$a_{221}$	$a_{2n1}$	$a_{212}$	$a_{222}$	$a_{2n2}$		$a_{21p}$	$a_{22p}$	$a_{2np}$
•	•	•	•	•	•	•••	•	•	•
•	•	•	•	•	•		•	•	•
	•	•	•	•	•			•	•
$a_{m11}$	$a_{m21}$ .	$ a_{mn1}$	$a_{m12}$	$a_{m22}$ .	$ a_{mn2}$		$a_{m1p}$	$a_{m2p}$ .	$ a_{mnp}$

## **Arrays**

Arrays contain vectors, matrices, or sequences. For a definition of array, see "How Do You Set Up Your Arrays?" on page 29.

## **One-Dimensional Arrays**

A one-dimensional array is represented as a single row of numeric elements enclosed in parentheses:

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown. In the following array, five elements are significant to the computation, and two elements not used in the computation exist between each of the elements shown:

$$(1.0, .., .., 2.0, .., .., 3.0, .., .., 4.0, .., .., 5.0)$$

This notation is used to show vector elements inside an array.

### **Two-Dimensional Arrays**

A two-dimensional array is represented as a block of numeric elements enclosed in square brackets:

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown. The following array contains three rows and two columns not used in the computation:

This notation is used to show matrix elements inside an array.

## Three-Dimensional Arrays

A three-dimensional array is represented as a series of blocks of elements separated by ellipses. Each block appears like a two-dimensional array:

$$\begin{bmatrix} 1.0 & 11.0 & 5.0 & 25.0 \\ 2.0 & 12.0 & 6.0 & 26.0 \\ 3.0 & 13.0 & 7.0 & 27.0 \\ 4.0 & 14.0 & 8.0 & 28.0 \end{bmatrix} \begin{bmatrix} 10.0 & 111.0 & 15.0 & 125.0 \\ 20.0 & 112.0 & 16.0 & 126.0 \\ 30.0 & 113.0 & 17.0 & 127.0 \\ 40.0 & 114.0 & 18.0 & 128.0 \end{bmatrix} ... \begin{bmatrix} 100.0 & 11.0 & 15.0 & 25.0 \\ 200.0 & 12.0 & 16.0 & 26.0 \\ 300.0 & 13.0 & 17.0 & 27.0 \\ 400.0 & 14.0 & 18.0 & 28.0 \end{bmatrix}$$

Elements not significant to the computation are usually not shown in the array. One dot appears for each element not shown, just as for two-dimensional arrays.

## Special Characters, Symbols, Expressions, and Abbreviations

The mathematical and programming notations used in this book are consistent with traditional mathematical and programming usage. These conventions are explained below, along with special abbreviations that are associated with specific values.

Item	Description
Greek letters: $\alpha$ , $\sigma$ , $\omega$ , $\Omega$	Symbolic scalar values
a	The absolute value of a
a•b	The dot product of <b>a</b> and <b>b</b>
$X_i$	The i-th element of vector x
c <sub>ij</sub>	The element in matrix $\boldsymbol{c}$ at row $i$ and column $j$
$x_1 \dots x_n$	Elements from $x_1$ to $x_n$
i = 1, n	i is assigned the values 1 to n
<i>y</i> ← <i>x</i>	Vector $\boldsymbol{y}$ is replaced by vector $\boldsymbol{x}$
xy	Vector <b>x</b> times vector <b>y</b>
AX ≅ B	AX is congruent to B
a <sup>k</sup>	a raised to the k power
e <sup>x</sup>	Exponential function of x
<b>A</b> T; <b>x</b> T	The transpose of matrix $\boldsymbol{A}$ ; the transpose of vector $\boldsymbol{x}$
$\bar{x}; \bar{A}$	The complex conjugate of vector <b>x</b> ; the complex conjugate of matrix <b>A</b>
$\bar{x}_i; \bar{c}_{jk}$	The complex conjugate of the complex vector element $x_{i}$ , where:
	if $x_i = (a_i, b_i)$ ,
	then $\bar{x}_i = (a_i, -b_i)$
	The complex conjugate of the complex matrix element $c_{jk}$
<b>x</b> H; <b>A</b> H	The complex conjugate transpose of vector <b>x</b> ; the complex conjugate transpose of matrix <b>A</b>

Item	Description
n	The sum of elements $x_1$ to $x_n$
$\sum_{i=1}^{n} x_{i}$	
i = 1	
$\sqrt{a+b}$	The square root of a+b
•	The integral from a to b of f(v) dv
$\int_{a}^{b} f(x) dx$	The integral from a to b of f(x) dx
$\ \mathbf{x}\ _2$	The Euclidean norm of vector <b>x</b> , defined as:
	$\sqrt{\sum_{j=1}^{n} \left  x_{j} \right ^{2}}$
$\ \boldsymbol{A}\ _1$	The one norm of matrix <b>A</b> , defined as:
	$\max \left\{ \sum_{i=1}^{m}  a_{ij} , \ 1 \le j \le n \right\}$
$\ \mathbf{A}\ _2$	The spectral norm of matrix <b>A</b> , defined as:
	$\max\{\ \mathbf{A}\mathbf{x}\ _2:\ \mathbf{x}\ _2 = 1\}$
∥ <b>A</b> ∥ <sub>F</sub>	The Frobenius norm of matrix <b>A</b> , defined as:
	$\sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2}$
<b>A</b> -1	The inverse of matrix <b>A</b>
<b>A</b> -T	The transpose of <b>A</b> inverse
<i>A</i>	The determinant of matrix A
m by n matrix A	Matrix <b>A</b> has m rows and n columns
sin a	The sine of a
cos b	The cosine of b
SIGN (a)	The sign of a; the result is either + or -
address {a}	The storage address of a
max( <b>x</b> )	The maximum element in vector <b>x</b>
min( <b>x</b> )	The minimum element in vector <b>x</b>
ceiling(x)	The smallest integer that is greater than or equal to x
floor(x)	The largest integer that is not greater than <i>x</i>
int(x)	The largest integer that is less than or equal to x
x mod(m)	x modulo $m$ ; the remainder when $x$ is divided by $m$
∞	Infinity
π	Pi, 3.14159265

## **How to Interpret the Subroutine Descriptions**

This section explains how to interpret the information in the subroutine descriptions in Part 2 of this book.

## **Description**

Each subroutine description begins with a brief explanation of what the subroutine does. When we combine the description of multiple versions of a subroutine, we give enough information to enable you to easily tell the differences among the subroutines. Differences usually occur in either the function performed or the data types required for each subroutine.

## **Syntax**

This shows the syntax for the Fortran, C, C++, and PL/I calling statements:

Fortran	CALL NAME-1   NAME-2     NAME-n ( <i>arg-1</i> , <i>arg-2</i> , , <i>arg-m</i> , )
C and C++	name-1   name-2     name-n ( <i>arg-1</i> , , <i>arg-m</i> );
PL/I	CALL NAME-1   NAME-2     NAME-n (arg-1, arg-2, ,arg-m, );

#### The syntax indicates:

- The programming language (Fortran, C, C++, or PL/I)
- Each possible subroutine name that you can code in the calling sequence. Each name is separated by the | (or) symbol. You specify only one of these names in your calling sequence. (You do not code the | in the calling sequence.)
- The arguments, listed in the order in which you code them in the calling sequence. You must code them all in your calling sequence.

You can distinguish between input arguments and output arguments by looking at the "On Entry" and "On Return" sections, respectively. An argument used for both input and output is described in both the "On Entry" and "On Return" sections. In this case, the input value for the argument is overlaid with the output value.

The names of the arguments give an indication of the type of data that you should specify for the argument; for example:

- Names beginning with the letters i through n, such as m, incx, iopt, and isign, indicate that you specify integer data.
- Names beginning with the letters a through h and o through z, such as b, t, alpha, sigma, and omega, indicate that you specify real or complex data.

# On Entry

This lists the input arguments, which are the arguments you pass to the ESSL subroutine. Each argument description first gives the meaning of the argument, and then gives the form of data required for the argument. (To help you avoid errors, output arguments are also listed, along with a reference to the On Return section.)

#### On Return

This lists the output arguments, which are the arguments passed back to your program from the ESSL subroutine. Each argument description first gives the meaning of the argument, and then gives the form of data passed back to your program for the argument.

#### **Notes**

The notes describe any programming considerations and restrictions that apply to the arguments or the data for the arguments. There may be references to other parts of the book for further information.

#### **Function**

This is a functional, or mathematical, description of the function performed by this subroutine. It explains what computation is performed, not the implementation. It explains the variations in the computation depending on the input arguments. References are made, where appropriate, to mathematical background books listed in the bibliography. References appear as a number enclosed in square brackets, where the number refers to the item listed under that number in the bibliography. For example, reference [1] cites the first item listed.

## Special Usage

These are unique ways you can use the subroutine in your application. In most cases, this book does not address applications of the ESSL subroutines; however, in special situations where the functional capability of the subroutine can be extended by following certain rules for its use, these rules are described in this section.

#### **Error Conditions**

These are all the ESSL run-time errors that can occur in the subroutine. They are organized under three headings; Computational Errors, Input-Argument Errors, and Resource Errors. The return code values resulting from these errors are also explained.

# **Examples**

The examples show how you would call the subroutine from a Fortran program. They show a variety of uses of the subroutine. Except where it is important to show differences in use between the various versions of the subroutine, the simplest version of the subroutine is used in the examples. In most cases, this is the short-precision real version of the subroutine. Each example provides a description of the important features of the example, followed by the Fortran calling sequence, the input data, and the resulting output data.

## What's New for ESSL for AIX

This section summarizes all the changes made to ESSL for AIX.

#### What's New for ESSL Version 3 Release 1.1

- The ESSL POWER Library, the ESSL Thread-Safe Library, and the ESSL SMP Library are tuned for the RS/6000 POWER3.
- The ESSL POWER Library, the ESSL Thread-Safe Library, and the ESSL Symmetric Multi-Processing (SMP) Library now support both 32-bit environment and 64-bit environment applications. For details on creating 64-bit environment applications see Chapter 4 on page 111 and Chapter 5 on page 163. If you are migrating to a 64-bit environment, you may need to make changes to your calls to ERRSET. For details see "ERRSET—ESSL ERRSET Subroutine for ESSL" on page 964.
- ESSL for AIX provides distinct libraries for AIX 4.2.1 and AIX 4.3.2:
  - The AIX 4.2.1 ESSL Thread-Safe Library, the ESSL Thread-Safe POWER2 Library, and the ESSL SMP Library were built using the pthreads draft 7 library supplied on AIX 4.2.1. This is the same as ESSL Version 3.1.
  - The AIX 4.3.2 ESSL Thread-Safe Library, the ESSL Thread-Safe POWER2 Library, and the ESSL SMP Library were built using the pthreads library that conforms to the IEEE POSIX 1003.1-1996 specification supplied on AIX 4.3.

# **Changes for ESSL Version 3**

- ESSL for AIX provides two new run-time libraries:
  - The ESSL Symmetric Multi-Processing (SMP) Library provides thread-safe versions of the ESSL subroutines for use on the RS/6000 SMP (for example 604e) processors. In addition, a subset of these subroutines are also multithreaded versions; that is, they support the shared memory parallel processing programming model. You do not have to change your existing application programs that call ESSL to take advantage of the increased performance of using the SMP processors. You can simply re-link your existing programs. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 21 on page 26.
  - The ESSL Thread-Safe Library provides thread-safe versions of the ESSL subroutines for use on all RS/6000 processors. You may use this library to develop your own multithreaded applications.
    - If your existing application program calls ESSL, you only need to re-link your program to take advantage of the increased performance of the ESSL SMP Library or to use the ESSL Thread-Safe Library.
- ESSL provides new subroutines (\_GETRF and \_GETRS), bringing the total number of subroutines to 458.
- For those ESSL subroutines that require extra working storage to perform computations, ESSL now provides a way to dynamically allocate storage when

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it does not need to persist after the subroutine call. See "Using Auxiliary Storage in ESSL" on page 31.

- The files for the Hypertext Markup Language (HTML) version of the ESSL Version 3 Guide and Reference are packaged with the ESSL product.
- All the ESSL messages are provided in an ESSL message catalog.

# **Future Migration**

If you are concerned with migration to possible future releases of ESSL or possible future hardware, you should read "Planning for Future Migration" on page 170. That section explains what you can do now to prevent future migration problems.

## In Brief—What's Provided in ESSL for AIX

- ESSL provides five run-time libraries:
  - The ESSL SMP Library provides thread-safe versions of the ESSL subroutines for use on the RS/6000 SMP (for example, 604e or 630) processors. In addition, a subset of these subroutines are also multithreaded versions; that is, they support the shared memory parallel processing programming model. You do not have to change your existing application programs that call ESSL to take advantage of the increased performance of using the SMP processors. You can simply re-link your existing application programs. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 21 on page 26.
  - The ESSL Thread-Safe Library provides thread-safe versions of the ESSL subroutines for use on all RS/6000 processors. You may use this library to develop your own multithreaded applications.
  - The ESSL Thread-Safe POWER2 Library provides thread-safe versions of the ESSL subroutines and is tuned for the RS/6000 POWER2 uniprocessors. You may use this library to develop your own multithreaded applications.
  - The ESSL POWER Library is tuned for the RS/6000 POWER, POWER3, and PowerPC uniprocessors.
  - The ESSL POWER2 Library is tuned for the RS/6000 POWER2 uniprocessors.

All libraries are designed to provide high levels of performance for numerically intensive computing jobs on these respective processors. All versions provide mathematically equivalent results.

The ESSL POWER Library, the ESSL Thread-Safe Library, and the ESSL SMP Library support both 32-bit environment and 64-bit environment applications.

- Callable from Fortran, C, C++, and PL/I programs.
- For a list of subroutines, refer to "List of ESSL Subroutines" on page 10.

# Part 1. Guide Information

This part of the book is organized into seven chapters, providing guidance information on how to use ESSL. It is organized as follows:

- · Learning about ESSL
- Designing your program
- Setting up your data structures
- Coding your program
- Processing your program
- Migrating your programs
- Handling problems

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# **Chapter 1. Introduction and Requirements**

This chapter introduces you to the Engineering and Scientific Subroutine Library (ESSL) for Advanced Interactive Executive (AIX\*).

#### Overview of ESSL

This section gives an overview of the ESSL capabilities and requirements.

ESSL is a state-of-the-art collection of subroutines providing a wide range of mathematical functions for many different scientific and engineering applications. Its primary characteristics are performance, functional capability, and usability.

## **Performance and Functional Capability**

The mathematical subroutines, in nine computational areas, are tuned for performance on the RS/6000\*. The computational areas are:

- · Linear Algebra Subprograms
- Matrix Operations
- Linear Algebraic Equations
- Eigensystem Analysis
- · Fourier Transforms, Convolutions and Correlations, and Related Computations
- Sorting and Searching
- Interpolation
- Numerical Quadrature
- Random Number Generation

ESSL provides five run-time libraries:

- The ESSL Symmetric Multi-Processing (SMP) Library provides thread-safe versions of the ESSL subroutines for use on the RS/6000 SMP (for example, 604e or 630) processors. In addition, a subset of these subroutines are also multithreaded versions; that is, they support the shared memory parallel processing programming model. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 21 on page 26.
- The **ESSL Thread-Safe Library** provides thread-safe versions of the ESSL subroutines for use on all RS/6000 processors. You may use this library to develop your own multithreaded applications.
- The ESSL Thread-Safe POWER2 Library provides thread-safe versions of the ESSL subroutines and is tuned for the RS/6000 POWER2 processors. You may use this library to develop your own multithreaded applications.
- The **ESSL POWER Library** is tuned for the RS/6000 POWER, POWER3, and PowerPC uniprocessors.
- The ESSL POWER2 Library is tuned for the RS/6000 POWER2 uniprocessors.

All libraries are designed to provide high levels of performance for numerically intensive computing jobs on these respective processors. All versions provide mathematically equivalent results.

The ESSL POWER Library, the ESSL Thread-Safe Library, and the ESSL SMP Library support both 32-bit environment and 64-bit environment applications.

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The ESSL subroutines can be called from application programs written in Fortran, C, C++, and Programming Language/I (PL/I). ESSL runs under the AIX operating system.

## **Usability**

ESSL is designed for usability:

- · It has an easy-to-use call interface.
- If your existing application programs call ESSL, you only need to re-link your program to take advantage of the increased performance of the ESSL SMP Library or to use the ESSL Thread-Safe Library.
- It supports a 64-bit environment.

64-bit applications can be created on any AIX 4.3.2 system, but can only run on 64-bit hardware.

The data model used for a 64-bit environment is referred to as LP64. This data model supports 32-bit integers and 64-bit pointers. In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the **iusadr** argument for ERRSET. See "ERRSET—ESSL ERRSET Subroutine for ESSL" on page 964.

- It has informative error-handling capabilities, enabling you to calculate auxiliary storage sizes and transform lengths.
- An online book that can be displayed using an Hypertext Markup Language (HTML) document browser, is available for use with ESSL.

## The Variety of Mathematical Functions

This section describes the mathematical functions included in ESSL.

#### **Areas of Application**

ESSL provides a variety of mathematical functions for many different types of scientific and engineering applications. Some of the industries using these applications are: Aerospace, Automotive, Electronics, Petroleum, Finance, Utilities, and Research. Examples of applications in these industries are:

Structural Analysis
Computational Chemistry
Fluid Dynamics Analysis
Seismic Analysis
Reservoir Modeling
Quantitative Analysis
Time Series Analysis
Computational Techniques
Mathematical Analysis
Dynamic Systems Simulation
Nuclear Engineering
Electronic Circuit Design

#### What ESSL Provides

The subroutines provided in ESSL, summarized in Table 1, fall into the following groups:

- Nine major areas of mathematical computation, providing the computations commonly used by the industry applications listed above
- Utilities, performing general-purpose functions

To help you select the ESSL subroutines that fulfill your needs for performance, accuracy, storage, and so forth, see "Selecting an ESSL Subroutine" on page 25.

Table 1. Summary of ESSL Subroutines		Short-	Long-
ESSL Area of Computation	Integer Subroutines	Precision Subroutines	Precision Subroutines
Linear Algebra Subprograms:			
Vector-scalar	0	41	41
Sparse vector-scalar	0	11	11
Matrix-vector	0	32	32
Sparse matrix-vector	0	0	3
Matrix Operations: Addition, subtraction, multiplications, rank-k updates, rank-2k updates, and matrix transposes	0	25	26
Linear Algebraic Equations:			
Dense linear algebraic equations	0	30	32
Banded linear algebraic equations	0	18	18
Sparse linear algebraic equations	0	0	11
Linear least squares	0	3	3
<b>Eigensystem Analysis</b> : Solutions to the algebraic eigensystem analysis problem and the generalized eigensystem analysis problem	0	8	8
(Signal Processing) Computations:		-	
Fourier transforms	0	15	11
Convolutions and correlations	0	10	2
Related computations	0	6	6
Sorting and Searching: Sorting, sorting with index, and binary and sequential searching	5	5	5
Interpolation: Polynomial and cubic spline interpolation	0	4	4
Numerical Quadrature: Numerical quadrature on a set of points or on a function	0	6	6
Random Number Generation: Generating vectors of uniformly distributed and normally distributed random numbers	0	3	3
Utilities: General service operations	11	0	3
Total ESSL Subroutines	16	217	225

# **ESSL—Processing Capabilities**

ESSL provides five run-time libraries, the ESSL SMP Library, the ESSL Thread-Safe Library, the ESSL Thread-Safe POWER2 Library, the ESSL POWER2 Library, and the ESSL POWER Library. These libraries are designed to provide high levels of performance for numerically intensive computing jobs on the RS/6000 processors. To order the IBM Engineering and Scientific Subroutine Library for AIX, Version 3 Release 1.1, specify program number 5765-C42. Most of the subroutine calls are compatible with those in the ESSL/370 product. See the

Engineering and Scientific Subroutine Library Version 2.2 Guide and Reference for details.

## **Accuracy of the Computations**

ESSL provides accuracy comparable to libraries using equivalent algorithms with identical precision formats. Both short- and long-precision real versions of the subroutines are provided in most areas of ESSL. In some areas, short- and long-precision complex versions are also provided, and, occasionally, an integer version is provided. The data types operated on by the short-precision, long-precision, and integer versions of the subroutines are RS/6000 architecture precisions: ANSI/IEEE 32-bit and 64-bit binary floating-point format, and 32-bit integer. See the ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754-1985, for more detail. (There are ESSL-specific rules that apply to the results of computations on workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.)

For more information on accuracy, see "Getting the Best Accuracy" on page 44.

## **High Performance of ESSL**

**Algorithms:** The ESSL subroutines have been designed to provide high performance. (See references [30], [41], and [42].) To achieve this performance, the subroutines use state-of-the-art algorithms tailored to specific operational characteristics of the hardware, such as cache size, Translation Lookaside Buffer (TLB) size, and page size.

Most subroutines use the following techniques to optimize performance:

- Managing the cache and TLB efficiently so the hit ratios are maximized; that is, data is blocked so it stays in the cache or TLB for its computation.
- Accessing data stored contiguously—that is, using stride-1 computations.
- Exploiting the large number of available floating-point registers.
- · Using algorithms that minimize paging.
- On the PowerPC SMP processor:
  - The ESSL SMP Library is designed to exploit the processing power and shared memory of the SMP processor. In addition, a subset of the ESSL SMP subroutines have been coded to take advantage of increased performance from multithreaded (parallel) programming techniques. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 21 on page 26.
  - Choosing the number of threads depends on the problem size, the specific subroutine being called, and the number of physical processors you are running on. To achieve optimal performance, experimentation is necessary; however, picking the number of threads equal to the number of online processors generally provides good performance in most cases. In some cases, performance may increase if you choose the number of threads to be less than the number of online processors.

You should use the the XL Fortran XLSMPOPTS environment variable to specify the number of threads you want to create.

• On the POWER3 processor:

- Structuring the ESSL subroutines so, where applicable, the compiled code fully utilizes the dual floating-point execution units. Because two Multiply-Add instructions can be executed each cycle, neglecting overhead, this allows four floating-point operations per cycle to be performed.
- Structuring the ESSL subroutines so, where applicable, the compiled code takes full advantage of the hardware data prefetching.

#### • On the POWER2 processor:

- Structuring the ESSL subroutines so, where applicable, the compiled code fully utilizes the dual fixed-point and floating-point execution units. Because two Multiply-Add instructions can be executed each cycle, neglecting overhead, this allows four floating-point operations per cycle to be performed.
- Structuring the ESSL subroutines so, where applicable, the compiled code uses the POWER2 Load and Store Floating Point Quad instructions. For example, in one cycle, two Load Floating Point Quad instructions can be executed. Neglecting overhead, this allows four doublewords to be loaded per cycle.

#### On the POWER processor:

- Using algorithms that balance floating-point operations with loads in the innermost loop.
- Using algorithms that minimize stores in the innermost loops.
- Structuring the ESSL subroutines so, where applicable, the compiled code uses the Multiply-Add instructions. Neglecting overhead, these instructions perform two floating-point operations per cycle.

**Mathematical Techniques:** All areas of ESSL use state-of-the-art mathematical techniques to achieve high performance. For example, the matrix-vector linear algebra subprograms operate on a higher-level data structure, matrix-vector rather than vector-scalar. As a result, they optimize performance directly for your program and indirectly through those ESSL subroutines using them.

# The Fortran Language Interface to the Subroutines

The ESSL subroutines follow standard Fortran calling conventions and must run in the Fortran run-time environment. When ESSL subroutines are called from a program in a language other than Fortran, such as C, C++, or PL/I, the Fortran conventions must be used. This applies to all aspects of the interface, such as the linkage conventions and the data conventions. For example, array ordering must be consistent with Fortran array ordering techniques. Data and linkage conventions for each language are given in Chapter 4 on page 111.

#### Software and Hardware Products That Can Be Used with ESSL

This section describes the hardware and software products you can use with ESSL, as well as those products for installing ESSL and displaying the online documentation.

#### For ESSL—Hardware

ESSL runs on the IBM\* RS/6000 processors supported by the AIX operating systems.

64-bit applications require 64-bit hardware.

### **ESSL—Operating Systems**

ESSL is supported in the following operating system environments:

- AIX Version 4.2.1 or later modification levels (either product number 5765-655 or 5765-C34)
- AIX Version 4.3.2 or later modification levels (product number 5765-C34)

#### **ESSL—Software Products**

ESSL requires the software products shown in Table 2 for compiling and running.

To assist C and C++ users, an ESSL header file is provided. Use of this file is described in "C Programs" on page 129 and "C++ Programs" on page 145.

For Compiling	For Linking, Loading, or Running		
XL Fortran for AIX, Version 5.1.1 or later (program number 5808-AAR part number 04L2110) <i>-or-</i>	XL Fortran Run-Time Environment for AIX, Version 5.1.1 or later (program number 5808-AAR part num 04L2123) <i>–or–</i>		
XL High Performance Fortran for AIX, Version 1.3.1 or			
later (program number 5765-613) -or-	XL High Performance Run-Time Environment for AIX,		
IBM C, C++ compilers Version 3.6.4 or later <sup>2</sup> –or–	Version 1.3.1 or later (program number 5765-612)		
C for AIX, Version 4.3 or later (program number 5765-AAR part number 04L0675 with feature number 2163) –or–	C libraries <sup>1</sup>		
PL/I Set for AIX, Version 1.1 or later (program number 5765-549)			
<sup>1</sup> The AIX Version 4 product includes the C and math libraries in the Application Development Toolkit.			
<sup>2</sup> Available as a component of the VisualAge C++ Professional for AIX, Version 4, product.			

#### **Installation and Customization Products**

The ESSL licensed program is distributed on a 4-millimeter or an 8-millimeter cartridge. The ESSL Version 3 Release 1.1 Installation Memo provides the detailed information you need to install ESSL.

The ESSL product is packaged according to the AIX guidelines, as described in the IBM AIX Version 4 General Programming Concepts: Writing and Debugging Programs manual. The product can be installed using the smit command, as described in the IBM AIX Version 4 System Management Guide: Operating System and Devices manual.

### Software Products for Displaying ESSL Online Information

The ESSL Guide and Reference Version 3 is available in PostScript and HTML format on the product media.

To view the online publications shipped on the product media, you need the following:

- Access to a common HTML document browser (such as Netscape Navigator).
- The location of the HTML index file provided with the file sets. Contact your system administrator or installer for this location.

#### **ESSL Internet Resources**

This section describes how you can use the ESSL resources available over the Internet.

### **Obtaining Documentation**

The ESSL Version 3 Release 1.1 Guide and Reference is available in PDF and HTML format at the IBM RS/6000 Web site at:

http://www.rs6000.ibm.com/resource/aix\_resource/sp\_books

To view the ESSL PDF publication, you need access to the Adobe Acrobat Reader 3.0.1. The Acrobat Reader is shipped with the AIX Version 4.3 Bonus Pack and is also freely available for downloading from the Adobe web site at:

http://www.adobe.com.

# **Accessing ESSL's Product Home Pages**

The following home pages contain information on ESSL and Parallel ESSL:

For ESSL for AIX, use:

http://www.rs6000.ibm.com/software/Apps/essl.html

• For Parallel ESSL, use:

http://www.rs6000.ibm.com/software/sp\_products/esslpara.html

# Getting on the ESSL Mailing List

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#### **List of ESSL Subroutines**

This section provides an overview of the subroutines in each of the areas of ESSL.

Appendix A on page APA-1 contains a list of Level 1, 2, and 3 Basic Linear Algebra Subprograms (BLAS) included in ESSL.

Appendix B on page APB-1 contains a list of Linear Algebra Package (LAPACK) subroutines included in ESSL.

## **Linear Algebra Subprograms**

The linear algebra subprograms consist of:

- Vector-scalar linear algebra subprograms (Table 3)
- Sparse vector-scalar linear algebra subprograms (Table 4)
- Matrix-vector linear algebra subprograms (Table 5)
- Sparse matrix-vector linear algebra subprograms (Table 6)

#### Notes:

- 1. The term **subprograms** is used to be consistent with the Basic Linear Algebra Subprograms (BLAS), because many of these subprograms correspond to the BLAS.
- 2. Some of the linear algebra subprograms were designed in accordance with the Level 1 and Level 2 BLAS de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program.

#### Vector-Scalar Linear Algebra Subprograms

The vector-scalar linear algebra subprograms include a subset of the standard set of Level 1 BLAS. For details on the BLAS, see reference [73]. The remainder of the vector-scalar linear algebra subprograms are commonly used computations provided for your applications. Both real and complex versions of the subprograms are provided.

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX†■ ICAMAX†■	IDAMAX†■ IZAMAX†■	201
Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value	ISAMIN†	IDAMIN†	204
Position of the First or Last Occurrence of the Vector Element Having Maximum Value	ISMAX†	IDMAX†	207
Position of the First or Last Occurrence of the Vector Element Having Minimum Value	ISMIN†	IDMIN†	210
Sum of the Magnitudes of the Elements in a Vector	SASUM†• SCASUM†•	DASUM†• DZASUM†•	213
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY• CAXPY•	DAXPY• ZAXPY•	216
Copy a Vector	SCOPY• CCOPY•	DCOPY• ZCOPY•	219
Dot Product of Two Vectors	SDOT† CDOTU† CDOTC†	DDOT† ZDOTU† ZDOTC†	222
Compute SAXPY or DAXPY N Times	SNAXPY	DNAXPY	226
Compute Special Dot Products N Times	SNDOT	DNDOT	231
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2† SCNRM2†	DNRM2†■ DZNRM2†■	236
Euclidean Length of a Vector with No Scaling of Input	SNORM2† CNORM2†	DNORM2† ZNORM2†	239
Construct a Givens Plane Rotation	SROTG* CROTG*	DROTG• ZROTG•	242
Apply a Plane Rotation	SROT* CROT* CSROT*	DROT• ZROT• ZDROT•	249
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL* CSCAL*	DSCAL* ZSCAL* ZDSCAL*	253
Interchange the Elements of Two Vectors	SSWAP• CSWAP•	DSWAP■ ZSWAP■	256
Add a Vector X to a Vector Y and Store in a Vector Z	SVEA CVEA	DVEA ZVEA	259
Subtract a Vector Y from a Vector X and Store in a Vector Z	SVES CVES	DVES ZVES	263
Multiply a Vector X by a Vector Y and Store in a Vector Z	SVEM CVEM	DVEM ZVEM	267
Multiply a Vector X by a Scalar and Store in a Vector Y	SYAX CYAX CSYAX	DYAX ZYAX ZDYAX	271
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z	SZAXPY CZAXPY	DZAXPY ZZAXPY	274

Table 3 (Page 2 of 2). List of Vector-Scalar Linear Algebra Subpro	ograms		
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
† This subprogram is invoked as a function in a Fortran program.			
■ Level 1 BLAS			

#### Sparse Vector-Scalar Linear Algebra Subprograms

The sparse vector-scalar linear algebra subprograms operate on sparse vectors; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the vector-scalar subprograms. These subprograms represent a subset of the sparse extensions to the Level 1 BLAS described in reference [29]. Both real and complex versions of the subprograms are provided.

Table 4. List of Sparse Vector-Scalar Linear Algebra Subprograms			
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode	SSCTR CSCTR	DSCTR ZSCTR	279
Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode	SGTHR CGTHR	DGTHR ZGTHR	282
Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y	SGTHRZ CGTHRZ	DGTHRZ ZGTHRZ	285
Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y	SAXPYI CAXPYI	DAXPYI ZAXPYI	288
Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode	SDOTI† CDOTCI† CDOTUI†	DDOTI† ZDOTCI† ZDOTUI†	291
† This subprogram is invoked as a function in a Fortran program.		•	•

#### Matrix-Vector Linear Algebra Subprograms

The matrix-vector linear algebra subprograms operate on a higher-level data structure—matrix-vector rather than vector-scalar—using optimized algorithms to improve performance. These subprograms include a subset of the standard set of Level 2 BLAS. For details on the Level 2 BLAS, see [34] and [35]. Both real and complex versions of the subprograms are provided.

Table 5. List of Matrix-Vector Linear Algebra Subprograms			
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV⁴ CGEMV⁴ SGEMX§ SGEMTX§	DGEMV⁴ ZGEMV⁴ DGEMX§ DGEMTX§	296
Rank-One Update of a General Matrix	SGER CGERUCE	DGER⁴ ZGERU⁴ ZGERC⁴	307
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV CHPMV SSYMV CHEMV SSLMX	DSPMV⁴ ZHPMV⁴ DSYMV⁴ ZHEMV⁴ DSLMX§	315
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR CHPR SSYR CHER SSLR1§	DSPR  ZHPR  DSYR  ZHER  DSLR1§	323
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR2* CHPR2* SSYR2* CHER2* SSLR2§	DSPR24 ZHPR24 DSYR24 ZHER24 DSLR28	331
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV⁴ CGBMV⁴	DGBMV◀ ZGBMV◀	340
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV⁴ CHBMV⁴	DSBMV◀ ZHBMV◀	347
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STRMV CTRMV STPMV CTPMV	DTRMV• ZTRMV• DTPMV• ZTPMV•	352
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV◀ CTBMV◀	DTBMV∢ ZTBMV∢	358

<sup>◆</sup> Level 2 BLAS

## **Sparse Matrix-Vector Linear Algebra Subprograms**

The sparse matrix-vector linear algebra subprograms operate on sparse matrices; that is, only the nonzero elements of the matrix are stored. These subprograms provide similar functions to the matrix-vector subprograms.

Table 6 (Page 1 of 2). List of Sparse Matrix-Vector Linear Algebra Subprograms		
Descriptive Name	Long- Precision Subprogram	Page
Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode	DSMMX	365

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs.

Table 6 (Page 2 of 2). List of Sparse Matrix-Vector Linear Algebra Subprograms			
Descriptive Name Long- Precision Subprogram P			
Transpose a Sparse Matrix in Compressed-Matrix Storage Mode	DSMTM	368	
Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode	DSDMX	372	

# **Matrix Operations**

Some of the matrix operation subroutines were designed in accordance with the Level 3 BLAS de facto standard. If these subroutines do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subroutines, the updates could require modifications of the calling application program. For details on the Level 3 BLAS, see reference [32]. The matrix operation subroutines also include the commonly used matrix operations: addition, subtraction, multiplication, and transposition.

Table 7 (Page 1 of 2). List of Matrix Operation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Matrix Addition for General Matrices or Their Transposes	SGEADD CGEADD	DGEADD ZGEADD	381
Matrix Subtraction for General Matrices or Their Transposes	SGESUB CGESUB	DGESUB ZGESUB	388
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes	SGEMUL CGEMUL	DGEMUL ZGEMUL DGEMLP§	395
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm	SGEMMS CGEMMS	DGEMMS ZGEMMS	405
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM◆ CGEMM◆	DGEMM◆ ZGEMM◆	411
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM◆ CSYMM◆ CHEMM◆	DSYMM◆ ZSYMM◆ ZHEMM◆	420
Triangular Matrix-Matrix Product	STRMM◆ CTRMM◆	DTRMM◆ ZTRMM◆	428
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK+ CSYRK+ CHERK+	DSYRK◆ ZSYRK◆ ZHERK◆	435
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K+ CSYR2K+ CHER2K+	DSYR2K* ZSYR2K* ZHER2K*	442
General Matrix Transpose (In-Place)	SGETMI CGETMI	DGETMI ZGETMI	450
General Matrix Transpose (Out-of-Place)	SGETMO CGETMO	DGETMO ZGETMO	453

Table 7 (Page 2 of 2). List of Matrix Operation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page

<sup>◆</sup> Level 3 BLAS

# **Linear Algebraic Equations**

The linear algebraic equations consist of:

- Dense linear algebraic equations (Table 8)
- · Banded linear algebraic equations (Table 9)
- Sparse linear algebraic equations (Table 10)
- Linear least squares (Table 11)

#### Notes:

1. Some of the linear algebraic equations were designed in accordance with the Level 2 BLAS, Level 3 BLAS, and LAPACK de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program. For details on the Level 2 and 3 BLAS, see [32] and [34]. For details on LAPACK, see [8].

#### **Dense Linear Algebraic Equations**

The dense linear algebraic equation subroutines provide solutions to linear systems of equations for both real and complex general matrices and their transposes, positive definite real symmetric and complex Hermitian matrices, and triangular matrices. Some of these subroutines correspond to the Level 2 BLAS, Level 3 BLAS, and LAPACK routines described in references [32], [34], and [8].

Table 8 (Page 1 of 2). List of Dense Linear Algebraic Equation Sul	broutines		
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
General Matrix Factorization	SGEF CGEF SGETRF <sup>Δ</sup> CGETRF <sup>Δ</sup>	DGEF ZGEF DGETRF ZGETRF DGEFP§	466 479
General Matrix, Its Transpose, or Its Conjugate Transpose Solve	SGES CGES	DGES ZGES	469
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGESM CGESM SGETRS <sup>A</sup> CGETRS <sup>A</sup>	DGESM ZGESM DGETRS <sup>A</sup> ZGETRS <sup>A</sup>	473 483
General Matrix Factorization, Condition Number Reciprocal, and Determinant	SGEFCD	DGEFCD	488

<sup>§</sup> This subroutine is provided only for migration from earlier release of ESSL and is not intended for use in new programs.

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization	SPPF SPOF CPOF	DPPF DPOF ZPOF DPPFP§	492
Positive Definite Real Symmetric Matrix Solve	SPPS	DPPS	500
Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve	SPOSM CPOSM	DPOSM ZPOSM	503
Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant	SPPFCD SPOFCD	DPPFCD DPOFCD	508
General Matrix Inverse, Condition Number Reciprocal, and Determinant	SGEICD	DGEICD	514
Positive Definite Real Symmetric Matrix Inverse, Condition Number Reciprocal, and Determinant	SPPICD SPOICD	DPPICD DPOICD	519
Solution of a Triangular System of Equations with a Single Right-Hand Side	STRSV4 CTRSV4 STPSV4 CTPSV4	DTRSV* ZTRSV* DTPSV* ZTPSV*	526
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM◆ CTRSM◆	DTRSM◆ ZTRSM◆	532
Triangular Matrix Inverse	STRI STPI	DTRI DTPI	540

<sup>◆</sup> Level 2 BLAS

#### **Banded Linear Algebraic Equations**

The banded linear algebraic equation subroutines provide solutions to linear systems of equations for real general band matrices, real positive definite symmetric band matrices, real or complex general tridiagonal matrices, real positive definite symmetric tridiagonal matrices, and real or complex triangular band matrices.

Table 9 (Page 1 of 2). List of Banded Linear Algebraic Equation Subroutines				
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page	
General Band Matrix Factorization	SGBF	DGBF	546	
General Band Matrix Solve	SGBS	DGBS	550	
Positive Definite Symmetric Band Matrix Factorization	SPBF SPBCHF	DPBF DPBCHF	553	

<sup>◆</sup> Level 3 BLAS

<sup>△</sup> LAPACK

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Positive Definite Symmetric Band Matrix Solve	SPBS SPBCHS	DPBS DPBCHS	557
General Tridiagonal Matrix Factorization	SGTF	DGTF	560
General Tridiagonal Matrix Solve	SGTS	DGTS	563
General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting	SGTNP CGTNP	DGTNP ZGTNP	565
General Tridiagonal Matrix Factorization with No Pivoting	SGTNPF CGTNPF	DGTNPF ZGTNPF	568
General Tridiagonal Matrix Solve with No Pivoting	SGTNPS CGTNPS	DGTNPS ZGTNPS	571
Positive Definite Symmetric Tridiagonal Matrix Factorization	SPTF	DPTF	574
Positive Definite Symmetric Tridiagonal Matrix Solve	SPTS	DPTS	576
Triangular Band Equation Solve	STBSV⁴ CTBSV⁴	DTBSV⁴ ZTBSV⁴	578

## **Sparse Linear Algebraic Equations**

The sparse linear algebraic equation subroutines provide direct and iterative solutions to linear systems of equations both for general sparse matrices and their transposes and for sparse symmetric matrices.

Table 10 (Page 1 of 2). List of Sparse Linear Algebraic Equation Subroutines		
Descriptive Name	Long- Precision Subroutine	Page
General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns	DGSF	585
General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns	DGSS	591
General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode	DGKFS DGKFSP§	595
Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode	DSKFS DSKFSP§	613
Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows	DSRIS	632
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMCG‡	643
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDCG	651
General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMGCG‡	659
General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDGCG	666

Table 10 (Page 2 of 2). List of Sparse Linear Algebraic Equation Subroutines		
Descriptive Name	Long- Precision Subroutine	Page

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

#### **Linear Least Squares**

The linear least squares subroutines provide least squares solutions to linear systems of equations for real general matrices. Two methods are provided: one that uses the singular value decomposition and another that uses a QR decomposition with column pivoting.

Table 11. List of Linear Least Squares Subroutines				
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page	
Singular Value Decomposition for a General Matrix	SGESVF	DGESVF	674	
Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition	SGESVS	DGESVS	682	
Linear Least Squares Solution for a General Matrix Using a QR Decomposition with Column Pivoting	SGELLS	DGELLS	687	

# **Eigensystem Analysis**

The eigensystem analysis subroutines provide solutions to the algebraic eigensystem analysis problem Az = wz and the generalized eigensystem analysis problem Az = wBz (Table 12). Many of the eigensystem analysis subroutines use the algorithms presented in *Linear Algebra* by Wilkinson and Reinsch [93] or use adaptations of EISPACK routines, as described in the *EISPACK Guide Lecture Notes in Computer Science* in reference [81] or in the *EISPACK Guide Extension Lecture Notes in Computer Science* in reference [55]. (EISPACK is available from the sources listed in reference [49].)

Table 12 (Page 1 of 2). List of Eigensystem Analysis Subroutines				
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page	
Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix	SGEEV CGEEV	DGEEV ZGEEV	696	
Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPEV CHPEV	DSPEV ZHPEV	707	
Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPSV CHPSV	DSPSV ZHPSV	716	
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, Az=wBz, where A and B Are Real General Matrices	SGEGV	DGEGV	724	

<sup>‡</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Use DSRIS instead.

Table 12 (Page 2 of 2). List of Eigensystem Analysis Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, Az=wBz, where A Is Real Symmetric and B Is Real Symmetric Positive Definite	SSYGV	DSYGV	730

# Fourier Transforms, Convolutions and Correlations, and Related Computations

This signal processing area provides:

- Fourier transform subroutines (Table 13)
- Convolution and correlation subroutines (Table 14)
- Related-computation subroutines (Table 15)

#### **Fourier Transforms**

The Fourier transform subroutines perform mixed-radix transforms in one, two, and three dimensions.

	Short- Precision	Long- Precision	
Descriptive Name	Subroutine	Subroutine	Page
Complex Fourier Transform	SCFT SCFTP§	DCFT	747
Real-to-Complex Fourier Transform	SRCFT	DRCFT	755
Complex-to-Real Fourier Transform	SCRFT	DCRFT	763
Cosine Transform	SCOSF SCOSFT§	DCOSF	771
Sine Transform	SSINF	DSINF	778
Complex Fourier Transform in Two Dimensions	SCFT2 SCFT2P§	DCFT2	785
Real-to-Complex Fourier Transform in Two Dimensions	SRCFT2	DRCFT2	792
Complex-to-Real Fourier Transform in Two Dimensions	SCRFT2	DCRFT2	799
Complex Fourier Transform in Three Dimensions	SCFT3 SCFT3P§	DCFT3	807
Real-to-Complex Fourier Transform in Three Dimensions	SRCFT3	DRCFT3	813
Complex-to-Real Fourier Transform in Three Dimensions	SCRFT3	DCRFT3	819

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

#### **Convolutions and Correlations**

The convolution and correlation subroutines provide the choice of using Fourier methods or direct methods. The Fourier-method subroutines contain a high-performance mixed-radix capability. There are also several direct-method subroutines that provide decimated output.

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Convolution or Correlation of One Sequence with One or More Sequences	SCON§ SCOR§		826
Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method	SCOND SCORD		832
Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method	SCONF SCORF		838
Convolution or Correlation with Decimated Output Using a Direct Method	SDCON SDCOR	DDCON DDCOR	847
Autocorrelation of One or More Sequences	SACOR§		851
Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method	SACORF		855

<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.

#### **Related Computations**

The related-computation subroutines consist of a group of computations that can be used in general signal processing applications. They are similar to those provided on the IBM 3838 Array Processor; however, the ESSL subroutines generally solve a wider range of problems.

Table 15. List of Related-Computation Subroutines				
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page	
Polynomial Evaluation	SPOLY	DPOLY	861	
I-th Zero Crossing	SIZC	DIZC	864	
Time-Varying Recursive Filter	STREC	DTREC	867	
Quadratic Interpolation	SQINT	DQINT	870	
Wiener-Levinson Filter Coefficients	SWLEV CWLEV	DWLEV ZWLEV	874	

## **Sorting and Searching**

The sorting and searching subroutines operate on three types of data: integer, short-precision real, and long-precision real (Table 16). The sorting subroutines perform sorts with or without index designations. The searching subroutines perform either a binary or sequential search.

Table 16. List of Sorting and Searching Subroutines				
Descriptive Name	Integer Subroutine	Short- Precision Subroutine	Long- Precision Subroutine	Page
Sort the Elements of a Sequence	ISORT	SSORT	DSORT	882
Sort the Elements of a Sequence and Note the Original Element Positions	ISORTX	SSORTX	DSORTX	884
Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions	ISORTS	SSORTS	DSORTS	887
Binary Search for Elements of a Sequence X in a Sorted Sequence Y	IBSRCH	SBSRCH	DBSRCH	890
Sequential Search for Elements of a Sequence X in the Sequence Y	ISSRCH	SSSRCH	DSSRCH	894

## Interpolation

The interpolation subroutines provide the capabilities of doing polynomial interpolation, local polynomial interpolation, and both one- and two-dimensional cubic spline interpolation (Table 17).

Table 17. List of Interpolation Subroutines				
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page	
Polynomial Interpolation	SPINT	DPINT	901	
Local Polynomial Interpolation	STPINT	DTPINT	906	
Cubic Spline Interpolation	SCSINT	DCSINT	909	
Two-Dimensional Cubic Spline Interpolation	SCSIN2	DCSIN2	915	

## **Numerical Quadrature**

The numerical quadrature subroutines provide Gaussian quadrature methods for integrating a tabulated function and a user-supplied function over a finite, semi-infinite, or infinite region of integration (Table 18).

Table 18 (Page 1 of 2). List of Numerical Quadrature Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Numerical Quadrature Performed on a Set of Points	SPTNQ	DPTNQ	923

Table 18 (Page 2 of 2). List of Numerical Quadrature Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature	SGLNQ†	DGLNQ†	926
Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature	SGLNQ2†	DGLNQ2†	929
Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature	SGLGQ†	DGLGQ†	935
Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature	SGRAQ†	DGRAQ†	938
Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature	SGHMQ†	DGHMQ†	942
† This subprogram is invoked as a function in a Fortran program.		•	•

# **Random Number Generation**

Random number generation subroutines generate uniformly distributed random numbers or normally distributed random numbers (Table 19).

Table 19. List of Random Number Generation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Generate a Vector of Uniformly Distributed Random Numbers	SURAND	DURAND	946
Generate a Vector of Normally Distributed Random Numbers	SNRAND	DNRAND	949
Generate a Vector of Long Period Uniformly Distributed Random Numbers	SURXOR	DURXOR	953

## **Utilities**

The utility subroutines perform general service functions that support ESSL, rather than mathematical computations (Table 20).

Table 20 (Page 1 of 2). List of Utility Subroutines		
Descriptive Name	Subroutine	Page
ESSL Error Information-Handler Subroutine	EINFO	960
ESSL ERRSAV Subroutine for ESSL	ERRSAV	963
ESSL ERRSET Subroutine for ESSL	ERRSET	964
ESSL ERRSTR Subroutine for ESSL	ERRSTR	966
Set the Vector Section Size (VSS) for the ESSL/370 Scalar Library	IVSSET§	
Set the Extended Vector Operations Indicator for the ESSL/370 Scalar Library	IEVOPS§	
Determine the Level of ESSL Installed	IESSL	967

Table 20 (Page 2 of 2). List of Utility Subroutines		
Descriptive Name	Subroutine	Page
Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines	STRIDE	969
Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode	DSRSM	979
For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DGKTRN	983
For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DSKTRN	989

<sup>§</sup> This subroutine is provided for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

# **Chapter 2. Planning Your Program**

This chapter provides information about ESSL that you need when planning your program. Its purpose is to help you in performing the following tasks:

- · Selecting an ESSL subroutine
- Avoiding Conflicts with Internal ESSL Routine Names That are Exported
- · Setting up your data
- Setting up your ESSL calling sequences
- Using auxiliary storage in ESSL
- · Providing a correct transform length to ESSL
- · Getting the best accuracy
- · Getting the best performance
- · Dealing with errors when using ESSL

If you are using ESSL with PL/I Set for AIX, Version 1, see the PL/I publications for details on calling subroutines and functions.

## Selecting an ESSL Subroutine

Your choice of which ESSL subroutine to use is based mainly on the functional needs of your program. However, you have a choice of several variations of many of the subroutines. In addition, there are instances where certain subroutines cannot be used. This section describes these variations and limitations. See the answers to each question below that applies to you.

# Which ESSL Library Do You Want to Use?

ESSL provides five run-time libraries:

- The ESSL SMP Library provides thread-safe versions of the ESSL subroutines for use on the RS/6000 SMP processors. In addition, a subset of these subroutines are also multithreaded versions; that is, they support the shared memory parallel processing programming model. For a list of the multithreaded subroutines in the ESSL SMP Library, see Table 21 on page 26.
- The ESSL Thread-Safe Library provides thread-safe versions of the ESSL subroutines for use on all RS/6000 processors. You may choose to use this library if you decide to develop your own multithreaded programs that call the thread-safe ESSL subroutines.

The number of threads you choose to use depends on the problem size, the specific subroutine being called, and the number of physical processors you are running on. To achieve optimal performance, experimentation is necessary; however, picking the number of threads equal to the number of online processors generally provides good performance in most cases. In a few cases, performance may increase if you choose the number of threads to be less than the number of online processors. For more information about thread concepts, see *IBM AIX Version 4 General Programming Concepts: Writing and Debugging Programs*.

- The ESSL Thread-Safe POWER2 Library provides thread-safe versions of the ESSL subroutines and is tuned for the RS/6000 POWER2 uniprocessors. You may use this library to develop your own multithreaded applications.
- The ESSL POWER2 Library is tuned for the RS/6000 POWER2 uniprocessors.

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The ESSL POWER Library, the ESSL Thread-Safe Library, and the ESSL SMP Library supports both 32-bit environment and 64-bit environment applications. For details see Chapter 4 on page 111 and Chapter 5 on page 163.

#### Table 21 (Page 1 of 2). Multithreaded ESSL SMP Subroutines

#### **Subroutine Names**

Vector-Scalar Linear Algebra Subprograms:

SASUM, DASUM, SCASUM, DZASUM

SAXPY, DAXPY, CAXPY, ZAXPY

SCOPY, DCOPY, CCOPY, ZCOPY

SDOT, DDOT, CDOTU, ZDOTU, CDOTC, ZDOTC

SNDOT, DNDOT

SNORM2, DNORM2, CNORM2, ZNORM2

SROT, DROT, CROT, ZROT, CSROT, ZDROT

SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, ZDSCAL

SSWAP, DSWAP, CSWAP, ZSWAP

SVEA, DVEA, CVEA, ZVEA

SVES, DVES, CVES, ZVES

SVEM, DVEM, CVEM, ZVEM

SYAX, DYAX, CYAX, ZYAX, CSYAX, ZDYAX

SZAXPY, DZAXPY, CZAXPY, ZZAXPY

Matrix-Vector Linear Algebra Subprograms:

SGEMV, DGEMV, CGEMV, ZGEMV

SGER, DGER, CGERU, ZGERU, CGERC, ZGERC

SSPMV, DSPMV, CHPMV, ZHPMV

SSYMV, DSYMV, CHEMV, ZHEMV

SSPR, DSPR, CHPR, ZHPR

SSYR, DSYR, CHER, ZHER

SSPR2, DSPR2, CHPR2, ZHPR2

SSYR2, DSYR2, CHER2, ZHER2

SGBMV+, DGBMV+

CGBMV◆, ZGBMV◆

SSBMV♦, DSBMV♦

CHBMV◆, ZHBMV◆

STRMV, DTRMV, CTRMV, ZTRMV

STPMV, DTPMV, CTPMV, ZTPMV

STBMV◆, DTBMV◆

CTBMV◆, ZTBMV◆

Matrix Operations:

SGEADD, DGEADD, CGEADD, ZGEADD

SGESUB, DGESUB, CGESUB, ZGESUB

**DGEMUL** 

DGEMM, ZGEMM

DSYMM, ZSYMM, ZHEMM

DTRMM, ZTRMM

DSYRK, ZSYRK, ZHERK

DSYR2K, ZSYR2K, ZHER2K

SGETMI, DGETMI, CGETMI, ZGETMI

SGETMO, DGETMO, CGETMO, ZGETMO

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#### **Subroutine Names**

Dense Linear Algebraic Equations:

SGEF, DGEF, CGEF, ZGEF

SGETRF, DGETRF, CGETRF, ZGETRF

**DPOF** 

STRSV, DTRSV, CTRSV, ZTRSV

STPSV, DTPSV, CTPSV, ZTPSV

DTRSM, ZTRSM

STRI, DTRI

Sparse Linear Algebraic Equations:

DSRIS†

Fourier Transforms:

SCFT, DCFT

SRCFT, DRCFT

SCRFT, DCRFT

SCFT2, DCFT2

SRCFT2, DRCFT2

SCRFT2, DCRFT2

SCFT3, DCFT3

SRCFT3, DRCFT3

DCRFT3, DCRFT3

Convolution and Correlation:

SCOND, SCORD

SDCON, SDCOR, DDCON, DDCOR

Many of the dense linear algebraic equations and eigensystem analysis subroutines make one or more calls to the multithreaded versions of the matrix-vector linear algebra and matrix operation subroutines shown in this table. SCOSF, DCOSF, SSINF, and DSINF make one or more calls to the multithreaded versions of the Fourier Transform subroutines shown in this table. These subroutines benefit from the increased performance of the multithreaded versions of the ESSL SMP subroutines.

† DSRIS only uses multiple threads when IPARM(4) = 1 or 2.

◆ The Level 2 Banded BLAS use multiple threads only when the bandwidth is sufficiently large.

# What Type of Data Are You Processing in Your Program?

The version of the ESSL subroutine you select should agree with the data you are using. ESSL provides a short- and long-precision version of most of its subroutines processing short- and long-precision data, respectively. In a few cases, it also provides an integer version processing integer data or returning just integer data. The subroutine names are distinguished by a one- or two-letter prefix based on the following letters:

S for short-precision real

D for long-precision real

C for short-precision complex

Z for long-precision complex

I for integer

The precision of your data affects the accuracy of your results. This is discussed in "Getting the Best Accuracy" on page 44. For a description of these data types, see "How Do You Set Up Your Scalar Data?" on page 28.

# How Is Your Data Structured? And What Storage Technique Are You Using?

Some subroutines process specific data structures, such as sparse vectors and matrices or dense and banded matrices. In addition, these data structures can be stored using various storage techniques. You should select the proper subroutine on the basis of the type of data structure you have and the storage technique you want to use. If possible, you should use a storage technique that conserves storage and potentially improves performance. For more about storage techniques, see "Setting Up Your Data."

### What about Performance and Accuracy?

ESSL provides variations among some of its subroutines. You should consider performance and accuracy when deciding which subroutine is the best to use. Study the "Function" section in each subroutine description. It helps you understand exactly what each subroutine does, and helps you determine which subroutine is best for you. For example, some subroutines perform multiple computations of a certain type. This might give you better performance than a subroutine that does each computation individually. In other cases, one subroutine may do scaling while another does not. If scaling is not necessary for your data, you get better performance by using the subroutine without scaling.

# **Avoiding Conflicts with Internal ESSL Routine Names That are Exported**

Do not use names for your own subroutines, functions, and global variables that are the same as the ESSL exported names. All internal ESSL routine names that are exported begin with the **ESV** prefix, so you should avoid using this prefix for your own names.

# **Setting Up Your Data**

This section explains how to set up your scalar and array data and points you to where you can find more detail.

# How Do You Set Up Your Scalar Data?

A scalar item is a single item of data, whether it is a constant, a variable, or an element of an array. ESSL assumes that your scalar data conforms to the appropriate standards, as described below. The scalar data types and how you should code them for each programming language are listed under "Coding Your Scalar Data" in each language section in Chapter 4 on page 111.

#### Internal Representation

Scalar data passed to ESSL from all types of programs, including Fortran, C, and C++, should conform to the ANSI/IEEE 32-bit and 64-bit binary floating-point format, as described in the ANSI/IEEE Standard for Binary Floating-Point Arithmetic. ANSI/IEEE Standard 754-1985

### How Do You Set Up Your Arrays?

An array represents an area of storage in your program, containing data stored in a series of locations. An array has a single name. It is made up of one or more pieces of scalar data, all the same type. These are the elements of the array. It can be passed to the ESSL subroutine as input, returned to your program as output, or used for both input and output, in which case the original contents are overwritten.

Arrays can contain conceptual (mathematical) data structures, such as vectors, matrices, or sequences. There are many different types of data structures. Each type of data structure requires a unique arrangement of data in an array and does not necessarily have to include all the elements of the array. In addition, the elements of these data structures are not always contiguous in storage within an array. Stride and leading dimension arguments passed to ESSL subroutines define the separations in array storage for the elements of the vector, matrix, and sequence. All these aspects of data structures are described in Chapter 3 on page 55. You must first understand array storage techniques to fully understand the concepts of data structures, stride, and leading dimension, especially if you are using them in unconventional ways.

ESSL subroutines assume that all arrays passed to them are stored using the Fortran array storage techniques (in column-major order), and they process your data accordingly. For details, see "Setting Up Arrays in Fortran" on page 112. On the other hand, C, C++, and PL/I programs store arrays in row-major order. For details on what you can do, see:

- For C, see page "Setting Up Arrays in C" on page 133.
- For C++, see page "Setting Up Arrays in C++" on page 149.
- For PL/I, see the PL/I publications.

# **How Should Your Array Data Be Aligned?**

All arrays, regardless of the type of data, should be aligned on a doubleword boundary to ensure optimal performance; however, when running on a POWER2 processor, it is best to align your long-precision arrays on a quadword boundary. For information on how your programming language aligns data, see your programming language manuals.

# What Storage Mode Should You Use for Your Data?

The amount of storage used by arrays and the storage arrangement of data in the arrays can affect overall program performance. As a result, ESSL provides subroutines that operate on different types of data structures, stored using various storage modes. You should chose a storage mode that conserves storage and potentially improves performance. For definitions of the various data structures and their corresponding storage modes, see Chapter 3 on page 55. You can also find special storage considerations, where applicable, in the "Notes" section of each subroutine description.

# How Do You Convert from One Storage Mode to Another?

This section describes how you can convert from one storage mode to another.

#### **Conversion Subroutines**

ESSL provides several subroutines that help you convert from one storage mode to another:

- DSRSM is used to migrate your existing program from sparse matrices stored by rows to sparse matrices stored in compressed-matrix storage mode. This converts the matrices into a storage format that is compatible with the input requirements for some ESSL sparse matrix subroutines, such as DSMMX.
- DGKTRN and DSKTRN are used to convert your sparse matrix from one skyline storage mode to another, if necessary, before calling the subroutines DGKFS/DGKFSP or DSKFS/DSKFSP, respectively.

#### Sample Programs

In addition, sample programs are provided with many of the storage mode descriptions in Chapter 3 on page 55. You can use these sample programs to convert your data to the desired storage mode by adapting them to your application program.

# **Setting Up Your ESSL Calling Sequences**

This section gives the general rules for setting up the ESSL calling sequences. The information given here applies to all types of programs, running in all environments. For a description and examples of how to code the ESSL calling sequences in your particular programming language, see the following sections:

- "Fortran Programs" on page 111
- "C Programs" on page 129
- "C++ Programs" on page 145

For details on the conventions used in this book to describe the calling sequence syntax, see "How to Interpret the Subroutine Descriptions" on page xxx. It describes how required and optional arguments are indicated in the calling sequence and the naming conventions used for different data types.

# What Is an Input-Output Argument?

Some arguments are used for both input and output. The contents of the input argument are overlaid with the output value(s) on return to your program. Be careful that you save any data you need to preserve before calling the ESSL subroutine.

# What Are the General Rules to Follow when Specifying Data for the Arguments?

You should follow the syntax rules given for each argument in "On Entry" in the subroutine description. Input-argument error messages may be issued, and your program may terminate when you make an error specifying the input arguments. For example:

- Data passed to ESSL must be of the correct type: integer, character, real, complex, short-precision, or long-precision. There is no conversion of data.
   Assuming you are using the ESSL header file with your C and C++ programs, you first need to define the following:
  - Complex and logical data in C programs, using the guidelines given on page 132.

- Short-precision complex and logical data in C++ programs, using the guidelines given on page 148.
- Character values must be one of the specified values. For example, it may
  have to be 'N', 'T', or 'C'.
- Numeric values must fall within the correct range for that argument. For example, a numeric value may need to be greater than or equal to 0, or it may have to be a nonzero value.
- Arrays must be defined correctly; that is, they must have the correct dimensions, or the dimensions must fall within the correct range. For example, input and output matrices may need to be conformable, or the number of rows in the matrix must be less than or equal to the leading dimension specified. (ESSL assumes all arrays are stored in column-major order.)

## What Happens When a Value of 0 Is Specified for N?

For most ESSL subroutines, if you specify 0 for the number of elements to be processed in a vector or the order of a matrix (usually argument *n*), no computation is performed. After checking for input-argument errors, the subroutine returns immediately and no result is returned. In the other subroutines, an error message may be issued.

# How Do You Specify the Beginning of the Data Structure in the ESSL Calling Sequence?

When you specify a vector, matrix, or sequence in your calling sequence, it does not necessarily have to start at the beginning of the array. It can begin at any point in the array. For example, if you want vector  $\mathbf{x}$  to start at element 3 in array A, which is declared A(1:12), specify A(3) in your calling sequence for argument  $\mathbf{x}$ , such as in the following SASUM calling sequence in your Fortran program:

Also, for example, if you want matrix A to start at the second row and third column of array A, which is declared A(0:10,2:8), specify A(1,4) in your calling sequence for argument a, such as in the following SGEADD calling sequence in your Fortran program:

For more examples of specifying vectors and matrices, see Chapter 3 on page 55.

# **Using Auxiliary Storage in ESSL**

For the ESSL subroutines listed in Table 22 on page 32, you need to provide extra working storage to perform the computation. This section describes the use of dynamic allocation for providing auxiliary storage in ESSL and how to calculate the amount of auxiliary storage you need by use of formulas or error-handling capabilities provided in ESSL, if dynamic allocation is not an option.

Auxiliary storage, or working storage, is supplied through one or more arguments, such as aux, in the calling sequence for the ESSL subroutine. If the working storage does not need to persist after the subroutine call, it is suggested you use dynamic allocation. For example, in the Fourier Transforms subroutines, you may allocate aux2 dynamically, but not aux1. See the subroutine descriptions in Part 2 of this book for details and variations.

Table 22. ESSL Subroutines Requiring Auxiliary Working Storage
Subroutine Names
Linear Algebra Subprograms: DSMTM
Matrix Operations: _GEMMS
Dense Linear Algebraic Equations: _GEFCD _PPFCD _GEICD _PPICD _POFCD _POICD DGEFP△ DPPFP△
Sparse Linear Algebraic Equations: DGSF DGSS DGKFS DGKFSP <sup>\(\Delta\)</sup> DSKFS DSKFSP <sup>\(\Delta\)</sup> DSRIS DSMCG DSDCG DSMGCG DSDGCG
Linear Least Squares: _GESVF _GELLS
Eigensystem Analysis: _GEEV _SPEV _HPEV _SPSV _HPSV _GEGV _SYGV
Fourier Transforms:  _CFT _RCFT _CRFT _COSF _SINF  SCOSFT^ _CFT2 _RCFT2 _CFT3  _RCFT3 _CRFT3 SCFTP^ SCFT2P^ SCFT3P^
Convolutions and Correlations: SCONF SCORF SACORF
Related Computations: _WLEV
Interpolation: _TPINT _CSIN2
Random Number Generation: _NRAND
Utilities: DGKTRN DSKTRN
$^{\Delta}$ Documentation for this subroutine is no longer provided. The <i>aux</i> and <i>naux</i> arguments for the subroutine are specified the same as for the corresponding serial ESSL subroutine.

# **Dynamic Allocation of Auxiliary Storage**

Dynamic allocation for the auxiliary storage is performed when error 2015 is unrecoverable and naux=0. For details on which aux arguments allow dynamic allocation, see the subroutine descriptions in Part 2 of this book.

### Setting Up Auxiliary Storage When Dynamic Allocation Is Not Used

You set up the storage area in your program and pass it to ESSL through arguments, specifying the size of the *aux* work area in the *naux* argument.

#### Who Do You Want to Calculate the Size? You or ESSL?

You have a choice of two methods for determining how much auxiliary storage you should specify:

- Use the formulas provided in the subroutine description to derive sufficient values for your current and future needs. Use them if ease of migration to future machines and future releases of ESSL is your primary concern. For details, see "How Do You Calculate the Size Using the Formulas?."
- Use the ESSL error-handling facilities to return to you a minimum value for the
  particular processor you are currently running on. (Values vary by platform.)
  Use this approach if conserving storage is your primary concern. For details,
  see "How Do You Get ESSL to Calculate the Size Using ESSL Error
  Handling?."

### How Do You Calculate the Size Using the Formulas?

The formulas provided for calculating *naux* indicate a **sufficient** amount of auxiliary storage required, which, in most cases, is larger than the minimum amount, returned by ESSL error handling. There are two types of formulas:

#### · Simple formulas

These are given in the *naux* argument syntax descriptions. In general, these formulas result in the minimum required value, but, in a few cases, they provide overestimates.

#### Processor-independent formulas

These are given in separate sections in the subroutine description. In general, these provide overestimates.

Both types of formulas provide values that are sufficient for all processors. As a result, you can migrate to any other processor and to future releases of ESSL without being concerned about having to increase the amount of storage for *aux*. You do, of course, need to weigh your storage requirements against the convenience of using this larger value.

To calculate the amount of storage using the formulas, you must substitute values for specific variables, such as n, m, n1, or n2. These variables are arguments specified in the ESSL calling sequence or derived from the arguments in the calling sequence.

# How Do You Get ESSL to Calculate the Size Using ESSL Error Handling?

This section describes how you can get ESSL to calculate auxiliary storage.

#### Here Are the Two Ways You Can Do It

Ask yourself which of the following ways you prefer to obtain the information from ESSL:

- By leaving error 2015 unrecoverable, you can obtain the minimum required value of naux from the input-argument error message, but your program terminates.
- By making error 2015 recoverable, you can obtain the minimum required value of *naux* from the input-argument error message and have the updated *naux* argument returned to your program.

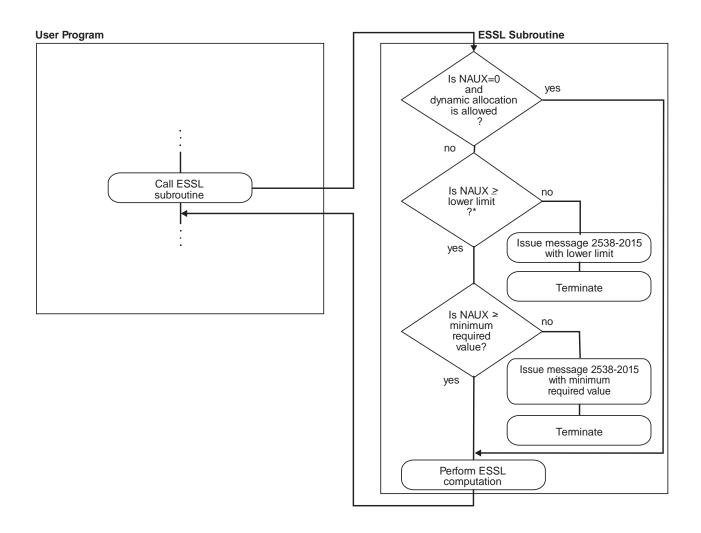
For both techniques, the amount returned by the ESSL error-handling facility is the **minimum** amount of auxiliary storage required to run your program successfully **on the particular processor you are currently running on.** The ESSL error-handling capability usually returns a smaller value than you derive by using the formulas listed for the subroutine. This is because the formulas provide a good estimate, but ESSL can calculate exactly what is needed on the basis of your data.

The values returned by ESSL error handling **may not apply to future processors.** You should not use them if you plan to run your program on a future processor. You should use them only if you are concerned with minimizing the amount of auxiliary storage used by your program.

#### The First Way

In this case, you obtain the minimum required value of *naux* from the error message, but your program terminates. The following description assumes that dynamic allocation is not selected as an option.

Leave error 2015 as unrecoverable, without calls to EINFO and ERRSET. Run your program with the *naux* values smaller than required by the subroutine for the particular processor you are running on. As a general guideline, specify values smaller than those listed in the formulas. However, if a lower limit is specified in the syntax (only for several *naux1* arguments in the Fourier transform, convolution, and correlation subroutines), you should not go below that limit. The ESSL error monitor returns the necessary sizes of the *aux* storage areas in the input-argument error message. This does, however, terminate your program when the error is encountered. (If you accidentally specify a sufficient amount of storage for the ESSL subroutine to perform the computation, error handling does not issue an error message and processing continues normally.) Figure 1 on page 35 illustrates what happens when error 2015 is unrecoverable.



<sup>\*</sup> This check applies only to several NAUX1 arguments in the Fourier transform, convolution, and correlation subroutines.

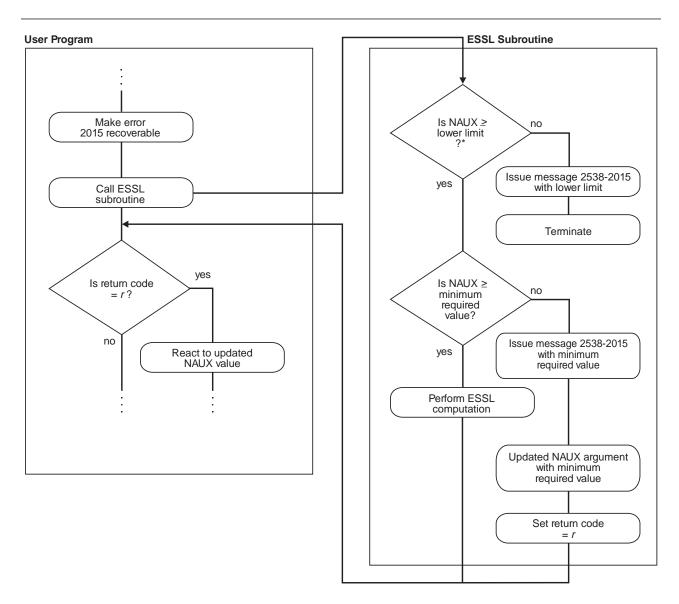
Figure 1. How to Obtain an NAUX Value from an Error Message, but Terminate

#### The Second Way

In this case, you obtain the minimum required value of *naux* from the error message and from the updated *naux* argument returned to your program.

Use EINFO and ERRSET with an ESSL error exit routine, ENOTRM, to make error 2015 recoverable. This allows you to dynamically determine in your program the minimum sizes required for the auxiliary working storage areas, specified in the *naux* arguments. Run your program with the *naux* values smaller than required by the subroutine for the particular processor you are running on. As a general guideline, specify values smaller than those listed in the formulas. However, if a lower limit is specified in the syntax (only for several *naux1* arguments in the

Fourier transform, convolution, and correlation subroutines), you should not go below that limit. The ESSL error monitor returns the necessary sizes of the *aux* storage areas in the input-argument error message and a return code is passed back to your program, indicating that updated values are also returned in the *naux* arguments. You can then react to these updated values during run time in your program. ESSL does not perform any computation when this error occurs. For details on how to do this, see Chapter 4 on page 111. (If you accidentally specify a sufficient amount of storage for the ESSL subroutine to perform the computation, error handling does not issue an error message and processing continues normally.) Figure 2 illustrates what happens when error 2015 is recoverable.



<sup>\*</sup> This check applies only to several NAUX1 arguments in the Fourier transform, convolution, and correlation subroutines.

Figure 2. How to Obtain an NAUX Value from an Error Message and in Your Program

# Here Is an Example of What Happens When You Use These Two Techniques

The following example illustrates all the actions taken by the ESSL error-handling facility for each possible value of a recoverable input argument, *naux*. A key point here is that if you want to have the updated argument value returned to your program, you must make error 2015 recoverable and then specify an *naux* value greater than or equal to 20 and less than 300. For values out of that range, the error recovery facility is not in effect. (These values of *naux*, 20 and 300, are used only for the purposes of this example and do not relate to any of the ESSL subroutines.)

# NAUX Meaning of the NAUX Value Lower limit of naux required for using recoverable input-argument error-handling facilities in ESSL. (This applies only to several naux1 arguments in the Fourier transform, convolution, and correlation subroutines. You can find the lower limit in the syntax description for the naux1 argument. For a list of subroutines, see Table 22 on page 32.) Minimum value of naux, required for successful running (on the

Table 23 describes the actions taken by ESSL in every possible situation for the values given in this example.

Table 23. Example of Input-Argument Error Recovery for Auxiliary Storage Sizes						
NAUX Value	Action When 2015 Is an Unrecoverable Input-Argument Error	Action When 2015 Is a Recoverable Input-Argument Error				
naux < 20	An input-argument error message is issued. The value in the error message is the lower limit, 20. The application program stops.	An input-argument error message is issued. The value in the error message is the lower limit, 20. The application program stops.				
20 ≤ naux < 300	An input-argument error message is issued. The value in the error message is the minimum required value, 300. The application program stops.	ESSL returns the value of <i>naux</i> as 300 to the application program, and an input-argument error message is issued. The value in the error message is the minimum required value, 300. ESSL does no computation, and control is returned to the application program.				
naux ≥ 300	Your application program runs successfully.	Your application program runs successfully.				

processor the program is being run on).

#### Here Is How You Code It in Your Program

If you leave error 2015 unrecoverable, you **do not code anything** in your program. You just look at the error messages to get the sizes of auxiliary storage. On the other hand, if you want to make error 2015 recoverable to obtain the auxiliary storage sizes dynamically in your program, you need to **add some coding statements** to your program. For details on coding these statements in each programming language, see the following examples:

- For Fortran, see page 121
- For C, see page 139
- For C++, see page 155

You may want to provide a separate subroutine to calculate the auxiliary storage size whenever you need it. Figure 3 on page 38 shows how you might code a separate Fortran subroutine. Before calling SCFT in your program, call this subroutine, SCFT which calculates the minimum size and stores it in the *naux* arguments. Upon return, your program checks the return code. If it is nonzero, the *naux* arguments were updated, as planned. You should then make sure adequate storage is available and call SCFT. On the other hand, if the return code is zero, error handling was not invoked, the *naux* arguments were not updated, and the initialization step was performed for SCFT.

```
SUBROUTINE SCFT
     * N, M, ISIGN, SCALE, AUX1, NAUX1, AUX2, NAUX2)
      REAL*4 X(0:*),Y(0:*),SCALE
      REAL*8 AUX1(7), AUX2(0:*)
      INTEGER*4 INIT, INC1X, INC2X, INC1Y, INC2Y, N, M, ISIGN, NAUX1, NAUX2
      EXTERNAL ENOTRM
      CHARACTER*8
                     S2015
          CALL EINFO(0)
          CALL ERRSAV (2015, S2015)
          CALL ERRSET(2015,0,-1,1,ENOTRM,0)
      SETS NAUX1 AND NAUX2 TO THE MINIMUM VALUES REQUIRED TO USE
C
С
      THE RECOVERABLE INPUT-ARGUMENT ERROR-HANDLING FACILITY
          NAUX1 = 7
          NAUX2 = 0
          CALL SCFT(INIT, X, INC1X, INC2X, Y, INC1Y, INC2Y,
                     N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
          CALL ERRSTR(2015, S2015)
          RETURN
10
          CONTINUE
          CALL ERRSTR(2015, S2015)
          RETURN 1
          END
```

Figure 3. Fortran Subroutine to Calculate Auxiliary Storage Sizes

# **Providing a Correct Transform Length to ESSL**

This section describes how to calculate the length of your transform by use of formulas or error-handling capabilities provided in ESSL.

# What ESSL Subroutines Require Transform Lengths?

For the ESSL subroutines listed in Table 24 on page 39, you need to provide one or more transform lengths for the computation of a Fourier transform. These transform lengths are supplied through one or more arguments, such as n, n1, n2, and n3, in the calling sequence for the ESSL subroutine. Only certain lengths of transforms are permitted in the computation.

Table 24. ESSL Subroutines Requiring Transform Lengths

#### **Subroutine Names**

Fourier Transforms:

\_CFT \_RCFT \_CRFT \_COSF \_SINF

SCOSFT \_CFT2 \_RCFT2 \_CRFT2 \_CFT3

\_RCFT3 \_CRFT3 SCFTP SCFT2P SCFT3P

## Who Do You Want to Calculate the Length? You or ESSL?

You have a choice of two methods for determining an acceptable length for your transform to be processed by ESSL:

- Use the formula or large table in "Acceptable Lengths for the Transforms" on page 739 to determine an acceptable length. For details, see "How Do You Calculate the Length Using the Table or Formula?."
- Use the ESSL error-handling facilities to return to you an acceptable length. For details, see "How Do You Get ESSL to Calculate the Length Using ESSL Error Handling?."

## How Do You Calculate the Length Using the Table or Formula?

The lengths ESSL accepts for transforms in the Fourier transform subroutines are listed in "Acceptable Lengths for the Transforms" on page 739. You should use the table in that section to find the two values your length falls between. You then specify the **larger** length for your transform. If you find a perfect match, you can use that value without having to change it. The formula provided in that section expresses how to calculate the acceptable values listed in the table. If necessary, you can use the formula to dynamically check lengths in your program.

# How Do You Get ESSL to Calculate the Length Using ESSL Error Handling?

This section describes how to get ESSL to calculate transform lengths.

#### Here Are the Two Ways You Can Do It

Ask yourself which of the following ways you prefer to obtain the information from ESSL:

- By leaving error 2030 unrecoverable, you can obtain an acceptable value for *n* from the input-argument error message, but your program terminates.
- By making error 2030 recoverable, you obtain an acceptable value for *n* from the input-argument error message and have the updated *n* argument returned to your program.

Because the Fourier transform subroutines allow only certain lengths for transforms, ESSL provides this error-handling capability to return acceptable lengths to your program. It returns them in the transform length arguments. The value ESSL returns is the **next larger acceptable length** for a transform, based on the length you specify in the *n* argument.

#### The First Way

In this case, you obtain an acceptable value of n from the error message, but your program terminates.

Leave error 2030 as unrecoverable, without calls to EINFO and ERRSET. Run your program with a close approximation of the transform length you want to use. If this happens not to be an acceptable length, the ESSL error monitor returns an acceptable length of the transform in input-argument error message. This does, however, terminates your program when the error is encountered. (If you do happen to specify an acceptable length for the transform, error handling does not issue an error message and processing continues normally.) Figure 4 illustrates what happens when error 2030 is unrecoverable.

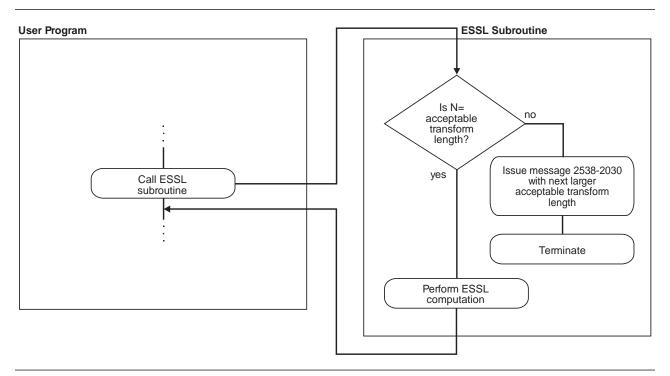


Figure 4. How to Obtain an N Value from an Error Message, but Terminate

#### The Second Way

In this case, you obtain an acceptable value of n from the error message and from the updated n argument returned to your program.

Use EINFO and ERRSET with an ESSL error exit routine, ENOTRM, to make error 2030 recoverable. This allows you to dynamically determine in your program an acceptable length for your transform, specified in the *n* argument(s). Run your program with a close approximation of the transform length you want to use. If this happens not to be an acceptable length, the ESSL error monitor returns an acceptable length of the transform in the input-argument error message and a return code is passed back to your program, indicating that updated values are also returned in the *n* argument(s). You can then react to these updated values during run time in your program. ESSL does not perform any computation when this error occurs. For details on how to do this, see Chapter 4 on page 111. (If you do happen to specify an acceptable length for the transform, error handling does not

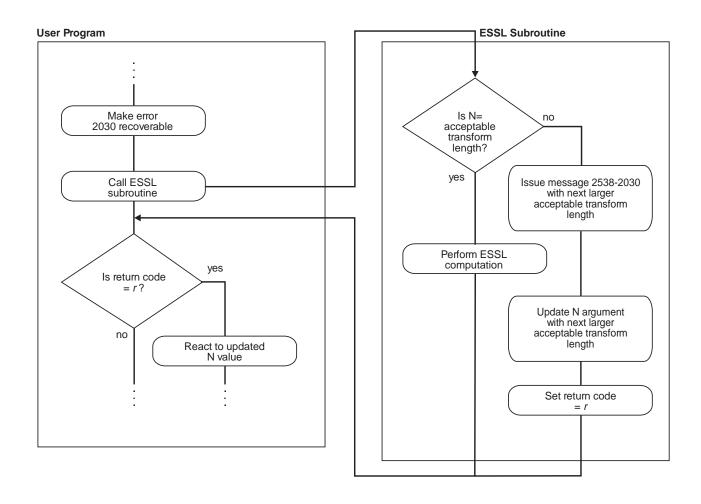


Figure 5. How to Obtain an N Value from an Error Message and in Your Program

# Here Is an Example of What Happens When You Use These Two Techniques

The following example illustrates all the actions taken by the ESSL error-handling facility for each possible value of a recoverable input argument, n. The values of n used in the example are as follows:

# N Meaning of the N Value

7208960 An acceptable transform length, required for successful computing of a Fourier transform

7340032 The next larger acceptable transform length, required for successful computing of a Fourier transform

Table 25 on page 42 describes the actions taken by ESSL in every possible situation for the values given in this example.

N Value	Action When 2030 Is an Unrecoverable Input-Argument Error	Action When 2030 Is a Recoverable Input-Argument Error	
n = 7208960	Your application program runs	Your application program runs successfully.	
-or-	successfully.		
n = 7340032			
7208960 < n < 7340032	An input-argument error message is issued. The value in the error message is 7340032. The application program stops.	ESSL returns the value of <i>n</i> as 7340032 to the application program, and an input-argument error message is issued. The value in the error message is 7340032. ESSL does no computation, and control is returned to the application program.	

#### Here Is How You Code It in Your Program

If you leave error 2030 unrecoverable, you do not code anything in your program. You just look at the error messages to get the transform lengths. On the other hand, if you want to make error 2030 recoverable to obtain the transform lengths dynamically in your program, you need to add some coding statements to your program. For details on coding these statements in each programming language, see the following examples:

- For Fortran, see page 121
- For C, see page 139
- For C++, see page 155

You may want to provide a separate subroutine to calculate the transform length whenever you need it. Figure 6 on page 43 shows how you might code a separate Fortran subroutine. Before calling SCFT in your program, you call this subroutine, SCFT which calculates the correct length and stores it in n. Upon return, your program checks the return code. If it is nonzero, the *n* argument was updated, as planned. You then do any necessary data setup and call SCFT. On the other hand, if the return code is zero, error handling was not invoked, the n argument was not updated, and the initialization step was performed for SCFT.

```
SUBROUTINE SCFT
     * N, M, ISIGN, SCALE, AUX1, NAUX1, AUX2, NAUX2)
      REAL*4 X(0:*), Y(0:*), SCALE
      REAL*8 AUX1(7), AUX2(0:*)
      INTEGER*4 INIT, INC1X, INC2X, INC1Y, INC2Y, N, M, ISIGN, NAUX1, NAUX2
      EXTERNAL ENOTRM
      CHARACTER*8
                     S2030
           CALL EINFO(0)
           CALL ERRSAV (2030, S2030)
           CALL ERRSET (2030, 0, -1, 1, ENOTRM, 0)
           CALL SCFT(INIT, X, INC1X, INC2X, Y, INC1Y, INC2Y,
                      N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
           CALL ERRSTR(2030, S2030)
           RETURN
10
           CONTINUE
           CALL ERRSTR(2030, S2030)
           RETURN 1
           END
```

Figure 6. Fortran Subroutine to Calculate Transform Length

You might want to combine the request for auxiliary storage sizes along with your request for transform lengths. Figure 7 shows how you might code a separate Fortran subroutine combining both requests. It combines the functions performed by the subroutines in Figure 3 on page 38 and Figure 6.

```
SUBROUTINE SCFT
     * N, M, ISIGN, SCALE, AUX1, NAUX1, AUX2, NAUX2)
      REAL*4 X(0:*), Y(0:*), SCALE
      REAL*8 AUX1(7), AUX2(0:*)
      INTEGER*4 INIT, INC1X, INC2X, INC1Y, INC2Y, N, M, ISIGN, NAUX1, NAUX2
      EXTERNAL ENOTRM
      CHARACTER*8
                     S2015, S2030
          CALL EINFO(0)
          CALL ERRSAV (2015, S2015)
          CALL ERRSAV (2030, S2030)
          CALL ERRSET(2015,0,-1,1,ENOTRM,0)
          CALL ERRSET (2030, 0, -1, 1, ENOTRM, 0)
C
      SETS NAUX1 AND NAUX2 TO THE MINIMUM VALUES REQUIRED TO USE
C
      THE RECOVERABLE INPUT-ARGUMENT ERROR-HANDLING FACILITY
          NAUX1 = 7
          NAUX2 = 0
          CALL SCFT(INIT,X,INC1X,INC2X,Y,INC1Y,INC2Y,
                     N,M,ISIGN,SCALE,AUX1,NAUX1,AUX2,NAUX2,*10)
          CALL ERRSTR(2015, S2015)
          CALL ERRSTR(2030, S2030)
          RETURN
10
          CONTINUE
          CALL ERRSTR(2015, S2015)
          CALL ERRSTR(2030, S2030)
          RETURN 1
          END
```

Figure 7. Fortran Subroutine to Calculate Auxiliary Storage Sizes and Transform Length

## **Getting the Best Accuracy**

This section explains how accuracy of your results can be affected in various situations and what you can do to achieve the best possible accuracy.

# What Precisions Do ESSL Subroutines Operate On?

Both short- and long-precision real versions of the subroutines are provided in most areas of ESSL. In some areas, short- and long-precision complex versions are also provided, and, occasionally, an integer version is provided. The subroutine names are distinguished by a one- or two-letter prefix based on the following letters:

S for short-precision real

D for long-precision real

C for short-precision complex

Z for long-precision complex

I for integer

For a description of these data types, see "How Do You Set Up Your Scalar Data?" on page 28. The scalar data types and how you should code them for each programming language are listed under "Coding Your Scalar Data" in each language section in Chapter 4 on page 111.

# How does the Nature of the ESSL Computation Affect Accuracy?

In subroutines performing operations such as copy and swap, the accuracy of data is not affected. In subroutines performing computations involving mathematical operations on array data, the accuracy of the result may be affected by the following:

- The algorithm, which can vary depending on values or array sizes within the computation or the number of threads used.
- · The matrix and vector sizes

For this reason, the ESSL subroutines do **not** have a closed formula for the error of computation. In other words, there is no formula with which you can calculate the error of computation in each subroutine.

Short-precision subroutines sometimes provide increased accuracy of results by accumulating intermediate results in long precision. This is also noted in the functional description for each subroutine. See the RS/6000 POWERstation and POWERserver Hardware Technical Reference Information—General Architectures manual for details.

For the RS/6000 POWER and POWER2, the short-precision, floating-point operands are stored by the hardware in the floating-point registers as long-precision values, and, as a result, all arithmetic operations are performed in long-precision. Where applicable, the ESSL subroutines use the Multiply-Add instructions, which combine a Multiply and Add operation without an intermediate rounding operation.

For the ESSL POWER Library, ESSL Thread-Safe Library, and ESSL SMP Library, results obtained by 32-bit environment and 64-bit environment applications using the same ESSL library are mathematically equivalent but may not be bit identical.

# What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?

The data types operated on by the short-precision, long-precision, and integer versions of the subroutines are ANSI/IEEE 32-bit and 64-bit binary floating-point format, and 32-bit integer. See the ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754-1985 for more detail.

There are ESSL-specific rules that apply to the results of computations using the ANSI/IEEE standards. When running your program, the result of a multiplication of NaN ("Not-a-Number") by a scalar zero, under certain circumstances, may differ in the ESSL subroutines from the result you expect.

Usually, when NaN is multiplied by a scalar zero, the result is NaN; however, in some ESSL subroutines where scaling is performed, the result may be zero. For example, in computing  $\alpha \textbf{A}$ , where  $\alpha$  is a scalar and A is a matrix, if  $\alpha$  is zero and one (or more) of the elements of A is NaN, the scaled result, using that element, may be a zero, rather than NaN. To avoid problems, you should consider this when designing your program.

#### **How is Underflow Handled?**

ESSL does not mask underflow. If your program incurs a number of unmasked underflows, its overall performance decreases. For the RS/6000, floating-point exception trapping is disabled by default. Therefore, you do not have to mask underflow unless you have changed the default.

## Where Can You Find More Information on Accuracy?

Information about accuracy can be found in the following places:

- Migration considerations concerning accuracy of results between releases, platforms, and so forth are described in Chapter 6 on page 169.
- Specific information on accuracy for each area of ESSL is given in "Performance and Accuracy Considerations" in each chapter introduction in Part 2.
- The functional description under "Function" for each subroutine explains what
  you need to know about the accuracy of the computation. Varying
  implementation techniques are sometimes used to improve performance. To let
  you know how accuracy is affected, the functional description may explain in
  general terms the different techniques used in the computation.

# **Getting the Best Performance**

This section describes how you can achieve the best possible performance from the ESSL subroutines.

# What General Coding Techniques Can You Use to Improve Performance?

There are many ways in which you can improve the performance of your program. Here are some of them:

• Use the basic linear algebra subprograms and matrix operations in the order of optimum performance: matrix-matrix computations, matrix-vector computations,

and vector-scalar computations. When data is presented in matrices or vectors, rather than vectors or scalars, multiple operations can be performed by a single ESSL subroutine.

- Where possible, use subroutines that do multiple computations, such as SNDOT and SNAXPY, rather than individual computations, such as SDOT and SAXPY.
- Use a stride of 1 for the data in your computations. Not having vector elements consecutively accessed in storage can degrade your performance. The closer the vector elements are to each other in storage, the better your performance.
   For an explanation of stride, see "How Stride Is Used for Vectors" on page 58.
- Do **not** specify the size of the leading dimension of an array (*Ida*) or stride of a vector (*inc*) equal to or near a multiple of:
  - 128 for a long-precision array
  - 256 for a short-precision array
- Do not specify the individual sizes of your one-dimensional arrays as multiples
  of 128. This is especially important when you are passing several
  one-dimensional arrays to an ESSL subroutine. (The multiplicity can cause a
  performance problem that otherwise might not occur.)
- For small problems, avoid using a large leading dimension (Ida) for your matrix.
- In general, align your arrays on doubleword boundaries, regardless of the type
  of data; however, when running on a POWER2 processor, it is best to align
  your long-precision arrays on a quadword boundary. For information on how
  your programming language aligns data, see your programming language
  manuals.
- One subroutine may do scaling while another does not. If scaling is not necessary for your data, you get better performance by using the subroutine without scaling. SNORM2 and DNORM2 are examples of subroutines that do not do scaling, versus SNRM2 and DNRM2, which do scaling.
- Use the STRIDE subroutine to calculate the optimal stride values for your input or output data when using any of the Fourier transform subroutines, except \_RCFT and \_CRFT. Using these stride values for your data allows the Fourier transform subroutines to achieve maximum performance. You first obtain the optimal stride values from STRIDE, calling it once for each stride value desired. You then arrange your data using these stride values. After the data is set up, you call the Fourier transform subroutine. For details on the STRIDE subroutine and how to use it for each Fourier transform subroutine, see "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969. For additional information, see "Setting Up Your Data" on page 742.

#### Where Can You Find More Information on Performance?

Information about performance can be found in the following places:

- Many of the techniques ESSL uses to achieve the best possible performance are described in the "High Performance of ESSL" on page 6.
- Migration considerations concerning performance are described in "Migrating ESSL Version 2 Programs to Version 3" on page 169.

- Specific information on performance for each area of ESSL is given in "Performance and Accuracy Considerations" in each chapter introduction in Part 2.
- Detailed performance information for selected subroutines can be found in reference [30], [41], [42] and on the IBM RS/6000 web site at:

http://www.rs6000.ibm.com/software/Apps/essl.html

# **Dealing with Errors when Using ESSL**

At run time, you can encounter different types of errors or messages that are related to the use of the ESSL subroutines:

- Program exceptions
- · ESSL input-argument errors
- ESSL computational errors
- · ESSL resource errors
- ESSL attention messages

This section explains how to handle all these situations.

# What Can You Do about Program Exceptions?

The program exceptions you can encounter in ESSL are described in the RS/6000 architecture manuals. For details, see:

- The ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754-1985
- The RS/6000 POWERstation and POWERserver Hardware Technical Reference Information—General Architectures manual

# What Can You Do about ESSL Input-Argument Errors?

This section gives an overview on how you can handle input-argument errors.

#### **All Input-Argument Errors**

ESSL checks the validity of most input arguments. If it finds that any are invalid, it issues the appropriate error messages. Also, except for the two recoverable errors described below, it terminates your program. You should use standard programming techniques to diagnose and fix unrecoverable input-argument errors, as described in Chapter 7 on page 173.

You can determine the input-argument errors that can occur in a subroutine by looking under "Error Conditions" in the subroutine description in Part 2 of this book. Error messages for all input-argument errors are listed in "Input-Argument Error Messages" on page 179.

# Recoverable Errors 2015 and 2030 Can Return Updated Values in the NAUX and N Arguments

For two input-argument errors, 2015 and 2030, in Fortran, C, C++, and PL/I programs, you have the option to continue running and have an updated value of the input argument returned to your program for subsequent use. These are called recoverable errors. This recoverable error-handling capability gives you flexibility in determining the correct values for the arguments. You can:

- Determine the correct size of an auxiliary work area by using error 2015. For help in deciding whether you want to use this capability and details on how to use it, see "Using Auxiliary Storage in ESSL" on page 31.
- Determine the correct length of a transform by using error 2030. For help in deciding whether you want to use this capability and details on how to use it, see "Providing a Correct Transform Length to ESSL" on page 38.

If you chose to leave errors 2015 and 2030 unrecoverable, you do not need to make any coding changes to your program. The input-argument error message is issued upon termination, containing the updated values you could have specified for the program to run successfully. You then make the necessary corrections in your program and rerun it.

If you choose to make errors 2015 and 2030 recoverable, you call the ERRSET subroutine to set up the ESSL error exit routine, ENOTRM, and then call the ESSL subroutine. When one or more of these errors occurs, the input-argument error message is issued with the updated values. In addition, the updated values are returned to your program in the input arguments named in the error message, along with a nonzero return code and processing continues. Return code values associated with these recoverable errors are described under "Error Conditions" for each ESSL subroutine in Part 2.

For details on how to code the necessary statements in your program to make 2015 and 2030 recoverable, see the following sections:

- "Input-Argument Errors in Fortran" on page 119
- "Input-Argument Errors in C" on page 136
- "Input-Argument Errors in C++" on page 152

# What Can You Do about ESSL Computational Errors?

This section gives an overview on how you can handle computational errors.

#### All Computational Errors

ESSL computational errors are errors occurring in the computational data, such as in your vectors and matrices. You can determine the computational errors that can occur in a subroutine by looking under "Error Conditions" in the subroutine description in Part 2 of this book. These errors cause your program to terminate abnormally unless you take preventive action. A message is also provided in your output, containing information about the error. Messages are listed in "Computational Error Messages" on page 187.

When a computational error occurs, you should assume that the results are unpredictable. The result of the computation is valid only if no errors have occurred. In this case, a zero return code is returned.

Figure 8 on page 49 shows what happens when a computational error occurs.

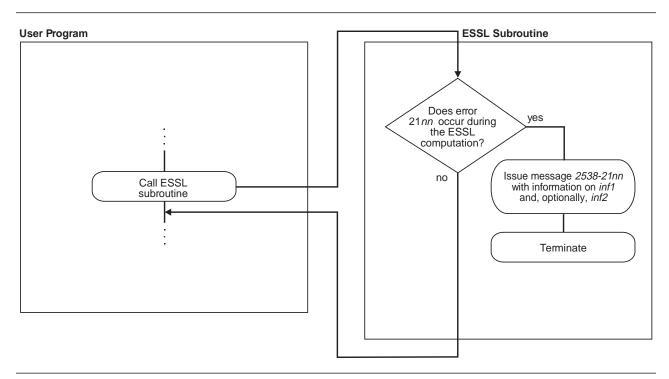


Figure 8. How to Obtain Computational Error Information from an Error Message, but Terminate

# Recoverable Computational Errors Can Return Values Through EINFO

In Fortran, C, C++, and PL/I programs, you have the capability to make certain computational errors recoverable and have information returned to your program about the errors. Recoverable computational errors are listed in Table 167 on page 960. First, you call EINFO in the beginning of your program to initialize the ESSL error option table. You then call ERRSET to reset the number of allowable errors for the computational error codes in which you are interested. When a computational error occurs, a nonzero return code is returned for each computational error. Return code values associated with these errors are described under "Error Conditions" in each subroutine description. Based on the return code, your program can branch to an appropriate statement to call the ESSL error information-handler subroutine, EINFO, to obtain specific information about the data involved in the error. This information is returned in the EINFO output arguments, inf1 and, optionally, inf2. You can then check the information returned and continue processing, if you choose. The syntax for EINFO is described under "EINFO—ESSL Error Information-Handler Subroutine" on page 960. You also get a message in your output for each computational error encountered, containing information about the error. The EINFO subroutine provides the same information in the messages as it provides to your program.

For details on how to code the necessary statements in your program to obtain specific information on computational errors, see the following sections:

- "Computational Errors in Fortran" on page 122
- "Computational Errors in C" on page 140
- "Computational Errors in C++" on page 157

Figure 9 on page 50 shows what happens if you make a computational error recoverable.

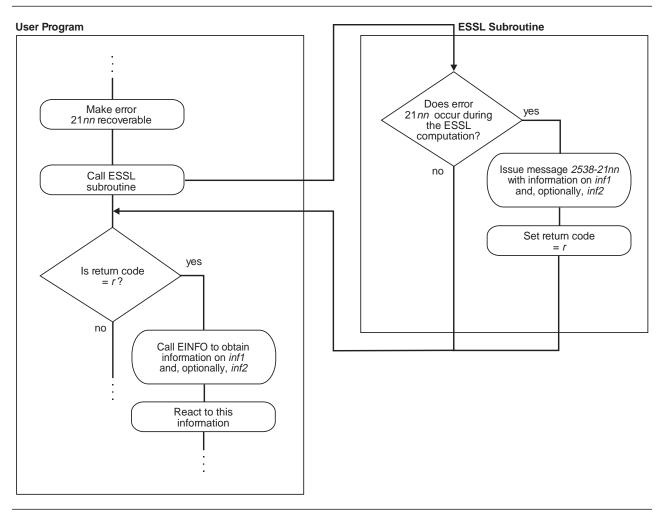


Figure 9. How to Obtain Computational Error Information in an Error Message and in Your Program

#### What Can You Do about ESSL Resource Errors?

This section gives an overview on how you can handle resource errors.

#### **All Resource Errors**

ESSL returns a resource error and terminates your program when an attempt to allocate work area fails. Some ESSL subroutines attempt to allocate work area for their internal use. Other ESSL subroutines attempt to dynamically allocate auxiliary storage when a user requests it through calling sequence arguments, such as *aux* and *naux*. For information on how you could reduce memory constraints on the system or increase the amount of memory available before rerunning the application program, see "ESSL Resource Error Messages" on page 176.

You can determine the resource errors that can occur in a subroutine by looking under "Error Conditions" in the subroutine description in Part 2 of this book. Error messages for all resource errors are listed in "Resource Error Messages" on page 190.

## What Can You Do about ESSL Attention Messages?

This section gives an overview on how you can handle attention messages.

#### All Attention Messages

ESSL returns an attention message to describe a condition that occurred, however, ESSL is able to continue processing. For information on how you could reduce memory constraints on the system or increase the amount of memory available, see "ESSL Resource Error Messages" on page 176.

For example, an attention message may be issued when enough work area was available to continue processing, but was not the amount initially requested. An attention message would be issued to indicate that performance may be degraded.

For a list of subroutines that may generate an attention message, see Table 31 on page 177. For a list of attention messages, see "Informational and Attention Error Messages" on page 190.

# How Do You Control Error Handling by Setting Values in the ESSL **Error Option Table?**

This section explains all aspects of using the ESSL error option table.

#### What Values Are Set in the ESSL Error Option Table?

The ESSL error option table contains information that tells ESSL what to do every time it encounters an ESSL-generated error. Table 26 shows the default values established in the table when ESSL is installed.

Table 26 (Page 1 of 2). ESSL Error Option Table Default Values					
Range of Error Messages (From–To)	Number of Allowable Errors (ALLOW)	Number of Messages Printed (PRINT)	Modifiable Table Entry (MODENT)		
2538–2000	Unlimited	255	NO		
2538-2001 through 2538-2073	Unlimited	255	YES		
2538–2074	Unlimited	5	YES		
2538-2075 through 2538-2098	Unlimited	255	YES		
2538–2099	1	255	YES		
2538-2100 through 2538-2101	1	255	YES		
2538–2102	Unlimited	255	YES		
2538-2103 through 2538-2113	1	255	YES		
2538–2114	Unlimited	255	YES		
2538-2115 through 2538-2122	1	255	YES		
2538-2123 through 2538-2124	Unlimited	255	YES		
2538-2125 through 2538-2126	1	255	YES		
2538–2127	Unlimited	255	YES		
2538-2128 through 2538-2137	1	255	YES		
2538-2138 through 2538-2143	Unlimited	255	YES		
2538-2144 through 2538-2145	1	255	YES		

Table 26 (Page 2 of 2). ESSL Error Option Table Default Values						
Range of Error Messages (From-To)	Number of Allowable Errors (ALLOW)	Number of Messages Printed (PRINT)	Modifiable Table Entry (MODENT)			
2538–2146	Unlimited	255	YES			
2538-2147 through 2538-2198	1	255	YES			
2538–2199	1	255	YES			
2538-2400 through 2538-2499	1	255	NO			
2538-2600 through 2538-2699	Unlimited	255	NO			
2538-2700 through 2538-2799	1	255	NO			

#### How Can You Change the Values in the Error Option Table?

You can change any of the values in the ESSL error option table by calling the ERRSET subroutine in your program. This dynamically changes values at run time. You can also save and restore entries in the table by using the ERRSAV and ERRSTR subroutines, respectively. For a description of the ERRSET, ERRSAV, and ERRSTR subroutines see Chapter 17 on page 957.

#### When Do You Change the Values in the Error Option Table?

Because you can change the information in the error option table, you can control what happens when any of the ESSL errors occur. There are a number of instances when you may want to do this:

To Customize Your Error-Handling Environment: You may simply want to adjust the number of times an error is allowed to occur before your program terminates. You can use any of the capabilities available in ERRSET.

To Obtain Auxiliary Storage Sizes and Transform Lengths: You may want to make ESSL input-argument error 2015 or 2030 recoverable, so ESSL returns updated auxiliary storage sizes or transform lengths, respectively, to your program. For a more detailed discussion, see "What Can You Do about ESSL Input-Argument Errors?" on page 47. For how to use ERRSET to do this, see the section for your programming language in Chapter 4 on page 111.

To Get More Information About a Computational Error: You may want ESSL to return information about a computational error to your program. For a more detailed discussion, see "What Can You Do about ESSL Computational Errors?" on page 48. For how to do use ERRSET to do this, see the section for your programming language in Chapter 4 on page 111.

#### To Allow Parts of Your Application to Have Unique Error-Handling

Environments: If your program is part of a large application, you may want to dynamically save and restore entries in the error option table that have been altered by ERRSET. This ensures the integrity of the error option table when it is used by multiple programs within an application. For a more detailed discussion, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53 For how to use ERRSAV and ERRSTR, see the section for your programming language in Chapter 4 on page 111.

# How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?

When your program is part of a larger application, you should consider that one of the following can occur:

- If you use ERRSET in your program to reset any of the values in the error
  option table for any of the ESSL input-argument errors or computational errors,
  some other program in the application may be adversely affected. It may be
  expecting its original values.
- If some other program in the application uses ERRSET to reset any of the
  values in the error option table for any of the ESSL input-argument errors or
  computational errors, your program may be adversely affected. You may need
  a certain value in the error option table, and the application may have reset that
  value.

These situations can be avoided if every program that uses ERRSET, in the large application, also uses the ERRSAV and ERRSTR facilities. For a particular error number, ERRSAV saves an entry from the error option table in an area accessible to your program. ERRSTR then stores the entry back into the error option table from the storage area. You code an ERRSAV and ERRSTR for each input-argument error number and computational error number for which you do an ERRSET to reset the values in the error option table. Call ERRSAV at the beginning of your program after you call EINFO, and then call ERRSTR at the end of your program after all ESSL computations are completed. This saves the original contents of the error option table while your program is running with different values, and then restores it to its original contents when your program is done. For details on how to code these statements in your program, see Chapter 4 on page 111.

# How does Error Handling Work in a Threaded Environment?

When your application program or Fortran first creates a thread, ESSL initializes the error option table information to the default settings shown in Table 26 on page 51. You can change the default settings for each thread you created by calling the appropriate error handling subroutines (ERRSET, ERRSAV, or ERRSTR) from each thread. An example of how to initialize the error option table and change the default settings on multiple threads is shown in "Example of Handling Errors in a Multithreaded Application Program" on page 127.

ESSL issues error messages as they occur in a threaded environment. Error messages issued from any of the existing threads are written to standard output in the order in which they occur.

When a terminating condition occurs on any of the existing threads (for example, the number of allowable errors was exceeded), ESSL terminates your application program. One set of summary information corresponding to the terminating thread is always printed. Summary information corresponding to other threads may also be printed.

#### Where Can You Find More Information on Errors?

Information about errors and how to handle them can be found in the following places:

- How to code your program to use the ESSL error-handling facilities is described in Chapter 4 on page 111.
- All ESSL error messages are listed under "Messages" on page 178.
- The errors and return codes associated with each ESSL subroutine are listed under "Error Conditions" in each subroutine description in Part 2.
- Complete diagnostic procedures for all types of ESSL programming and documentation problems, along with how to collect information and report a problem, are provided in Chapter 7 on page 173.

# Chapter 3. Setting Up Your Data Structures

This chapter provides you with information that you need to set up your data structures, consisting of vectors, matrices, and sequences. These techniques apply to programs in all programming languages.

# **Concepts**

Vectors, matrices, and sequences are conceptual data structures contained in arrays. In many cases, ESSL uses stride or leading dimension to select the elements of the vector, matrix, or sequence from an array. In other cases, ESSL uses a specific mapping, or storage layout, that identifies the elements of the vector, matrix, or sequence in an array, sometimes requiring several arrays to help define the mapping. These elements selected from the array(s) make up the conceptual data structure.

When you call an ESSL subroutine, it assumes that the data structure is set up properly in the array(s) you pass to it. If it is not, your results are unpredictable. ESSL also uses these same storage layouts for data structures passed back to your program.

The use of the terms vector, matrix, and sequence in this book is consistent with standard mathematical definitions, and their representations are consistent with conventions used in mathematical texts. Special notations and conventions used in this book for describing vectors, matrices, and sequences are explained in "Special Notations and Conventions" on page xxv.

**Overlapping Data Structures:** Most of the subroutines do not allow vectors, matrices, or sequences to overlap. If this occurs, results are unpredictable. Where this applies, it is explained in Notes in each subroutine description. This means the elements of the data structure cannot reside in the same storage locations as any of the other data structures. It is possible, however, to have elements of different data structures in the same array, as long as the elements are interleaved through storage using strides greater than 1. For example, using vectors  $\mathbf{x}$  and  $\mathbf{y}$  with strides of 2, where  $\mathbf{x}$  starts at A(1) and  $\mathbf{y}$  starts at A(2), the elements reside in array A in the order  $x_1, y_1, x_2, y_2, x_3, y_3, \dots$  and so forth.

When you use this technique, you should be careful that you specify different starting locations for each data structure contained in the array.

#### Vectors

A vector is a one-dimensional, ordered collection of numbers. It can be a column vector, which represents an *n* by 1 ordered collection, or a row vector, which represents a 1 by *n* ordered collection.

The column vector appears symbolically as follows:

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$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

A row vector appears symbolically as follows:

$$\mathbf{x} = [x_1 x_2 x_3 \dots x_n]$$

Vectors can contain either real or complex numbers. When they contain real numbers, they are sometimes called real vectors. When they contain complex numbers, they are called complex vectors.

## Transpose of a Vector

The transpose of a vector changes a column vector to a row vector, or vice versa:

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} \quad \boldsymbol{x}^{\mathrm{T}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} \quad (\boldsymbol{x}^{\mathrm{T}})^{\mathrm{T}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

The ESSL subroutines use the vector as it is intended in the computation, as either a column vector or a row vector; therefore, no movement of data is necessary.

In the examples provided with the subroutine descriptions in Part 2 of this book, both types of vectors are represented in the same way, showing the elements of the array that make up the vector  $\mathbf{x}$ , as follows:

# **Conjugate Transpose of a Vector**

The conjugate transpose of a vector  $\mathbf{x}$ , containing complex numbers, is denoted by  $\mathbf{x}^{H}$  and is expressed as follows:

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} \quad \boldsymbol{x}^{H} = \begin{bmatrix} \overline{x}_1 \ \overline{x}_2 \ \overline{x}_3 ... \overline{x}_n \end{bmatrix}$$

Just as for the transpose of a vector, no movement of data is necessary for the conjugate transpose of a vector.

## In Storage

A vector is usually stored within a one- or two-dimensional array. Its elements are stored sequentially in the array, but not necessarily contiguously.

The location of the vector in the array is specified by the argument for the vector in the ESSL calling sequence. It can be specified in a number of ways. For example, if A is an array of length 12, and you want to specify vector x as starting at the first element of array A, specify A as the argument, such as in:

$$X = SASUM (4,A,2)$$

where the number of elements to be summed in the vector is 4, the location of the vector is A, and the stride is 2.

If you want to specify vector **x** as starting at element 3 in array A, which is declared as A(1:12), specify:

```
X = SASUM (4,A(3),2)
```

If A is declared as A(-1:8), specify the following for element 3:

$$X = SASUM (4,A(1),2)$$

If A is a two-dimensional array and declared as A(1:4,1:10), and you want vector xto start at the second row and third column of A, specify the following:

```
X = SASUM (4,A(2,3),2)
```

The **stride** specified in the ESSL calling sequence is used to step through the array to select the vector elements. The direction in which the vector elements are selected from the array—that is, front to back or back to front—is indicated by the sign (+ or -) of the stride. The absolute value of the stride gives the spacing between each element selected from the array.

To calculate the total number of elements needed in an array for a vector, you can use the following formula, which takes into account the number of elements, n, in the array and the stride, inc, specified for the vector:

$$1+(n-1)|inc|$$

An array can be much larger than the vector that it contains; that is, there can be many elements following the vector in the array, as well as elements preceding the vector.

For a complete description of how vectors are stored within arrays, see "How Stride Is Used for Vectors" on page 58.

For a complex vector, a special storage arrangement is used to accommodate the two parts, a and b, of each complex number (a+bi) in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex vectors and matrices as for real vectors and matrices of the same precision. See "How Do You Set Up Your Scalar Data?" on page 28 for a description of real and complex numbers, and

"How Do You Set Up Your Arrays?" on page 29 for a description of how real and complex data is stored in arrays.

#### How Stride Is Used for Vectors

The stride for a vector is an increment that is used to step through array storage to select the vector elements from an array. To define exactly which elements become the conceptual vector in the array, the following items are used together:

- · The location of the vector within the array
- The stride for the vector
- The number of elements, n, to be processed

The stride can be positive, negative, or 0. For positive and negative strides, if you specify vector elements beyond the range of the array, your results are be unpredictable, and you may get program errors.

This section explains how each of the three types of stride is used to select the vector elements from the array.

#### **Positive Stride**

When a positive stride is specified for a vector, the location specified by the argument for the vector is the location of the first element in the vector, element  $x_1$ . The vector is in forward order in the array:  $(x_1, x_2, ..., x_n)$ . For example, if you specify X(1) for vector  $\mathbf{x}$ , where X is declared as X(0:12) and defined as:

```
X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0, 12.0, 13.0)
```

then processing begins at the second element in X, which is 2.0.

To find each successive element, the stride is added cumulatively to the starting point of vector  $\mathbf{x}$  in the array. In this case, the starting point is X(1). If the stride specified for vector  $\mathbf{x}$  is 3 and the number of elements to be processed is 4, then the resulting elements selected from X for vector  $\mathbf{x}$  are: X(1), X(4), X(7), and X(10).

Vector **x** is then:

```
(2.0, 5.0, 8.0, 11.0)
```

As shown in this example, a vector does not have to extend to the end of the array. Elements are selected from the second to the eleventh element of the array, and the array elements after that are not used.

This element selection can be expressed in general terms. Using BEGIN as the starting point in an array X and *inc* as the stride, this results in the following elements being selected from the array:

```
X(BEGIN)
X(BEGIN+inc)
X(BEGIN+(2)inc)
X(BEGIN+(3)inc)
.
.
.
X(BEGIN+(n-1)inc)
```

The following general formula can be used to calculate each vector element position in a one-dimensional array:

$$x_i = X(BEGIN + (i-1)(inc))$$
 for  $i = 1, n$ 

When using an array with more than one dimension, you should understand how the array elements are stored to ensure that elements are selected properly. For a description of array storage, see "Setting Up Arrays in Fortran" on page 112. You should remember that the elements of an array are selected as they are arranged in storage, regardless of the number of dimensions defined in the array. Stride is used to step through array storage until n elements are selected. ESSL processing stops at that point. For example, given the following two-dimensional array, declared as A(1:7,1:4).

Matrix A is:

with A(3,1) specified for vector  $\mathbf{x}$ , a stride of 2, and the number of elements to be processed as 12, the resulting vector  $\mathbf{x}$  is:

```
(3.0, 5.0, 7.0, 9.0, 11.0, 13.0, 15.0, 17.0, 19.0, 21.0, 23.0, 25.0)
```

This is not a conventional use of arrays, and you should be very careful when using this technique.

#### Zero Stride

When a zero stride is specified for a vector, the starting point for the vector is the only element used in the computation. The starting point for the vector is at the location specified by the argument for the vector, just as though you had specified a positive stride. For example, if you specify X for vector X, where X is defined as:

$$X = (5.0, 4.0, 3.0, 2.0, 1.0)$$

and you specify the number of elements, n, to be processed as 6, then processing begins at the first element, which is 5.0. This element is used for each of the six elements in vector x.

This makes the conceptual vector **x** appear as:

The following general formula shows how to calculate each vector position in a one-dimensional array:

$$x_i = X(BEGIN)$$
 for  $i = 1$ ,  $n$ 

#### **Negative Stride**

When a negative stride is specified for a vector, the location specified for the vector is actually the location of the last element in the vector. In other words, the vector is in reverse order in the array:  $(x_n, x_{n-1}, ..., x_1)$ . You specify the end of the vector,  $(x_n)$ . ESSL then calculates where the starting point  $(x_1)$  is by using the following arguments:

- The location of the vector in the array
- The stride for the vector, inc
- The number of elements, n, to be processed

If you specify vector  $\mathbf{x}$  at location X(BEGIN) in array X with a negative stride of *inc* and n elements to be processed, then the following formula gives the starting point of vector  $\mathbf{x}$  in the array:

```
X(BEGIN + (-n+1)(inc))
```

For example, if you specify X(2) for vector  $\mathbf{x}$ , where X is declared as X(1:9) and defined as:

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)$$

and if you specify a stride of -2, and four elements to be processed, processing begins at the following element in X:

$$X(2+(-4+1)(-2)) = X(8)$$

where element X(8) is 8.0.

To find each of the n successive element positions in the array, you successively add the stride to the starting point n-1 times. Suppose the formula calculated a starting point of X(SP); the elements selected are:

```
X(SP)
X(SP+inc)
X(SP+(2)inc)
X(SP+(3)inc)
.
.
.
X(SP+(n-1)inc)
```

In the above example, the resulting elements selected from X for vector  $\mathbf{x}$  are X(8), X(6), X(4), and X(2). This makes the resulting vector  $\mathbf{x}$  appear as follows:

The following general formula can be used to calculate each vector element position in a one-dimensional array:

$$x_i = X(BEGIN + (-n+i)(inc))$$
 for  $i = 1, n$ 

# **Sparse Vector**

A sparse vector is a vector having a relatively small number of nonzero elements.

Consider the following as an example of a sparse vector  $\mathbf{x}$  with n elements, where n is 11, and vector  $\mathbf{x}$  is:

$$(0.0, 0.0, 1.0, 0.0, 2.0, 3.0, 0.0, 4.0, 0.0, 5.0, 0.0)$$

#### In Storage

There are two storage modes that apply to sparse vectors: full-vector storage mode and compressed-vector storage mode. When a sparse vector is stored in **full-vector storage mode**, all its elements, including its zero elements, are stored in an array.

For example, sparse vector  $\mathbf{x}$  is stored in full-vector storage mode in a one-dimensional array X, as follows:

$$X = (0.0, 0.0, 1.0, 0.0, 2.0, 3.0, 0.0, 4.0, 0.0, 5.0, 0.0)$$

When a sparse vector is stored in **compressed-vector storage mode**, it is stored without its zero elements. It consists of two one-dimensional arrays, each with a length of nz, where nz is the number of nonzero elements in vector x:

• The first array contains the nonzero elements of the sparse vector **x**, stored contiguously within the array.

**Note:** The ESSL subroutines do not check that all elements are nonzero. You do not get an error if any elements are zero.

• The second array contains a sequence of integers indicating the element positions (indices) of the nonzero elements of the sparse vector **x** stored in full-vector storage mode. This is referred to as the indices array.

For example, the sparse vector  $\mathbf{x}$  shown above might have its five nonzero elements stored in ascending order in array X of length 5, as follows:

$$X = (1.0, 2.0, 3.0, 4.0, 5.0)$$

in which case, the array of indices, INDX, also of length 5, contains:

$$INDX = (3, 5, 6, 8, 10)$$

If the sparse vector **x** has its elements stored in random order in the array X as:

$$X = (5.0, 3.0, 4.0, 1.0, 2.0)$$

then the array INDX contains:

$$INDX = (10, 6, 8, 3, 5)$$

In general terms, this storage technique can be expressed as follows:

```
For each x_j \neq 0, for j = 1, n
there exists i, where 1 \leq i \leq nz,
such that X(i) = x_i and INDX(i) = j.
```

where:

 $x_1, ..., x_n$  are the *n* elements of sparse vector  $\mathbf{x}$ , stored in full-vector storage mode.

X is the array containing the nz nonzero elements of sparse vector  $\mathbf{x}$ ; that is, vector  $\mathbf{x}$  is stored in compressed-vector storage mode.

INDX is the array containing the *nz* indices indicating the element positions.

To avoid an error when using the INDX array to access the elements in any other target vector, the length of the target vector must be greater than or equal to max(INDX(i)) for i = 1, nz.

#### **Matrices**

A matrix, also referred to as a general matrix, is an m by n ordered collection of numbers. It is represented symbolically as:

$$\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \ddots \\ \vdots & & \ddots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

where the matrix is named **A** and has m rows and n columns. The elements of the matrix are  $a_{ij}$ , where i = 1, m and j = 1, n.

Matrices can contain either real or complex numbers. Those containing real numbers are called real matrices; those containing complex numbers are called complex matrices.

## Transpose of a Matrix

The transpose of a matrix  $\mathbf{A}$  is a matrix formed from  $\mathbf{A}$  by interchanging the rows and columns such that row i of matrix  $\mathbf{A}$  becomes column i of the transposed matrix. The transpose of  $\mathbf{A}$  is denoted by  $\mathbf{A}^T$ . Each element  $a_{ij}$  in  $\mathbf{A}$  becomes element  $a_{ji}$  in  $\mathbf{A}^T$ . If  $\mathbf{A}$  is an m by n matrix, then  $\mathbf{A}^T$  is an n by m matrix. The following represents a matrix and its transpose:

$$A = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \ddots \\ \vdots & & \ddots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \qquad A^{T} = \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \vdots & & \ddots \\ \vdots & & \ddots \\ a_{1n} & \dots & a_{mn} \end{bmatrix}$$

ESSL assumes that all matrices are stored in untransformed format, such as matrix **A** shown above. No movement of data is necessary in your application program when you are processing transposed matrices. The ESSL subroutines adjust their selection of elements from the matrix when an argument in the calling sequence indicates that the transposed matrix is to be used in the computation. Examples of this are the *transa* and *transb* arguments specified for SGEADD, matrix addition.

# **Conjugate Transpose of a Matrix**

The conjugate transpose of a matrix  $\mathbf{A}$ , containing complex numbers, is denoted by  $\mathbf{A}^{H}$  and is expressed as follows:

$$\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \qquad \mathbf{A}^{H} = \begin{bmatrix} \overline{a}_{11} & \dots & \overline{a}_{m1} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ \overline{a}_{1n} & \dots & \overline{a}_{mn} \end{bmatrix}$$

Just as for the transpose of a matrix, the conjugate transpose of a matrix is stored in untransformed format. No movement of data is necessary in your program.

# In Storage

A matrix is usually stored in a two-dimensional array. Its elements are stored successively within the array. Each column of the matrix is stored successively in the array. The leading dimension argument is used to select the matrix elements from each successive column of the array. The starting point of the matrix in the array is specified as the argument for the matrix in the ESSL calling sequence. For example, if matrix  $\boldsymbol{A}$  is contained in array A and starts at the first element in the first row and first column of A, you should specify A as the argument for matrix  $\boldsymbol{A}$ , such as in:

CALL SGEMX 
$$(5,2,1.0,A,6,X,1,Y,1)$$

where, in the matrix-vector product, the number of rows in matrix  $\mathbf{A}$  is 5, the number of columns in matrix  $\mathbf{A}$  is 2, the scaling constant is 1.0, the location of the matrix is A, the leading dimension is 6, the vectors used in the matrix-vector product are X and Y, and their strides are 1.

If matrix  $\mathbf{A}$  is contained in the array BIG, declared as BIG(1:20,1:30), and starts at the second row and third column of BIG, you should specify BIG(2,3) as the argument for matrix  $\mathbf{A}$ , such as in:

CALL SGEMX 
$$(5,2,1.0,BIG(2,3),6,X,1,Y,1)$$

See "How Leading Dimension Is Used for Matrices" for a complete description of how matrices are stored within arrays.

For a complex matrix, a special storage arrangement is used to accommodate the two parts, a and b, of each complex number (a+bi) in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex matrices as for real matrices of the same precision. See "How Do You Set Up Your Scalar Data?" on page 28 for a description of real and complex numbers, and "How Do You Set Up Your Arrays?" on page 29 for a description of how real and complex data is stored in arrays.

# **How Leading Dimension Is Used for Matrices**

The leading dimension for a two-dimensional array is an increment that is used to find the starting point for the matrix elements in each successive column of the array. To define exactly which elements become the conceptual matrix in the array, the following items are used together:

- The location of the matrix within the array
- The leading dimension
- The number of rows, m, to be processed in the array

• The number of columns, n, to be processed in the array

The leading dimension must always be positive. It must always be greater than or equal to m, the number of rows in the matrix to be processed. For an array, A, declared as A(E1:E2,F1:F2), the leading dimension is equal to:

```
(E2-E1+1)
```

The starting point for selecting the matrix elements from the array is at the location specified by the argument for the matrix in the ESSL calling sequence. For example, if you specify A(3,0) for a 4 by 4 matrix A, where A is declared as A(1:7,0:4):

```
      1.0
      8.0
      15.0
      22.0
      29.0

      2.0
      9.0
      16.0
      23.0
      30.0

      3.0
      10.0
      17.0
      24.0
      31.0

      4.0
      11.0
      18.0
      25.0
      32.0

      5.0
      12.0
      19.0
      26.0
      33.0

      6.0
      13.0
      20.0
      27.0
      34.0

      7.0
      14.0
      21.0
      28.0
      35.0
```

then processing begins at the element at row 3 and column 0 in array A, which is 3.0.

The leading dimension is used to find the starting point for the matrix elements in each of the n successive columns in the array. ESSL subroutines assume that the arrays are stored in column-major order, as described under "How Do You Set Up Your Arrays?" on page 29, and they add the leading dimension (times the size of the element in bytes) to the starting point. They do this n-1 times. This finds the starting point in each of the n columns of the array.

In the above example, the leading dimension is:

```
E2-E1+1 = 7-1+1 = 7
```

If the number of columns, n, to be processed is 4, the starting points are: A(3,0), A(3,1), A(3,2), and A(3,3). These are elements 3.0, 10.0, 17.0, and 24.0 for  $a_{11}$ ,  $a_{12}$ ,  $a_{13}$ , and  $a_{14}$ , respectively.

In general terms, this results in the following starting positions of each column in the matrix being calculated as follows:

```
A(BEGINI, BEGINJ)
A(BEGINI, BEGINJ+1)
A(BEGINI, BEGINJ+2)
.
.
.
A(BEGINI, BEGINJ+n-1)
```

To find the elements in each column of the array, 1 is added successively to the starting point in the column until m elements are selected. This is why the leading dimension must be greater than or equal to m; otherwise, you go past the end of each dimension of the array. In the above example, if the number of elements, m, to be processed in each column is 4, the following elements are selected from array A for the first column of the matrix: A(3,0), A(4,0), A(5,0), and A(6,0).

These are elements 3.0, 4.0, 5.0, and 6.0, corresponding to the matrix elements  $a_{11}$ ,  $a_{21}$ ,  $a_{31}$ , and  $a_{41}$ , respectively.

Column element selection can also be expressed in general terms. Using A(BEGINI, BEGINJ) as the starting point in the array, this results in the following elements being selected from each column in the array:

```
A(BEGINI, BEGINJ)
A(BEGINI+1, BEGINJ)
A(BEGINI+2, BEGINJ)
.
.
.
A(BEGINI+m-1, BEGINJ)
```

Combining this with the technique already described for finding the starting point in each column of the array, the resulting matrix in the example is:

$$A = \begin{bmatrix} a_{11} & \dots & a_{14} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{41} & \dots & a_{44} \end{bmatrix} = \begin{bmatrix} 3.0 & 10.0 & 17.0 & 24.0 \\ 4.0 & 11.0 & 18.0 & 25.0 \\ 5.0 & 12.0 & 19.0 & 26.0 \\ 6.0 & 13.0 & 20.0 & 27.0 \end{bmatrix}$$

As shown in this example, a matrix does not have to include all columns and rows of an array. The elements of matrix **A** are selected from rows 3 through 6 and columns 0 through 3 of the array. Rows 1, 2, and 7 and column 4 of the array are not used.

# **Symmetric Matrix**

The matrix  $\mathbf{A}$  is symmetric if it has the property  $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$ , which means:

- It has the same number of rows as it has columns; that is, it has n rows and n columns.
- The value of every element  $a_{ij}$  on one side of the main diagonal equals its mirror image  $a_{ij}$  on the other side:  $a_{ij} = a_{ji}$  for  $1 \le i \le n$  and  $1 \le j \le n$ .

The following matrix illustrates a symmetric matrix of order *n*; that is, it has *n* rows and *n* columns. The subscripts on each side of the diagonal appear the same to show which elements are equal:

#### In Storage

The four storage modes used for storing symmetric matrices are described in the following sections:

- "Lower-Packed Storage Mode"
- "Upper-Packed Storage Mode" on page 67
- "Lower Storage Mode" on page 68
- "Upper Storage Mode" on page 69

The storage technique you should use depends on the ESSL subroutine you are using and is given under Notes in each subroutine description.

**Lower-Packed Storage Mode:** When a symmetric matrix is stored in lower-packed storage mode, the lower triangular part of the symmetric matrix is stored, including the diagonal, in a one-dimensional array. The lower triangle is packed by columns. (This is equivalent to packing the upper triangle by rows.) The matrix is packed sequentially column by column in n(n+1)/2 elements of a one-dimensional array. To calculate the location of each element  $a_{ij}$  of matrix  $\bf A$  in an array, AP, using the lower triangular packed technique, use the following formula:

```
AP(i + ((2n-j)(j-1)/2)) = a_{ij} where i \ge j
```

This results in the following storage arrangement for the elements of a symmetric matrix  $\mathbf{A}$  in an array AP:

```
= a_{11} (start the first column)
AP(1)
AP(2)
                                = a_{21}
AP(3)
                                = a_{31}
AP(n)
                                = a_{n1}
                                = a_{22} (start the second column)
AP(n+1)
AP(n+2)
                                = a_{32}
AP(2n-1)
                                = a_{33} (start the third column and so forth)
AP(2n)
AP(2n+1)
                                = a_{43}
AP(n(n+1)/2)
                                = a_{nn}
```

Following is an example of a symmetric matrix that uses the element values to show the order in which the matrix elements are stored in the array.

Given the following matrix **A**:

```
1 2 3 4 5
2 6 7 8 9
3 7 10 11 12
4 8 11 13 14
5 9 12 14 15
```

the array is:

```
AP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)
```

**Note:** Additional work storage is required in the array for some ESSL subroutines; for example, in the simultaneous linear algebraic equation subroutines SPPF, DPPF, SPPS, and DPPS. See the description of those subroutines in Part 2 for details.

Following is an example of how to transform your symmetric matrix to lower-packed storage mode:

```
K = 0
DO 1 J=1,N
DO 2 I=J,N
K = K+1
AP(K)=A(I,J)
CONTINUE
CONTINUE
```

**Upper-Packed Storage Mode:** When a symmetric matrix is stored in upper-packed storage mode, the upper triangular part of the symmetric matrix is stored, including the diagonal, in a one-dimensional array. The upper triangle is packed by columns. (This is equivalent to packing the lower triangle by rows.) The matrix is packed sequentially column by column in n(n+1)/2 elements of a one-dimensional array. To calculate the location of each element  $a_{ij}$  of matrix  $\bf{A}$  in an array AP using the upper triangular packed technique, use the following formula:

```
AP(i+(j(j-1)/2)) = a_{ii} where j \ge i
```

This results in the following storage arrangement for the elements of a symmetric matrix  $\boldsymbol{A}$  in an array AP:

```
AP(1)
                                 = a_{11} (start the first column)
AP(2)
                                 = a_{12} (start the second column)
AP(3)
                                 = a_{22}
AP(4)
                                 = a_{13} (start the third column)
AP(5)
                                = a_{23}
AP(6)
                                = a_{33}
                                 = a_{14} (start the fourth column)
AP(7)
AP(j(j-1)/2+1)
                                 = a_{1i} (start the j-th column)
AP(j(j-1)/2+2)
                                 = a_{2i}
AP(j(j-1)/2+3)
                                 = a_{3i}
AP(j(j-1)/2+j)
                                = a_{ii} (end of the j-th column)
```

Following is an example of a symmetric matrix that uses the element values to show the order in which the matrix elements are stored in the array. Given the following matrix **A**:

the array is:

$$AP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

Following is an example of how to transform your symmetric matrix to upper-packed storage mode:

```
K = 0
D0 1 J=1,N
D0 2 I=1,J
K = K+1
AP(K)=A(I,J)
CONTINUE
CONTINUE
```

**Lower Storage Mode:** When a symmetric matrix is stored in lower storage mode, the lower triangular part of the symmetric matrix is stored, including the diagonal, in a two-dimensional array. These elements are stored in the array in the same way they appear in the matrix. The upper part of the matrix is not required to be stored in the array.

Following is an example of a symmetric matrix  $\boldsymbol{A}$  of order 5 and how it is stored in an array AL.

Given the following matrix **A**:

the array is:

$$AL = \begin{bmatrix} 1 & * & * & * & * \\ 2 & 6 & * & * & * \\ 3 & 7 & 10 & * & * \\ 4 & 8 & 11 & 13 & * \\ 5 & 9 & 12 & 14 & 15 \end{bmatrix}$$

where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

**Upper Storage Mode:** When a symmetric matrix is stored in upper storage mode, the upper triangular part of the symmetric matrix is stored, including the diagonal, in a two-dimensional array. These elements are stored in the array in the same way they appear in the matrix. The lower part of the matrix is not required to be stored in the array.

Following is an example of a symmetric matrix **A** of order 5 and how it is stored in an array AU.

Given the following matrix A:

the array is:

$$AU = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ * & 6 & 7 & 8 & 9 \\ * & * & 10 & 11 & 12 \\ * & * & * & 13 & 14 \\ * & * & * & * & 15 \end{bmatrix}$$

where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

# Positive Definite or Negative Definite Symmetric Matrix

A real symmetric matrix  $\boldsymbol{A}$  is positive definite if and only if  $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$  is positive for all nonzero vectors  $\boldsymbol{x}$ .

A real symmetric matrix  $\boldsymbol{A}$  is negative definite if and only if  $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$  is negative for all nonzero vectors  $\boldsymbol{x}$ .

#### In Storage

The positive definite or negative definite symmetric matrix is stored in the same way the symmetric matrix is stored. For a description of this storage technique, see "Symmetric Matrix" on page 65.

## **Complex Hermitian Matrix**

A complex matrix is Hermitian if it is equal to its conjugate transpose:

$$H = H^{H}$$

#### In Storage

The complex Hermitian matrix is stored using the same four techniques used for symmetric matrices:

- Lower-packed storage mode, as described in "Lower-Packed Storage Mode" on page 66. (The complex Hermitian matrix is not symmetric; therefore, lower-packed storage mode is not equivalent to packing the upper triangle by rows, as it is for a symmetric matrix.)
- Upper-packed storage mode, as described in "Upper-Packed Storage Mode" on page 67. (The complex Hermitian matrix is not symmetric; therefore, upper-packed storage mode is not equivalent to packing the lower triangle by rows, as it is for a symmetric matrix.)
- Lower storage mode, as described in "Lower Storage Mode" on page 68.
- Upper storage mode, as described in "Upper Storage Mode" on page 69.

Following is an example of a complex Hermitian matrix **H** of order 5.

Given the following matrix *H*:

it is stored in a one-dimensional array, HP, in n(n+1)/2 = 15 elements as follows:

In lower-packed storage mode:

```
HP = ((11, *), (21, 1), (31, -1), (41, 1), (51, 1), (22, *), (32, 1), (42, 1), (52, -1), (33, *), (43, 1), (53, 1), (44, *), (54, 1), (55, *)
```

• In upper-packed storage mode:

```
HP = ((11, *), (21, -1), (22, *), (31, 1), (32, -1), (33, *), (41, -1), (42, -1), 43, -1), (44, *), (51, -1), (52, 1), (53, -1), (54, -1), (55, *)
```

or it is stored in a two-dimensional array, HP, as follows:

In lower storage mode:

$$HP = \begin{bmatrix} (11, & *) & * & * & * & * & * \\ (21, & 1) & (22, & *) & * & * & * \\ (31, & -1) & (32, & 1) & (33, & *) & * & * \\ (41, & 1) & (42, & 1) & (43, & 1) & (44, & *) & * \\ (51, & 1) & (52, & -1) & (53, & 1) & (54, & 1) & (55, & *) \end{bmatrix}$$

In upper storage mode

HP = 
$$\begin{bmatrix} (11, *) & (21, -1) & (31, 1) & (41, -1) & (51, -1) \\ * & (22, *) & (32, -1) & (42, -1) & (52, 1) \\ * & * & (33, *) & (43, -1) & (53, -1) \\ * & * & * & (44, *) & (54, -1) \\ * & * & * & * & (55, *) \end{bmatrix}$$

where "\*" means you do not have to store a value in that position in the array. The imaginary parts of the diagonal elements of a complex Hermitian matrix are always 0, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 0.

## Positive Definite or Negative Definite Complex Hermitian Matrix

A complex Hermitian matrix  $\boldsymbol{A}$  is positive definite if and only if  $\boldsymbol{x}^H \boldsymbol{A} \boldsymbol{x}$  is positive for all nonzero vectors  $\boldsymbol{x}$ .

A complex Hermitian matrix  $\mathbf{A}$  is negative definite if and only if  $\mathbf{x}^H \mathbf{A} \mathbf{x}$  is negative for all nonzero vectors  $\mathbf{x}$ .

### In Storage

The positive definite or negative definite complex Hermitian matrix is stored in the same way the complex Hermitian matrix is stored. For a description of this storage technique, see "Complex Hermitian Matrix" on page 70.

## Positive Definite or Negative Definite Symmetric Toeplitz Matrix

A positive definite or negative definite symmetric matrix  $\boldsymbol{A}$  of order n is also a Toeplitz matrix if and only if:

$$a_{ij} = a_{i-1,j-1}$$
 for  $i = 2$ ,  $n$  and  $j = 2$ ,  $n$ 

The elements on each diagonal of the Toeplitz matrix have a constant value. For the definition of a positive definite or negative definite symmetric matrix, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.

The following matrix illustrates a symmetric Toeplitz matrix of order n; that is, it has n rows and n columns:

A symmetric Toeplitz matrix of order n is represented by a vector  $\mathbf{x}$  of length n containing the elements of the first column of the matrix (or the elements of the first row), such that  $x_i = a_{i1}$  for i = 1, n.

The following vector represents the matrix **A** shown above:

$$\mathbf{x} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{bmatrix}$$

#### In Storage

The elements of the vector **x**, which represent a positive definite symmetric Toeplitz matrix, are stored sequentially in an array. This is called packed-symmetric-Toeplitz storage mode. Following is an example of a positive definite symmetric Toeplitz matrix A and how it is stored in an array X.

Given the following matrix **A**:

the array is:

$$X = (99, 12, 13, 14, 15, 16)$$

## Positive Definite or Negative Definite Complex Hermitian Toeplitz **Matrix**

A positive definite or negative definite complex Hermitian matrix  $\bf{A}$  of order n is also a Toeplitz matrix if and only if:

$$a_{ij} = a_{i-1,j-1}$$
 for  $i = 2$ ,  $n$  and  $j = 2$ ,  $n$ 

The real part of the diagonal elements of the Toeplitz matrix must have a constant value. The imaginary part of the diagonal elements must be zero.

For the definition of a positive definite of negative definite complex Hermitian matrix, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 71.

The following matrix illustrates a complex Hermitian Toeplitz matrix of order *n*; that is, it has *n* rows and *n* columns:

A complex Hermitian Toeplitz matrix of order n is represented by a vector  $\mathbf{x}$  of length n containing the elements of the first row of the matrix.

The following vector represents the matrix **A** shown above.

$$\mathbf{x} = \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ \vdots \\ a_{1n} \end{bmatrix}$$

### In Storage

The elements of the vector  $\mathbf{x}$ , which represent a positive definite complex Hermitian Toeplitz matrix, are stored sequentially in an array. This is called packed-Hermitian-Toeplitz storage mode. Following is an example of a positive definite complex Hermitian Toeplitz matrix  $\mathbf{A}$  and how it is stored in an array X.

Given the following matrix A:

$$\begin{bmatrix} (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) & (1.0, 1.0) \\ (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) & (-3.0, 1.0) \\ (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) & (2.0, -3.0) \\ (1.0, -1.0) & (-3.0, -1.0) & (2.0, 3.0) & (10.0, 0.0) \end{bmatrix}$$

the array is:

$$X = ((10.0, 0.0), (2.0, -3.0), (-3.0, 1.0), (1.0, 1.0))$$

# Triangular Matrix

There are two types of triangular matrices: upper triangular matrix and lower triangular matrix. Triangular matrices have the same number of rows as they have columns; that is, they have *n* rows and *n* columns.

A matrix U is an upper triangular matrix if its nonzero elements are found only in the upper triangle of the matrix, including the main diagonal; that is:

$$u_{ij} = 0$$
 if  $i > j$ 

A matrix *L* is an lower triangular matrix if its nonzero elements are found only in the lower triangle of the matrix, including the main diagonal; that is:

$$I_{ii} = 0$$
 if  $i < j$ 

The following matrices,  $\boldsymbol{U}$  and  $\boldsymbol{L}$ , illustrate upper and lower triangular matrices of order n, respectively:

$$\boldsymbol{U} = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \dots & u_{1n} \\ 0 & u_{22} & u_{23} & & & \\ 0 & 0 & u_{33} & & & \\ \vdots & & & \ddots & & \\ \vdots & & & \ddots & & \\ 0 & \vdots & \ddots & \vdots & & & \\ 0 & \vdots & \ddots & \vdots & & & \\ 0 & \vdots & \ddots & \vdots & & & \\ 0 & \vdots & \ddots & \vdots & & & \\ \end{bmatrix} \qquad \boldsymbol{L} = \begin{bmatrix} l_{11} & 0 & 0 & \dots & 0 \\ l_{21} & l_{22} & 0 & & & \\ l_{31} & l_{32} & l_{33} & & & \\ \vdots & & & \ddots & & \\ \vdots & & & \ddots & & \\ \vdots & & & \ddots & \ddots & \\ l_{n1} & \vdots & \ddots & \ddots & l_{nn} \end{bmatrix}$$

A unit triangular matrix is a triangular matrix in which all the diagonal elements have a value of one; that is:

- For an upper triangular matrix,  $u_{ii} = 1$  if i = j.
- For an lower triangular matrix,  $l_{ii} = 1$  if i = j.

The following matrices,  $\boldsymbol{U}$  and  $\boldsymbol{L}$ , illustrate upper and lower unit real triangular matrices of order n, respectively:

#### In Storage

The four storage modes used for storing triangular matrices are described in the following sections:

- "Upper-Triangular-Packed Storage Mode"
- "Lower-Triangular-Packed Storage Mode" on page 75
- "Upper-Triangular Storage Mode" on page 75
- "Lower-Triangular Storage Mode" on page 76

It is important to note that because the diagonal elements of a unit triangular matrix are always one, you do not need to set these values in the array for these four storage modes. ESSL always assumes that the values in these positions are one.

**Upper-Triangular-Packed Storage Mode:** When an upper-triangular matrix is stored in upper-triangular-packed storage mode, the upper triangle of the matrix is stored, including the diagonal, in a one-dimensional array. The upper triangle is packed by columns. The elements are packed sequentially, column by column, in n(n+1)/2 elements of a one-dimensional array. To calculate the location of each element of the triangular matrix in the array, use the technique described in "Upper-Packed Storage Mode" on page 67.

Following is an example of an upper triangular matrix  $\boldsymbol{U}$  of order 5 and how it is stored in array UP. It uses the element values to show the order in which the elements are stored in the one-dimensional array.

Given the following matrix *U*:

the array is:

$$UP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

**Lower-Triangular-Packed Storage Mode:** When a lower-triangular matrix is stored in lower-triangular-packed storage mode, the lower triangle of the matrix is stored, including the diagonal, in a one-dimensional array. The lower triangle is packed by columns. The elements are packed sequentially, column by column, in n(n+1)/2 elements of a one-dimensional array. To calculate the location of each element of the triangular matrix in the array, use the technique described in "Lower-Packed Storage Mode" on page 66.

Following is an example of a lower triangular matrix *L* of order 5 and how it is stored in array LP. It uses the element values to show the order in which the elements are stored in the one-dimensional array.

Given the following matrix L:

the array is:

$$LP = (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15)$$

**Upper-Triangular Storage Mode:** A triangular matrix is stored in upper-triangular storage mode in a two-dimensional array. Only the elements in the upper triangle of the matrix, including the diagonal, are stored in the upper triangle of the array.

Following is an example of an upper triangular matrix  $\boldsymbol{U}$  of order 5 and how it is stored in array UTA.

Given the following matrix *U*:

the array is:

where "\*" means you do not have to store a value in that position in the array.

Lower-Triangular Storage Mode: A triangular matrix is stored in lower-triangular storage mode in a two-dimensional array. Only the elements in the lower triangle of the matrix, including the diagonal, are stored in the lower triangle of the array.

Following is an example of a lower triangular matrix L of order 5 and how it is stored in array LTA.

Given the following matrix L:

the array is:

LTA = 
$$\begin{bmatrix} 11 & * & * & * & * \\ 21 & 22 & * & * & * \\ 31 & 32 & 33 & * & * \\ 41 & 42 & 43 & 44 & * \\ 51 & 52 & 53 & 54 & 55 \end{bmatrix}$$

where "\*" means you do not have to store a value in that position in the array.

### **General Band Matrix**

A general band matrix has its nonzero elements arranged uniformly near the diagonal, such that:

$$a_{ii} = 0$$
 if  $(i-j) > ml$  or  $(j-i) > mu$ 

where ml and mu are the lower and upper band widths, respectively, and ml+mu+1 is the total band width.

The following matrix illustrates a **square** general band matrix of order n, where the band widths are ml = q-1 and mu = p-1:

Some special types of band matrices are:

- Tridiagonal matrix: ml = mu = 1
- 9-diagonal matrix: ml = mu = 4

The following two matrices illustrate m by n rectangular general band matrices, where the band widths are ml = q-1 and mu = p-1. For both matrices, the leading diagonal is  $a_{11}$ ,  $a_{22}$ ,  $a_{33}$ , ...,  $a_{nn}$ . Following is a general band matrix with m > n:

$$\begin{vmatrix} \leftarrow mu \rightarrow | \\ a_{11} a_{12} a_{13} & \cdot \cdot a_{1p} 0 & \cdot \cdot & 0 \\ a_{21} a_{22} a_{23} & \cdot \cdot & 0 & \cdot \\ a_{31} a_{32} a_{33} & \cdot \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & a_{q1} & \cdot & \cdot & \cdot & \cdot \\ a_{q1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ - & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & a_{mn} \end{bmatrix}$$

Following is a general band matrix with m < n:

## In Storage

The two storage modes used for storing general band matrices are described in the following sections:

- "General-Band Storage Mode"
- "BLAS-General-Band Storage Mode" on page 80

**General-Band Storage Mode:** (This storage mode is used only for square matrices.) Only the band elements of a general band matrix are stored for general-band storage mode. Additional storage must also be provided for fill- in. General-band storage mode packs the matrix elements by columns into a two-dimensional array, such that each diagonal of the matrix appears as a row in the packed array.

For a matrix  $\mathbf{A}$  of order n with band widths ml and mu, the array must have a leading dimension, lda, greater than or equal to 2ml+mu+16. The size of the second dimension must be (at least) n, the number of columns in the matrix.

Using array AGB, which is declared as AGB(2ml+mu+16, n), the columns of elements in matrix **A** are stored in each column in array AGB as follows, where  $a_{11}$  is stored at AGB(ml+mu+1, 1):

where "\*" means you do not store an element in that position in the array.

In the ESSL subroutine computation, some of the positions in the array indicated by an "\*" are used for fill- in. Other positions may not be accessed at all.

Following is an example of a band matrix  $\bf{A}$  of order 9 and band widths of ml = 2 and mu = 3.

Given the following matrix A:

you store it in general-band storage mode in a 23 by 9 array AGB as follows, where  $a_{11}$  is stored in AGB(6,1):

```
14
                         25
                                           69
                              36
                                  47
                                       58
                 13
                          35
                              46
                                   57
                                       68
                                           79
             12
                 23
                     34
                          45
                              56
                                   67
                                       78
                                           89
         11
             22
                 33
                     44
                          55
                              66
                                  77
                                       88
                                           99
        21
            32
                 43
                                       98
                     54
                          65
                              76
                                  87
            42
        31
                 53
                          75
                              86
AGB =
```

Following is an example of how to transform your general band matrix, of order *n*, to general-band storage mode:

```
MD=ML+MU+1
DO 1 J=1,N
DO 1 I=MAX(J-MU,1),MIN(J+ML,N)
AGB(I-J+MD,J)=A(I,J)

CONTINUE
```

**BLAS-General-Band Storage Mode:** (This storage mode is used for both square and rectangular matrices.) Only the band elements of a general band matrix are stored for BLAS-general-band storage mode. The storage mode packs the matrix elements by columns into a two-dimensional array, such that each diagonal of the matrix appears as a row in the packed array.

For an m by n matrix  $\mathbf{A}$  with band widths ml and mu, the array AGB must have a leading dimension, lda, greater than or equal to ml+mu+1. The size of the second dimension must be (at least) n, the number of columns in the matrix.

Using the array AGB, which is declared as AGB(ml+mu+1, n), the columns of elements in matrix **A** are stored in each column in array AGB as follows, where  $a_{11}$  is stored at AGB(mu+1, 1):

where "\*" means you do not store an element in that position in the array. These positions are not accessed by ESSL. Unused positions in the array always occur in the upper left triangle of the array, but may not occur in the lower right triangle of the array, as you can see from the examples given here.

Following is an example where m > n, and general band matrix **A** is 9 by 8 with band widths of ml = 2 and mu = 3.

Given the following matrix **A**:

you store it in array AGB, declared as AGB(6,8), as follows, where  $a_{11}$  is stored in AGB(4,1):

AGB = 
$$\begin{bmatrix} * & * & * & 14 & 25 & 36 & 47 & 58 \\ * & * & 13 & 24 & 35 & 46 & 57 & 68 \\ * & 12 & 23 & 34 & 45 & 56 & 67 & 78 \\ 11 & 22 & 33 & 44 & 55 & 66 & 77 & 88 \\ 21 & 32 & 43 & 54 & 65 & 76 & 87 & 98 \\ 31 & 42 & 53 & 64 & 75 & 86 & 97 & * \end{bmatrix}$$

Following is an example where m < n, and general band matrix **A** is 7 by 9 with band widths of ml = 2 and mu = 3.

Given the following matrix A:

you store it in array AGB, declared as AGB(6,9), as follows, where  $a_{11}$  is stored in AGB(4,1) and the leading diagonal does not fill up the whole row:

AGB = 
$$\begin{bmatrix} * & * & * & 14 & 25 & 36 & 47 & 58 & 69 \\ * & * & 13 & 24 & 35 & 46 & 57 & 68 & 79 \\ * & 12 & 23 & 34 & 45 & 56 & 67 & 78 & * \\ 11 & 22 & 33 & 44 & 55 & 66 & 77 & * & * \\ 21 & 32 & 43 & 54 & 65 & 76 & * & * & * \\ 31 & 42 & 53 & 64 & 75 & * & * & * & * \end{bmatrix}$$

and where "\*" means you do not store an element in that position in the array.

Following is an example of how to transform your general band matrix, for all values of m and n, to BLAS-general-band storage mode:

```
DO 20 J=1,N

K=MU+1-J

DO 10 I=MAX(1,J-MU),MIN(M,J+ML)

AGB(K+I,J)=A(I,J)

10 CONTINUE

20 CONTINUE
```

# **Symmetric Band Matrix**

A symmetric band matrix is a symmetric matrix whose nonzero elements are arranged uniformly near the diagonal, such that:

$$a_{ii} = 0$$
 if  $|i-j| > k$ 

where *k* is the half band width.

The following matrix illustrates a symmetric band matrix of order n, where the half band width k = q-1:

$$A = \begin{bmatrix} a_{11} a_{21} a_{31} & . & . & a_{q1} 0 & . & . & 0 \\ a_{21} a_{22} a_{32} & & & 0 & . & . \\ a_{31} a_{32} a_{33} & & & 0 & . & . \\ . & & . & & & 0 \\ . & & & . & & . & . \\ a_{q1} & & & . & & . & . \\ 0 & & & . & & . & . \\ . & 0 & & & . & . & . \\ . & 0 & & & . & . & . \\ 0 & . & . & 0 & . & . & . & . \end{bmatrix}$$

#### In Storage

The two storage modes used for storing symmetric band matrices are described in the following sections:

- "Upper-Band-Packed Storage Mode"
- "Lower-Band-Packed Storage Mode" on page 84

**Upper-Band-Packed Storage Mode:** Only the band elements of the upper triangular part of a symmetric band matrix, including the main diagonal, are stored for upper-band-packed storage mode.

For a matrix  $\mathbf{A}$  of order n and a half band width of k, the array must have a leading dimension, lda, greater than or equal to k+1, and the size of the second dimension must be (at least) n.

Using array ASB, which is declared as ASB(Ida, n), where p = Ida = k+1, the elements of a symmetric band matrix are stored as follows:

where "\*" means you do not store an element in that position in the array.

Following is an example of a symmetric band matrix **A** of order 6 and a half band width of 3.

Given the following matrix A:

you store it in upper-band-packed storage mode in array ASB, declared as ASB(4,6), as follows.

ASB = 
$$\begin{bmatrix} * & * & * & 14 & 25 & 36 \\ * & * & 13 & 24 & 35 & 46 \\ * & 12 & 23 & 34 & 45 & 56 \\ 11 & 22 & 33 & 44 & 55 & 66 \end{bmatrix}$$

Following is an example of how to transform your symmetric band matrix to upper-band-packed storage mode:

```
DO 20 J=1,N

M=K+1-J

DO 10 I=MAX(1,J-K),J

ASB(M+I,J)=A(I,J)

10 CONTINUE

20 CONTINUE
```

**Lower-Band-Packed Storage Mode:** Only the band elements of the lower triangular part of a symmetric band matrix, including the main diagonal, are stored for lower-band-packed storage mode.

For a matrix  $\mathbf{A}$  of order n and a half band width of k, the array must have a leading dimension, lda, greater than or equal to k+1, and the size of the second dimension must be (at least) n.

Using array ASB, which is declared as ASB(Ida, n), where q = Ida = k+1, the elements of a symmetric band matrix are stored as follows:

$$ASB = \begin{bmatrix} a_{11} & a_{22} & \dots & a_{nn} \\ a_{21} & a_{32} & & * \\ a_{31} & a_{42} & & \dots \\ & \ddots & & & \ddots \\ & \ddots & & & \ddots \\ & a_{q1} & a_{q+1,2} & \dots & a_{n,n-k} * \dots * \end{bmatrix}$$

where "\*" means you do not store an element in that position in the array.

Following is an example of a symmetric band matrix **A** of order 6 and a half band width of 2.

Given the following matrix A:

you store it in lower-band-packed storage mode in array ASB, declared as ASB(3,6), as follows:

$$ASB = \begin{bmatrix} 11 & 22 & 33 & 44 & 55 & 66 \\ 21 & 32 & 43 & 54 & 65 & * \\ 31 & 42 & 53 & 64 & * & * \end{bmatrix}$$

Following is an example of how to transform your symmetric band matrix to lower-band-packed storage mode:

```
DO 20 J=1,N

DO 10 I=J,MIN(J+K,N)

ASB(I-J+1,J)=A(I,J)

10 CONTINUE

20 CONTINUE
```

## **Positive Definite Symmetric Band Matrix**

A real symmetric band matrix  $\mathbf{A}$  is positive definite if and only if  $\mathbf{x}^T \mathbf{A} \mathbf{x}$  is positive for all nonzero vectors  $\mathbf{x}$ .

#### In Storage

The positive definite symmetric band matrix is stored in the same way a symmetric band matrix is stored. For a description of this storage technique, see "Symmetric Band Matrix" on page 82.

# **Complex Hermitian Band Matrix**

A complex band matrix is Hermitian if it is equal to its conjugate transpose:

$$H = H^{H}$$

#### In Storage

The complex Hermitian band matrix is stored using the same two techniques used for symmetric band matrices:

- Lower-band-packed storage mode, as described in "Lower-Band-Packed Storage Mode" on page 84
- Upper-band-packed storage mode, as described in "Upper-Band-Packed Storage Mode" on page 83

Following is an example of a complex Hermitian band matrix  $\boldsymbol{H}$  of order 5, having a half band width of 2.

Given the following matrix H:

you store it in a two-dimensional array HP, as follows:

In lower-band-packed storage mode:

$$HP = \begin{bmatrix} (11, & *) & (22, & *) & (33, & *) & (44, & *) & (55, & *) \\ (21, & 1) & (32, & 1) & (43, & 1) & (54, & 1) & & * \\ (31, & -1) & (42, & 1) & (53, & 1) & & & & * \end{bmatrix}$$

• In upper-band-packed storage mode:

$$HP = \begin{bmatrix} * & * & (31, 1) & (42, -1) & (53, -1) \\ * & (21, -1) & (32, -1) & (43, -1) & (54, -1) \\ (11, *) & (22, *) & (33, *) & (44, *) & (55, *) \end{bmatrix}$$

where "\*" means you do not have to store a value in that position in the array. The imaginary parts of the diagonal elements of a complex Hermitian band matrix are always 0, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 0.

# **Triangular Band Matrix**

There are two types of triangular band matrices: upper triangular band matrix and lower triangular band matrix. Triangular band matrices have the same number of rows as they have columns; that is, they have n rows and n columns. They have an upper or lower band width of k.

A band matrix  $\boldsymbol{U}$  is an upper triangular band matrix if its nonzero elements are found only in the upper triangle of the matrix, including the main diagonal; that is:

$$u_{ii} = 0$$
 if  $i > j$ 

Its band elements are arranged uniformly near the diagonal in the upper triangle of the matrix, such that:

$$u_{ii} = 0$$
 if  $j-i > k$ 

The following matrix  $\boldsymbol{U}$  illustrates an upper triangular band matrix of order n with an upper band width k=q-1:

$$U = \begin{bmatrix} u_{11} u_{21} u_{31} & \dots & u_{q1} 0 & \dots & 0 \\ 0 u_{22} u_{32} & & 0 & \dots \\ \vdots & & \ddots & & \vdots \\ 0 & \dots & \ddots & & \ddots \\ \vdots & & \ddots & \ddots & \ddots \\ \vdots &$$

A band matrix **L** is a lower triangular band matrix if its nonzero elements are found only in the lower triangle of the matrix, including the main diagonal; that is:

$$I_{ij} = 0$$
 if  $i < j$ 

Its band elements are arranged uniformly near the diagonal in the lower triangle of the matrix such that:

$$I_{ii} = 0$$
 if  $i-j > k$ 

The following matrix L illustrates an upper triangular band matrix of order n with a lower band width k = q-1:

A triangular band matrix can also be a unit triangular band matrix if all the diagonal elements have a value of 1. For an illustration of a unit triangular matrix, see "Triangular Matrix" on page 73.

#### In Storage

The two storage modes used for storing triangular band matrices are described in the following sections:

- "Upper-Triangular-Band-Packed Storage Mode" on page 88
- "Lower-Triangular-Band-Packed Storage Mode" on page 89

It is important to note that because the diagonal elements of a unit triangular band matrix are always one, you do not need to set these values in the array for these two storage modes. ESSL always assumes that the values in these positions are one. **Upper-Triangular-Band-Packed Storage Mode:** Only the band elements of the upper triangular part of an upper triangular band matrix, including the main diagonal, are stored for upper-triangular-band-packed storage mode.

For a matrix U of order n and an upper band width of k, the array must have a leading dimension, Ida, greater than or equal to k+1, and the size of the second dimension must be (at least) n.

Using array UTB, which is declared as UTB(Ida, n), where p = Ida = k+1, the elements of an upper triangular band matrix are stored as follows:

where "\*" means you do not store an element in that position in the array.

Following is an example of an upper triangular band matrix  $\boldsymbol{U}$  of order 6 and an upper band width of 3.

Given the following matrix *U*:

you store it in upper-triangular-band-packed storage mode in array UTB, declared as UTB(4,6), as follows:

Following is an example of how to transform your upper triangular band matrix to upper-triangular-band-packed storage mode:

```
DO 20 J=1,N

M=K+1-J

DO 10 I=MAX(1,J-K),J

UTB(M+I,J)=U(I,J)

10 CONTINUE

20 CONTINUE
```

**Lower-Triangular-Band-Packed Storage Mode:** Only the band elements of the lower triangular part of a lower triangular band matrix, including the main diagonal, are stored for lower-triangular-band-packed storage mode.

**Note:** As an alternative to this storage mode, you can specify your arguments in your subroutine in a special way so that ESSL selects the matrix elements properly, and you can leave your matrix stored in full-matrix storage mode. For details, see the Notes in the subroutine description in Part 2 of this book.

For a matrix L of order n and a lower band width of k, the array must have a leading dimension, lda, greater than or equal to k+1, and the size of the second dimension must be (at least) n.

Using array LTB, which is declared as LTB(Ida,n), where q = Ida = k+1, the elements of a lower triangular band matrix are stored as follows:

$$\mathsf{LTB} \ = \begin{bmatrix} l_{11} & l_{22} & \dots & & l_{nn} \\ l_{21} & l_{32} & & & * \\ l_{31} & l_{42} & & & \vdots \\ \vdots & \vdots & & & \ddots \\ l_{q1} & l_{q+1,2} & \dots & l_{n,n-k} * & \dots * \end{bmatrix}$$

where "\*" means you do not store an element in that position in the array.

Following is an example of a lower triangular band matrix L of order 6 and a lower band width of 2.

Given the following matrix *L*:

you store it in lower-triangular-band-packed storage mode in array LTB, declared as LTB(3,6), as follows:

Following is an example of how to transform your lower triangular band matrix to lower-triangular-band-packed storage mode:

```
DO 20 J=1,N

M=1-J

DO 10 I=J,MIN(N,J+K)

LTB(M+I,J)=L(I,J)

10 CONTINUE

20 CONTINUE
```

## **General Tridiagonal Matrix**

A general tridiagonal matrix is a matrix whose nonzero elements are found only on the diagonal, subdiagonal, and superdiagonal of the matrix; that is:

$$a_{ii} = 0$$
 if  $|i-j| > 1$ 

The following matrix illustrates a general tridiagonal matrix of order *n*:

## In Storage

Only the diagonal, subdiagonal, and superdiagonal elements of the general tridiagonal matrix are stored. This is called tridiagonal storage mode. The elements of a general tridiagonal matrix,  $\boldsymbol{A}$ , of order n are stored in three one-dimensional arrays, C, D, and E, each of length n, where array C contains the subdiagonal elements, stored as follows:

$$C = (*, a_{21}, a_{32}, a_{43}, ..., a_{n-1})$$

and array D contains the main diagonal elements, stored as follows:

$$D = (a_{11}, a_{22}, a_{33}, ..., a_{nn})$$

and array E contains the superdiagonal elements, stored as follows:

$$E = (a_{12}, a_{23}, a_{34}, ..., a_{n-1,n}, *)$$

where "\*" means you do not store an element in that position in the array.

Following is an example of a general tridiagonal matrix A of order 5:

which you store in tridiagonal storage mode in arrays C, D, and E, each of length 5, as follows:

**Note:** Some ESSL subroutines provide an option for specifying at least *n* additional locations at the end of each of the arrays C, D, and E. These additional locations are used for working storage by the ESSL subroutine. The reasons for choosing this option are explained in the subroutine descriptions.

# Symmetric Tridiagonal Matrix

A tridiagonal matrix  $\mathbf{A}$  is also symmetric if and only if its nonzero elements are found only on the diagonal, subdiagonal, and superdiagonal of the matrix, and its subdiagonal elements and superdiagonal elements are equal; that is:

$$(a_{ij} = 0 \text{ if } |i-j| > 1)$$
 and  $(a_{ij} = a_{ji} \text{ if } |i-j| = 1)$ 

The following matrix illustrates a symmetric tridiagonal matrix of order *n*:

#### In Storage

Only the diagonal and subdiagonal elements of the positive definite symmetric tridiagonal matrix are stored. This is called symmetric-tridiagonal storage mode. The elements of a symmetric tridiagonal matrix  $\boldsymbol{A}$  of order  $\boldsymbol{n}$  are stored in two one-dimensional arrays  $\mathbb C$  and  $\mathbb D$ , each of length  $\boldsymbol{n}$ , where array  $\mathbb C$  contains the subdiagonal elements, stored as follows:

$$C = (*, a_{21}, a_{32}, a_{43}, ..., a_{n,n-1})$$

where "\*" means you do not store an element in that position in the array. Then array D contains the main diagonal elements, stored as follows:

$$D = (a_{11}, a_{22}, a_{33}, ..., a_{nn})$$

Following is an example of a symmetric tridiagonal matrix **A** of order 5:

which you store in symmetric-tridiagonal storage mode in arrays C and D, each of length 5, as follows:

$$C = (*, 1, 2, 3, 4)$$
  
 $D = (10, 20, 30, 40, 50)$ 

**Note:** Some ESSL subroutines provide an option for specifying at least *n* additional locations at the end of each of the arrays C and D. These additional locations are used for working storage by the ESSL subroutine. The reasons for choosing this option are explained in the subroutine descriptions.

## **Positive Definite Symmetric Tridiagonal Matrix**

A real symmetric tridiagonal matrix  $\mathbf{A}$  is positive definite if and only if  $\mathbf{x}^T \mathbf{A} \mathbf{x}$  is positive for all nonzero vectors x.

## In Storage

The positive definite symmetric tridiagonal matrix is stored in the same way the symmetric tridiagonal matrix is stored. For a description of this storage technique, see "Symmetric Tridiagonal Matrix" on page 91.

# Sparse Matrix

A sparse matrix is a matrix having a relatively small number of nonzero elements.

Consider the following as an example of a sparse matrix **A**:

### In Storage

A sparse matrix can be stored in full-matrix storage mode or a packed storage mode. When a sparse matrix is stored in full-matrix storage mode, all its elements, including its zero elements, are stored in an array.

The seven packed storage modes used for storing sparse matrices are described in the following sections:

- "Compressed-Matrix Storage Mode" on page 93
- "Compressed-Diagonal Storage Mode" on page 94

- "Storage-by-Indices" on page 97
- "Storage-by-Columns" on page 98
- "Storage-by-Rows" on page 99
- "Diagonal-Out Skyline Storage Mode" on page 101
- "Profile-In Skyline Storage Mode" on page 103

**Note:** When the elements of a sparse matrix are stored using any of these storage modes, the ESSL subroutines do not check that all elements are nonzero. You do not get an error if any elements are zero.

**Compressed-Matrix Storage Mode:** The sparse matrix  $\boldsymbol{A}$ , stored in compressed-matrix storage mode, uses two two-dimensional arrays to define the sparse matrix storage, AC and KA. See reference [67]. Given the m by n sparse matrix  $\boldsymbol{A}$ , having a maximum of nz nonzero elements in each row:

- AC is defined as AC(Ida,nz), where the leading dimension, Ida, must be greater than or equal to m. Each row of array AC contains the nonzero elements of the corresponding row of matrix A. For each row in matrix A containing less than nz nonzero elements, the corresponding row in array AC is padded with zeros. The elements in each row can be stored in any order.
- KA is an integer array defined as KA(Ida,nz), where the leading dimension, Ida, must be greater than or equal to m. It contains the column numbers of the matrix A elements that are stored in the corresponding positions in array AC. For each row in matrix A containing less than nz nonzero elements, the corresponding row in array KA is padded with any values from 1 to n. Because this array is used by the ESSL subroutines to access other target vectors in the computation, you must adhere to these required values to avoid errors.

Unless all the rows of sparse matrix A contain approximately the same number of nonzero elements, this storage mode requires a large amount of storage. This diminishes the performance you can obtain by using this storage mode.

Consider the following as an example of a 6 by 6 sparse matrix  $\boldsymbol{A}$  with a maximum of four nonzero elements in each row. It shows how matrix  $\boldsymbol{A}$  can be stored in arrays AC and KA.

Given the following matrix **A**:

the arrays are:

$$AC = \begin{bmatrix} 11 & 13 & 0 & 0 \\ 22 & 21 & 24 & 0 \\ 33 & 32 & 35 & 0 \\ 44 & 43 & 46 & 0 \\ 55 & 51 & 54 & 0 \\ 66 & 61 & 62 & 65 \end{bmatrix}$$

where "\*" means you can store any value from 1 to 6 in that position in the array.

Symmetric sparse matrices use the same storage technique as nonsymmetric sparse matrices; that is, all nonzero elements of a symmetric matrix  $\boldsymbol{A}$  must be stored in array AC, not just the elements of the upper triangle and diagonal of matrix  $\boldsymbol{A}$ .

In general terms, this storage technique can be expressed as follows:

```
For each a_{ij} \neq 0, for i = 1, m and j = 1, n there exists k, where 1 \leq k \leq nz, such that AC(i,k) = a_{ij} and KA(i,k) = j.
For all other elements of AC and KA, AC(i,k) = 0 and 1 \leq KA(i,k) \leq n
```

#### where:

- a<sub>ij</sub> are the elements of the m by n matrix A that has a maximum of nz nonzero elements in each row.
- Array AC is defined as AC(Ida,nz), where  $Ida \ge m$ .
- Array KA is defined as KA(Ida,nz), where  $Ida \ge m$ .

**Compressed-Diagonal Storage Mode:** The storage mode used for square sparse matrices stored in compressed-diagonal storage mode has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. This section explains both of these variations. This section begins, however, by explaining the conventions used for numbering the diagonals in the matrix, which apply to the storage descriptions.

Matrix  $\mathbf{A}$  of order n has 2n-1 diagonals. Because k = j-i is constant for the elements  $a_{ij}$  along each diagonal, each diagonal can be assigned a diagonal number, k, having a value from 1-n to n-1. Then the diagonals can be referred to as  $\mathbf{d}_k$ , where k = 1-n, n-1.

The following matrix shows the starting position of each diagonal,  $d_k$ :

For a **general** (square) sparse matrix **A**, compressed-diagonal storage mode uses two arrays to define the sparse matrix storage, AD and LA. Using the above convention for numbering the diagonals, and given that sparse matrix **A** contains *nd* diagonals having nonzero elements, arrays AD and LA are set up as follows:

- AD is defined as AD(Ida,nd), where the leading dimension, Ida, must be greater than or equal to n. Each diagonal of matrix A that has at least one nonzero element is stored in a column of array AD. All of the elements of the diagonal, including its zero elements, are stored in n contiguous locations in the array, in the same order as they appear in the diagonal. Padding with zeros is required as follows to fill the n locations in each column of array AD:
  - Each superdiagonal (k > 0), which has n-k elements, is padded with k trailing zeros.
  - The main diagonal (k = 0), which has n elements, does not require padding.
  - Each subdiagonal (k < 0), which has n-|k| elements, is padded with |k| leading zeros.

The diagonals can be stored in any columns in array AD.

• LA is a one-dimensional integer array of length *nd*, containing the diagonal numbers *k* for the diagonals stored in each corresponding column in array AD.

Because this storage mode requires entire diagonals to be stored, if the nonzero elements in matrix A are not concentrated along a few diagonals, this storage mode requires a large amount of storage. This diminishes the performance you obtain by using this storage mode.

Consider the following as an example of how a 6 by 6 general sparse matrix  $\boldsymbol{A}$  with 5 nonzero diagonals is stored in arrays AD and LA.

Given the following matrix **A**:

the arrays are:

$$AD = \begin{bmatrix} 11 & 13 & 0 & 0 & 0 \\ 22 & 24 & 21 & 0 & 0 \\ 33 & 35 & 32 & 0 & 0 \\ 44 & 46 & 43 & 0 & 0 \\ 55 & 0 & 54 & 51 & 0 \\ 66 & 0 & 65 & 62 & 61 \end{bmatrix}$$

$$LA = (0, 2, -1, -4, -5)$$

For a **symmetric** sparse matrix, where each superdiagonal k is equal to subdiagonal -k, compressed-diagonal storage mode uses the same storage technique as for the general sparse matrix, except that only the nonzero main diagonal and one diagonal of each couple of nonzero diagonals, k and -k, are used in setting up arrays AD and LA. You can store either the upper or the lower diagonal of each couple.

Consider the following as an example of a symmetric sparse matrix of order 6 and how it is stored in arrays AD and LA, using only three nonzero diagonals in the matrix.

Given the following matrix A:

the arrays are:

$$AD = \begin{bmatrix} 11 & 13 & 0 \\ 22 & 24 & 0 \\ 33 & 35 & 0 \\ 44 & 46 & 0 \\ 55 & 0 & 51 \\ 66 & 0 & 62 \end{bmatrix}$$

$$LA = (0, 2, -4)$$

In general terms, this storage technique can be expressed as follows:

```
For each d_k \neq (0, ..., 0), for k = 1-n, n-1 for general square sparse matrices, or for each unique d_k \neq (0, ..., 0), for k = 1-n, n-1 for symmetric sparse matrices, there exists l, where 1 \leq l \leq nd, such that LA(l) = k and column l in array AD contains dp_k.
```

where:

- Array AD is defined as AD(Ida, nd), where  $Ida \ge n$ , and where nd is the number of nonzero diagonals,  $d_k$  that are stored in array AD.
- Array LA has nd elements.
- k is the diagonal number of each diagonal,  $d_k$ , where k = i-j.
- dp<sub>k</sub> are the diagonals, d<sub>k</sub>, with padding, which are constructed from the sparse matrix A elements, a<sub>ii</sub>, for i, j = 1, n as follows:

```
For superdiagonals (k > 0), d\boldsymbol{p}_k has k trailing zeros: d\boldsymbol{p}_k = (a_{1,k+1}, a_{2,k+2}, ..., a_{n-k,n}, 0_1, ..., 0_k)
For the main diagonal (k = 0), d\boldsymbol{p}_0 has no padding: d\boldsymbol{p}_0 = (a_{11}, a_{22}, ..., a_{nn})
For subdiagonals (k < 0), d\boldsymbol{p}_k has |k| leading zeros: d\boldsymbol{p}_k = (0_1, ..., 0_{|k|}, a_{|k|+1,1}, a_{|k|+2,2}, ..., a_{n,n-|k|})
```

**Storage-by-Indices:** For a sparse matrix A, storage-by-indices uses three one-dimensional arrays to define the sparse matrix storage, AR, IA, and JA. Given the m by n sparse matrix A having ne nonzero elements, the arrays are set up as follows:

- AR of (at least) length ne contains the ne nonzero elements of the sparse matrix
   A, stored contiguously in any order.
- IA, an integer array of (at least) length ne contains the corresponding row numbers of each nonzero element, a<sub>ii</sub>, in matrix A.
- JA, an integer array of (at least) length ne contains the corresponding column numbers of each nonzero element,  $a_{ii}$ , in matrix A.

Consider the following as an example of a 6 by 6 sparse matrix **A** and how it can be stored in arrays AR, IA, and JA.:

Given the following matrix A:

the arrays are:

In general terms, this storage technique can be expressed as follows:

```
For each a_{ij} \neq 0, for i = 1, m and j = 1, n there exists k, where 1 \leq k \leq ne, such that:
AR(k) = a_{ij}
IA(k) = i
JA(k) = j
```

where:

- $a_{ii}$  are the elements of the m by n sparse matrix  $\boldsymbol{A}$ .
- Arrays AR, IA, and JA each have ne elements.

**Storage-by-Columns:** For a sparse matrix,  $\mathbf{A}$ , storage-by-columns uses three one-dimensional arrays to define the sparse matrix storage, AR, IA, and JA. Given the m by n sparse matrix  $\mathbf{A}$  having ne nonzero elements, the arrays are set up as follows:

- AR of (at least) length ne contains the ne nonzero elements of the sparse matrix
   A, stored contiguously. The columns of matrix A are stored consecutively from
   1 to n in AR. The elements in each column of A are stored in any order in AR.
- IA, an integer array of (at least) length ne contains the corresponding row numbers of each nonzero element, a<sub>ii</sub>, in matrix A.
- JA, an integer array of (at least) length n+1 contains the relative starting position of each column of matrix A in array AR; that is, each element JA(j) of the column pointer array indicates where column j begins in array AR. If all elements in column j are zero, then JA(j) = JA(j+1). The last element, JA(n+1), indicates the position after the last element in array AR, which is ne+1.

Consider the following as an example of a 6 by 6 sparse matrix **A** and how it can be stored in arrays AR, IA, and JA.

Given the following matrix A:

the arrays are:

In general terms, this storage technique can be expressed as follows:

```
For each a_{ij} \neq 0, for i=1, m and j=1, n there exists k, where 1 \leq k \leq ne, such that AR(k) = a_{ij} IA(k) = i And for j=1, n, JA(j) = k, where a_{ij}, in AR(k), is the first element stored in AR for column j JA(j) = JA(j+1), where all a_{ij} = 0 in column j JA(n+1) = ne+1
```

where:

•  $a_{ii}$  are the elements of the m by n sparse matrix  $\boldsymbol{A}$ .

- Arrays AR and IA each have ne elements.
- Array JA has *n*+1 elements.

**Storage-by-Rows:** The storage mode used for sparse matrices stored by rows has three variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. This section explains these variations.

For a **general** sparse matrix A, storage-by-rows uses three one-dimensional arrays to define the sparse matrix storage, AR, IA, and JA. Given the m by n sparse matrix A having ne nonzero elements, the arrays are set up as follows:

- AR of (at least) length ne contains the ne nonzero elements of the sparse matrix
   A, stored contiguously. The rows of matrix A are stored consecutively from 1 to
   m in AR. The elements in each row of A are stored in any order in AR.
- IA, an integer array of (at least) length m+1 contains the relative starting position of each row of matrix  $\mathbf{A}$  in array AR; that is, each element IA(i) of the row pointer array indicates where row i begins in array AR. If all elements in row i are zero, then IA(i) = IA(i+1). The last element, IA(m+1), indicates the position after the last element in array AR, which is m=1.
- JA, an integer array of (at least) length ne contains the corresponding column numbers of each nonzero element,  $a_{ii}$ , in matrix A.

Consider the following as an example of a 6 by 6 general sparse matrix  $\boldsymbol{A}$  and how it can be stored in arrays AR, IA, and JA.

Given the following matrix A:

the arrays are:

For a **symmetric** sparse matrix of order *m*, storage-by-rows uses the same storage technique as for the general sparse matrix, except that only the upper or lower triangle and diagonal elements are used in setting up arrays AR, IA, and JA.

Consider the following as an example of a symmetric sparse matrix  $\boldsymbol{A}$  of order 6 and how it can be stored in arrays AR, IA, and JA using upper-storage-by-rows, which stores only the upper triangle and diagonal elements.

Given the following matrix A:

the arrays are:

```
AR = (11, 13, 22, 24, 23, 33, 35, 46, 44, 55)

IA = (1, 3, 6, 8, 10, 11, 11)

JA = (1, 3, 2, 3, 4, 3, 5, 4, 6, 5)
```

Using the same symmetric matrix A, consider the following as an example of how it can be stored in arrays AR, IA, and JA using lower-storage-by-rows, which stores only the lower triangle and diagonal elements:

```
AR = (11, 22, 23, 33, 13, 24, 44, 55, 35, 46)

IA = (1, 2, 3, 6, 8, 10, 11)

JA = (1, 2, 2, 3, 1, 2, 4, 5, 3, 4)
```

In general terms, this storage technique can be expressed as follows:

```
For each a_{ij} \neq 0, for i=1, m and j=1, n for general sparse matrices or for i=1, m and j=i, m for symmetric sparse matrices using the lower triangle or for i=1, m and j=1, i for symmetric sparse matrices using the upper triangle there exists k, where 1 \leq k \leq ne, such that AR(k) = a_{ij} JA(k) = j And for i=1, m, IA(i) = k, where a_{ij} in AR(k), is the first element stored in AR for row i IA(i) = IA(i+1), where all a_{ij} = 0 in row i IA(m+1) = ne+1
```

#### where:

- a<sub>ij</sub> are the elements of sparse matrix A, which is either an m by n general sparse matrix or a symmetric sparse matrix of order m containing ne nonzero elements.
- Arrays AR and JA each have ne elements.
- Array IA has m+1 elements.

**Diagonal-Out Skyline Storage Mode:** The diagonal-out skyline storage mode used for sparse matrices has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. Both of these variations are explained here.

For a **general** sparse matrix A, diagonal-out skyline storage mode uses four one-dimensional arrays to define the sparse matrix storage, AU, IDU, AL, and IDL. Given the sparse matrix A of order n, containing nu+nl-n elements under the top and left profiles, the arrays are set up as follows:

- AU of (at least) length nu contains the upper triangle of the sparse matrix A, where the columns are stored consecutively from 1 to n in AU in the following way. For each column, the elements starting at the diagonal element and ending at the topmost nonzero element in the column are stored contiguously in AU. The elements stored may include zero elements along with the nonzero elements. If all elements in the column to be stored are zero, the diagonal element, a<sub>ii</sub>, having a value of zero, is stored in AU for that column. A total of nu elements are stored for the upper triangle of A.
- IDU, an integer array of (at least) length n+1 contains the relative position of each diagonal element of matrix A in array AU; that is, each element IDU(i) of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AU. One-origin is used, so the first element of IDU is always 1. The last element, IDU(n+1), indicates the position after the last element in array AU, which is nu+1.
- AL of (at least) length *nl* contains the lower triangle of the sparse matrix *A*, where the rows are stored consecutively from 1 to *n* in AL in the following way. For each row, the elements starting at the diagonal element and ending at the leftmost nonzero element in the row are stored contiguously in AL. The elements stored may include zero elements along with the nonzero elements. If all elements in the row to be stored are zero, the diagonal element, *a<sub>ij</sub>*, having a value of zero, is stored in AL for that row. A total of *nl* elements are stored for the lower triangle of *A*. The values of the diagonal elements are meaningless, so you can store any values in those positions in AL.
- IDL, an integer array of (at least) length n+1 contains the relative position of each diagonal element of matrix A in array AL; that is, each element IDL(i) of the diagonal pointer array indicates where diagonal element  $a_{ii}$  is stored in array AL. One-origin is used, so the first element of IDL is always 1. The last element, IDL(n+1), indicates the position after the last element in array AL, which is n+1.

Consider the following as an example of a 6 by 6 general sparse matrix **A** and how it is stored in arrays AU, IDU, AL, and IDL.

Given the following matrix **A**:

the arrays are:

AU = 
$$(0, 22, 12, 33, 0, 13, 44, 34, 24, 55, 45, 66, 56, 0, 36)$$
  
IDU =  $(1, 2, 4, 7, 10, 12, 16)$  where  $nu=15$   
AL =  $(*, *, 21, *, 0, 31, *, 43, 42, 41, *, 54, *, 65, 0, 63)$   
IDL =  $(1, 2, 4, 7, 11, 13, 17)$  where  $nl=16$ 

and where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

For a **symmetric** sparse matrix of order *n*, diagonal-out skyline storage mode uses the same storage technique as for the upper triangle and diagonal elements of the general sparse matrix; therefore, only the AU and IDU arrays are needed.

Consider the following as an example of a symmetric sparse matrix A of order 6 and how it is stored in arrays AU and IDU.

Given the following matrix **A**:

the arrays are:

AU = 
$$(0, 22, 12, 33, 0, 13, 44, 34, 24, 55, 45, 66, 56, 0, 36)$$
  
IDU =  $(1, 2, 4, 7, 10, 12, 16)$  where  $nu=15$ 

In general terms, this storage technique can be expressed as follows:

```
For general sparse matrices and symmetric sparse matrices:
    For each a_{ii} for j = 1, n and i = j, k,
    where a_{ki} is the topmost a_{ij} \neq 0 in each column j,
    there exists m, where 1 \le m \le nu, such that
        AU(m+j-i) = a_{ii}
         IDU(j) = m for each a_{ii}
        IDU(n+1) = nu+1
Also, for general sparse matrices:
    For each a_{ii} for i = 1, n and i = j, k,
    where a_{ik} is the leftmost a_{ii} \neq 0 in each row i,
    there exists m, where 1 \le m \le nl, such that
        AL(m+i-j) = a_{ii}
         IDL(i) = m for each a_{ii}
         IDL(n+1) = nl+1
```

where:

a<sub>ii</sub> are the elements of sparse matrix A, of order n.

- Array AU has nu elements.
- Array AL has nl elements.
- Arrays IDU and IDL each have n+1 elements.

**Profile-In Skyline Storage Mode:** The profile-in skyline storage mode used for sparse matrices has two variations, depending on whether the matrix is a general sparse matrix or a symmetric sparse matrix. Both of these variations are explained here.

For a **general** sparse matrix A, profile-in skyline storage mode uses four one-dimensional arrays to define the sparse matrix storage, AU, IDU, AL, and IDL. Given the sparse matrix A of order n, containing nu+nl-n elements under the top and left profiles, the arrays are set up as follows:

- AU of (at least) length nu contains the upper triangle of the sparse matrix A, where the columns are stored consecutively from 1 to n in AU in the following way. For each column, the elements starting at the topmost nonzero element in the column and ending at the diagonal element are stored contiguously in AU. The elements stored may include zero elements along with the nonzero elements. If all elements in the column to be stored are zero, the diagonal element, a<sub>ji</sub>, having a value of zero, is stored in AU for that column. A total of nu elements are stored for the upper triangle of A.
- IDU, an integer array of (at least) length n+1 contains the relative position of each diagonal element of matrix A in array AU; that is, each element IDU(i) of the diagonal pointer array indicates where diagonal element a<sub>ii</sub> is stored in array AU. One-origin is used, so the first element of IDU is always 1. The last element, IDU(n+1), indicates the position after the last element in array AU, which is nu+1.
- AL of (at least) length nl contains the lower triangle of the sparse matrix A, where the rows are stored consecutively from 1 to n in AL in the following way. For each row, the elements starting at the leftmost nonzero element in the row and ending at the diagonal element are stored contiguously in AL. The elements stored may include zero elements along with the nonzero elements. If all elements in the row to be stored are zero, the diagonal element, a<sub>ij</sub>, having a value of zero, is stored in AL for that row. A total of nl elements are stored for the lower triangle of A. The values of the diagonal elements are meaningless, so you can store any values in those positions in AL.
- IDL, an integer array of (at least) length n+1 contains the relative position of each diagonal element of matrix A in array AL; that is, each element IDL(i) of the diagonal pointer array indicates where diagonal element a<sub>ii</sub> is stored in array AL. One-origin is used, so the first element of IDL is always 1. The last element, IDL(n+1), indicates the position after the last element in array AL, which is nl+1.

Consider the following as an example of a 6 by 6 general sparse matrix **A** and how it is stored in arrays AU, IDU, AL, and IDL.

Given the following matrix **A**:

```
    0
    12
    13
    0
    0
    0

    21
    22
    0
    24
    0
    0

    31
    0
    33
    34
    0
    36

    41
    42
    43
    44
    45
    0

    0
    0
    0
    54
    55
    56

    0
    0
    63
    0
    65
    66
```

the arrays are:

AU = 
$$(0, 12, 22, 13, 0, 33, 24, 34, 44, 45, 55, 36, 0, 56, 66)$$

IDU =  $(1, 3, 6, 9, 11, 15, 16)$  where  $nu=15$ 

AL =  $(*, 21, *, 31, 0, *, 41, 42, 43, *, 54, *, 63, 0, 65, *)$ 

IDL =  $(1, 3, 6, 10, 12, 16, 17)$  where  $nl=16$ 

and where "\*" means you do not have to store a value in that position in the array. However, these storage positions are required.

For a **symmetric** sparse matrix of order *n*, profile-in skyline storage mode uses the same storage technique as for the upper triangle and diagonal elements of the general sparse matrix; therefore, only the AU and IDU arrays are needed.

Consider the following as an example of a symmetric sparse matrix A of order 6 and how it is stored in arrays AU and IDU.

Given the following matrix **A**:

the arrays are:

AU = 
$$(0, 12, 22, 13, 0, 33, 24, 34, 44, 45, 55, 36, 0, 56, 66)$$
  
IDU =  $(1, 3, 6, 9, 11, 15, 16)$  where  $nu=15$ 

In general terms, this storage technique can be expressed as follows:

```
For general sparse matrices and symmetric sparse matrices:
    For each a_{ii} for j = 1, n and i = k, j,
    where a_{kj} is the topmost a_{ij} \neq 0 in each column j,
    there exists m, where 1 \le m \le nu, such that
        AU(m-j+i) = a_{ii}
        IDU(j) = m for each a_{ii}
        IDU(n+1) = nu+1
Also, for general sparse matrices:
    For each a_{ii} for i = 1, n and j = k, i,
```

```
where a_{ik} is the leftmost a_{ij} \neq 0 in each row i, there exists m, where 1 \leq m \leq nl, such that AL(m-i+j) = a_{ij}

IDL(i) = m for each a_{ii}

IDL(n+1) = nl+1
```

#### where:

- $a_{ii}$  are the elements of sparse matrix **A**, of order *n*.
- Array AU has nu elements.
- Array AL has *nl* elements.
- Arrays IDU and IDL each have n+1 elements.

## Sequences

A sequence is an ordered collection of numbers. It can be a one-, two-, or three-dimensional sequence. Sequences are used in the areas of sorting, searching, Fourier transforms, convolutions, and correlations.

## Real and Complex Elements in Storage

Sequences can contain either real or complex data. For sequences containing complex data, a special storage arrangement is used to accommodate the two parts, *a* and *b*, of each complex number, *a+bi*, in the array. For each complex number, two sequential storage locations are required in the array. Therefore, exactly twice as much storage is required for complex sequences as for real sequences of the same precision. See "How Do You Set Up Your Scalar Data?" on page 28 for a description of real and complex numbers, and "How Do You Set Up Your Arrays?" on page 29 for a description of how real and complex data is stored in arrays.

# **One-Dimensional Sequences**

A one-dimensional sequence appears symbolically as follows, where the subscripts indicate the element positions within the sequence:

$$(x_1, x_2, x_3, \dots x_n)$$

### In Storage

A one-dimensional sequence is stored in an array using stride in the same way a vector uses stride. For details, see "How Stride Is Used for Vectors" on page 58.

# **Two-Dimensional Sequences**

A two-dimensional sequence appears symbolically as a series of columns of elements. (They are represented in the same way as a matrix without the square brackets.) The two subscripts indicate the element positions in the first and second dimensions, respectively:

### In Storage

A two-dimensional sequence is stored in an array using the stride for the second dimension in the same way that a matrix uses leading dimension. It uses a stride of 1 for the first dimension. For details, see "How Leading Dimension Is Used for Matrices" on page 63. (In the area of Fourier transforms, a two-dimensional sequence may be stored in transposed form in an array. In this case, the stride for the second dimension is 1, and the stride for the first dimension is the leading dimension of the array.)

## **Three-Dimensional Sequences**

A three-dimensional sequence is represented as a series of blocks of elements. Each block is equivalent to a two-dimensional sequence. The number of blocks indicates the length of the third dimension. The three subscripts indicate the element positions in the first, second, and third dimensions, respectively:

### Plane 0:

#### Plane 1:

# Plane (p-1):

# In Storage

Each block of elements in a three-dimensional sequence is stored successively in an array. The stride for the third dimension is used to select the elements for each successive block of elements in the array. The starting point of the three-dimensional sequence is specified as the argument for the sequence in the ESSL calling statement. For example, if the three-dimensional sequence is contained in array BIG, declared as BIG(1:20,1:30,1:10), and starts at the second element in the first dimension, the third element in the second dimension, and the first element in the third dimension of array BIG, you should specify BIG(2,3,1) as the argument for the sequence, such as in:

```
CALL SCFT3 (BIG(2,3,1),20,600,Y,32,2056,16,20,10,1,1.0,AUX,30000)
```

See "How Stride Is Used for Three-Dimensional Sequences" on page 108 for a detailed description of how three-dimensional sequences are stored within arrays using strides.

# How Stride Is Used for Three-Dimensional Sequences

The elements of the three-dimensional sequence can be defined as  $a_{ijk}$  for i=1, m, j=1, n, and k=1, p. The first two subscripts, i and j, define the elements in the first two dimensions of the sequence, and the third subscript, k, defines the elements in the third dimension. Using this definition of three-dimensional sequences, this section explains how these elements are mapped into an array using the concepts of stride. (Remember that the elements  $a_{ijk}$  are the elements of the conceptual data structure, the three-dimensional sequence to be processed by ESSL. The sequence does not have to include all the elements in the array. Strides are used by the ESSL subroutines to select the desired elements to be processed in the array.)

The sequence elements in the first two dimensions are mapped into an array in the same way a matrix or two-dimensional sequence is mapped into an array. It uses all the items listed in "How Leading Dimension Is Used for Matrices" on page 63, such as the starting point, the number of rows and columns, and the leading dimension. The stride for the first dimension, *inc1*, of a three-dimensional sequence is assumed to be 1, as for matrices. The stride for the second dimension, *inc2*, of a three-dimensional sequence is equivalent to the leading dimension for a matrix.

The stride for the third dimension, inc3, is used to define the array elements that make up the third dimension of the three-dimensional sequence. The stride for the third dimension is used as an increment to step through the array to find the starting point for each of the p successive blocks of elements in the array. The stride, inc3, must always be positive. It must always be greater than or equal to the number of elements to be processed in the first two dimensions; that is,  $inc3 \ge (inc2)(n)$ .

A three-dimensional sequence is usually stored in a one-, two-, or three-dimensional array; however, for the sake of this discussion, a three-dimensional array is used here. For an array, A, declared as A(E1:E2,F1:F2,G1:G2), the strides in the first, second, and third dimensions are:

```
inc1 = 1

inc2 = (E2-E1+1)

inc3 = (E2-E1+1)(F2-F1+1)
```

Given an array A, declared as A(1:7,1:3,0:3), where the lengths of the first, second, and third dimensions are 7, 3, and 4, respectively, the resulting strides are inc1 = 1, inc2 = 7, and inc3 = 21.

The starting point for a three-dimensional sequence in an array is at the location specified by the argument for the sequence in the ESSL calling statement. Using the array A, described above, if you specify A(2,2,1) for a three-dimensional sequence, where A is defined as follows, in four blocks, for planes 0 - 3, respectively:

```
1.0 8.0 15.0
               22.0 29.0 36.0
                                43.0 50.0 57.0
                                                 64.0 71.0 78.0
2.0 9.0 16.0
               23.0 30.0 37.0
                                44.0 51.0 58.0
                                                 65.0 72.0 79.0
               24.0 31.0 38.0 45.0 52.0 59.0
3.0 10.0 17.0
                                                 66.0 73.0 80.0
4.0 11.0 18.0
               25.0 32.0 39.0 46.0 53.0 60.0
                                                 67.0 74.0 81.0
5.0 12.0 19.0
               26.0 33.0 40.0 47.0 54.0 61.0
                                                 68.0 75.0 82.0
6.0 13.0 20.0
               27.0 34.0 41.0
                                48.0 55.0 62.0
                                                 69.0 76.0 83.0
7.0 14.0 21.0
               28.0 35.0 42.0 49.0 56.0 63.0
                                                 70.0 77.0 84.0
```

then processing begins in the second block of elements at row 2 and column 2 in array A, which is 30.0. The stride in the third dimension is then used to find the starting point for each of the next p-1 successive blocks of elements in the array. The stride, *inc3*, is added to the starting point p-1 times. In this example, the stride for the third dimension is 21, and the number of blocks of elements, p, to be processed is 3, so the starting points in array A are A(2,2,1), A(2,2,2), and A(2,2,3). These are elements 30.0, 51.0, and 72.0. These array elements then correspond to the sequence elements  $a_{111}$ ,  $a_{112}$ , and  $a_{113}$ , respectively.

In general terms, this results in the following starting positions for the blocks of elements in the array:

```
A(BEGINI, BEGINJ, BEGINK)
A(BEGINI, BEGINJ, BEGINK+1)
A(BEGINI, BEGINJ, BEGINK+2)
.
.
A(BEGINI, BEGINJ, BEGINK+p-1)
```

Using m = 4, n = 2, and p = 3 to define the elements of the three-dimensional data structure in this example, the resulting three-dimensional sequence is defined as follows, in three blocks, for planes 0 - 2, respectively:

Plane 0:	Plane 1:	Plane 2:	
$a_{000}$ $a_{010}$	$a_{001}$ $a_{011}$	$a_{002}$ $a_{012}$	
$a_{100}$ $a_{110}$	$a_{101}$ $a_{111}$	$a_{102}$ $a_{112}$	=
$a_{200}$ $a_{210}$	$a_{201}$ $a_{211}$	$a_{202}$ $a_{212}$	
$a_{300}$ $a_{310}$	$a_{301}$ $a_{311}$	$a_{302}$ $a_{312}$	
Plane 0:	Plane 1:	Plane 2:	
<b>Plane 0:</b> 30.0 37.0	<b>Plane 1:</b> 51.0 58.0	<b>Plane 2:</b> 72.0 79.0	
30.0 37.0	51.0 58.0	72.0 79.0	

As shown in this example, the three-dimensional sequence does not have to include all the blocks of elements in the array. In this case, the three-dimensional sequence includes only the second through the fourth block of elements in the array. The first block is not used. Elements of an array are selected as they are arranged in storage, regardless of the number of dimensions defined in the array. Therefore, when using a one- or two-dimensional array to store your three-dimensional sequence, you should understand how your array elements are stored to ensure that elements are selected properly. See "Setting Up Arrays in Fortran" on page 112 for a description of array storage.

**Note:** Three-dimensional sequences are used by the three-dimensional Fourier transform subroutines. By specifying certain stride values for *inc2* and *inc3* and declaring your arrays to have certain number of dimensions, you achieve optimal performance in these subroutines. For details, see "Setting Up Your Data" on page 742 and the Notes section for each subroutine.

# **Chapter 4. Coding Your Program**

This chapter provides you with information you need to code your Fortran, C, C++, and PL/I programs using ESSL.

# **Fortran Programs**

This section describes how to code your Fortran program using any of the ESSL run-time libraries.

# Calling ESSL Subroutines and Functions in Fortran

In Fortran programs, most ESSL subroutines are invoked with the CALL statement:

```
CALL subroutine-name (argument-1, . . . , argument-n)
```

An example of a calling sequence for the SAXPY subroutine might be:

```
CALL SAXPY (5,A,X,J+INC,Y,1)
```

The remaining ESSL subroutines are invoked as functions by coding a function reference. You first declare the type of value returned by the function: short- or long-precision real, short- or long-precision complex, or integer. Then you code the function reference as part of an expression in a statement. An example of declaring and invoking the DASUM function might be:

```
DOUBLE PRECISION DASUM, SUM, X
.
.
.
SUM = DASUM (N.X.INCX)
```

Values are returned differently for ESSL subroutines and functions. For subroutines, the results of the computation are returned in an argument specified in the calling sequence. In the CALL statement above, the result is returned in argument Y. For functions, the result is returned as the value of the function. In the assignment statement above, the result is assigned to SUM.

See the Fortran publications for details on how to code the CALL statement and a function reference.

# Setting Up a User-Supplied Subroutine for ESSL in Fortran

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in Fortran, there are some coding rules you must follow:

- You must declare subf as EXTERNAL in your program.
- You should code the *subf* subroutine to the specifications given in "
   Programming Considerations for the SUBF Subroutine" on page 920. For
   examples of coding a *subf* subroutine in Fortran, see the subroutine
   descriptions in that chapter.

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# **Setting Up Scalar Data in Fortran**

Table 27 lists the scalar data types in Fortran that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 27. Scalar Data Types in Fortran Programs	
Terminology Used by ESSL	Fortran Equivalent
Character item1	CHARACTER*1
'N', 'T', 'C' or 'n', 't', 'c'	'N', 'T', 'C'
Logical item	LOGICAL
.TRUE., .FALSE.	.TRUE., .FALSE.
32-bit environment integer	INTEGER or INTEGER*4
12345, –12345	12345, –12345
64-bit environment integer <sup>2</sup>	INTEGER*83
12345, –12345	12345_8, -12345_8
Short-precision real number4	REAL or REAL*4
12.345	0.12345E2
Long-precision real number4	DOUBLE PRECISION or REAL*8
12.345	0.12345D2
Short-precision complex number <sup>4</sup>	COMPLEX or COMPLEX*8
(123.45, -54321.0)	(123.45E0, -543.21E2)
Long-precision complex number <sup>4</sup>	COMPLEX*16
(123.45, -54321.0)	(123.45D0, -543.21D2)
1	

<sup>&</sup>lt;sup>1</sup> ESSL accepts character data in either upper- or lowercase in its calling sequences.

# **Setting Up Arrays in Fortran**

Arrays are declared in Fortran by specifying the array name, the number of dimensions, and the range of each dimension in a DIMENSION statement or an explicit data type statement, such as REAL, DOUBLE PRECISION, and so forth.

### Real and Complex Array Elements

Each array element can be either a real or complex data item of short or long precision. The type of the array determines the size of the element storage locations. Short-precision data requires 4 bytes, and long-precision data requires 8 bytes. Complex data requires two storage locations of either 4 or 8 bytes each, for short or long precision, respectively, to accommodate the two parts of the complex number: c = a+bi. Therefore, exactly twice as much storage is required for complex data as for real data of the same precision. See "How Do You Set Up Your Scalar Data?" on page 28 for a description of real and complex numbers.

Even though complex data items require two storage locations, the same number of elements exist in the array as for real data. A reference to an element—for example, C(3)—in an array containing complex data gives you the whole complex

<sup>&</sup>lt;sup>2</sup> In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the iusadr argument for ERRSET.

<sup>3</sup> INTEGER may be used if you specify the compiler option -qintsize=8.

<sup>&</sup>lt;sup>4</sup> Short- and long-precision numbers look the same in this book.

number; that is, it contains both a and b, where the complex number is expressed as follows:

```
C(I) \leftarrow (a_i, b_i) for a one-dimensional array
C(I,J) \leftarrow (a_{ii}, b_{ii}) for a two-dimensional array
C(I,J,K) \leftarrow (a_{iik}, b_{iik}) for a three-dimensional arra y
```

### **One-Dimensional Array**

For a one-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2)
```

where A is the name of the array, E1 is the lower bound, and E2 is the upper bound of the single dimension in the array. If the lower bound is not specified, such as in A(E2), the value is assumed to be 1. The upper bound is required.

A one-dimensional array is stored in ascending storage locations (relative to some base storage address) in the following order:

Relative Location	Array Element
1	A(E1)
2	A(E1+1)
3	A(E1+2)
	i
E2-E1+1	A(E2)

For example, the array A of length 4 specified in the DIMENSION statement as A(0:3) and containing the following elements:

$$A = (1, 2, 3, 4)$$

has its elements arranged in storage as follows:

Array Element Value
1
2
3
4

### Two-Dimensional Array

For a two-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2,F1:F2)
```

where A is the name of the array. E1 and F1 are the lower bounds of the first and second dimensions, respectively, and E2 and F2 are the upper bounds of the first and second dimensions, respectively. If either of the lower bounds is not specified, such as in A(E2,F1:F2), the value is assumed to be 1. The upper bounds are always required for each dimension. For examples of Fortran 77 usage, see "SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX—Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose" on page 296.

The elements of a two-dimensional array are stored in column-major order; that is, they are stored in the following ascending storage locations (relative to some base storage address) with the value of the first (row) subscript expression increasing

most rapidly and the value of the second (column) subscript expression increasing least rapidly. Following are the locations of the elements in the array:

Relative Location	Array Element
1	A(E1,F1) (starting column 1)
2	A(E1+1,F1)
•	
•	•
E2-E1+1	A(E2,F1)
(E2-E1+1)+1	A(E1,F1+1) (starting column 2)
(E2-E1+1)+2	A(E1+1,F1+1)
•	
•	•
(E2–E1+1)(2)	A(E2,F1+1)
(E2-E1+1)(2)+1	A(E1,F1+2) (starting column 3)
(E2-E1+1)(2)+2	A(E1+1,F1+2)
•	
•	• .
(E2-E1+1)(F2-F1)	A(E2,F2-1)
(E2-E1+1)(F2-F1)+1	A(E1,F2) (starting column F2–F1+1)
(E2-E1+1)(F2-F1)+2	A(E1+1,F2)
(E2-E1+1)(F2-F1+1)	A(E2,F2)

For example, the 3 by 4 array A specified in the DIMENSION statement as A(2:4,1:4) and containing the following elements:

$$A = \begin{bmatrix} 11 & 12 & 13 & 14 \\ 21 & 22 & 23 & 24 \\ 31 & 32 & 33 & 34 \end{bmatrix}$$

has its elements arranged in storage as follows:

Array Element Value
11 (starting column 1)
21
31
12 (starting column 2)
22
32
13 (starting column 3)
23
33
14 (starting column 4)
24
34

Each element A(I,J) of the array A, declared A(1:n, 1:m), containing real or complex data, occupies the storage location whose address is given by the following formula:

```
address \{A(I,J)\} = address \{A\} + (I-1 + n(J-1))f
```

for:

I = 1, n and J = 1, m

#### where:

f = 4 for short-precision real numbers

f = 8 for long-precision real numbers

f = 8 for short-precision complex numbers

f = 16 for long-precision complex numbers

### **Three-Dimensional Array**

For a three-dimensional array in Fortran 77, you can code:

```
DIMENSION A(E1:E2,F1:F2,G1:G2)
```

where A is the name of the array. E1, F1, and G1 are the lower bounds of the first, second, and third dimensions, respectively, and E2, F2, and G2 are the upper bounds of the first, second, and third dimensions, respectively. If any of the lower bounds are not specified, such as in A(E1:E2,F1:F2,G2), the value is assumed to be 1. The upper bounds are always required for each dimension. For examples of Fortran 77 usage, see "SCFT3 and DCFT3—Complex Fourier Transform in Three Dimensions" on page 807.

The elements of a three-dimensional array can be thought of as a set of two-dimensional arrays, stored sequentially in ascending storage locations in the array. The elements in each two-dimensional array are stored as defined in the previous section. In the three-dimensional array, the value of the first (row) subscript expression increases most rapidly, the second (column) subscript expression increases less rapidly, and the third subscript expression (set of rows and columns) increases least rapidly. Following are the locations of the elements in the array:

Relative Location	Array Element
1	A(E1,F1,G1) (starting the first set)
2	A(E1+1,F1,G1)
	•
(E2-E1+1)(F2-F1+1)	A(E2,F2,G1)
(E2-E1+1)(F2-F1+1)+1	A(E1,F1,G1+1) (starting the second set)
(E2-E1+1)(F2-F1+1)+2	A(E1+1,F1,G1+1)
•	•
	•
(E2-E1+1)(F2-F1+1)(2)	A(E2,F2,G1+1)
(E2-E1+1)(F2-F1+1)(2)+1	A(E1,F1,G1+2) (starting the third set)
(E2-E1+1)(F2-F1+1)(2)+2	A(E1+1,F1+2)
	•

```
(E2-E1+1)(F2-F1+1)(G2-G1)
                                     A(E2,F2,G2-1)
(E2-E1+1)(F2-F1+1)(G2-G1)+1
                                     A(E1,F1,G2) (starting the last set*)
(E2-E1+1)(F2-F1+1)(G2-G1)+2
                                     A(E1+1,F1,G2)
(E2-E1+1)(F2-F1+1)(G2-G1+1)
                                     A(E2,F2,G2)
```

For example, the 3 by 2 by 4 array A specified in the DIMENSION statement as A(1:3,0:1,2:5) and containing the following sets of rows and columns of elements:

has its elements arranged in storage as follows:

Relative Location	Array Element Value
1	111 (starting the first set)
2	211
3	311
4	121
5	221
6	321
7	112 (starting the second set)
8	212
9	312
10	122
11	222
12	322
13	113 (starting the third set)
14	213
15	313
16	123
17	223
18	323
19	114 (starting the fourth set)
20	214
21	314
22	124
23	224
24	324

Each element A(I,J,K) of the array A, declared A(1:n, 1:m, 1:p), containing real or complex data, occupies the storage location whose address is given by the following formula:

address 
$$\{A(I,J,K)\}$$
 = address  $\{A\}$  +  $(I-1 + n(J-1) + mn(K-1))f$ 

for:

$$I = 1, n$$

<sup>\*</sup> The last set is the G2-G1+1 set.

```
J = 1, m
K = 1, p

where:

f = 4 for short-precision real numbers
f = 8 for long-precision real numbers
f = 8 for short-precision complex numbers
f = 16 for long-precision complex numbers
```

# **Creating Multiple Threads and Calling ESSL from Your Fortran Program**

The example shown below shows how to create up to a maximum of eight threads, where each thread calls the DURAND and DGEICD subroutines.

Be sure to compile this program with the xlf r command and the -qnosave option.

```
program matinv example
       implicit none
!
  program to invert m nxn random matrices
       real(8), allocatable :: A(:,:,:), det(:,:), rcond(:)
       real(8)
                            :: dummy_aux, seed=1998, sd
       integer
                           :: rc, i, m=8, n=500, iopt=3, naux=0
! allocate storage
       allocate(A(n,n,m),stat=rc)
       call error exit(rc, "Allocation of matrix A")
       allocate(det(2,m),stat=rc)
       call error exit(rc, "Allocation of det")
       allocate(rcond(m), stat=rc)
       call error_exit(rc,"Allocation of rcond")
! Calculate inverses in parallel
!SMP$ parallel do private(i,sd), schedule(static),
!SMP$&
          share(n,a,iopt,rcond,det,dummy aux,naux)
       do i=1,m
         sd = seed + 100*i
         call durand(sd,n*n,A(1,1,i))
         call dgeicd(A(1,1,i),n,n,iopt,rcond(i),det(1,i),
                     dummy aux, naux)
       enddo
```

```
write(*,*)'Reciprocal condition numbers of the matrices are:'
       write(*,'(4E12.4)') rcond
!
!
!
       deallocate(A,stat=rc)
       call error exit(rc, "Deallocation of matrix A")
       deallocate(det,stat=rc)
       call error exit(rc, "Deallocation of det")
       deallocate(rcond,stat=rc)
       call error exit(rc, "Deallocation of rcond")
       stop
       contains
         subroutine error_exit(error_code,string)
         character(*) :: string
         integer
                        :: error code
         if(error code .eq. 0 ) return
         write(0,*)string,": failing return code was ",error_code
         end subroutine error exit
       end
```

# Handling Errors in Your Fortran Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

 For input-argument errors 2015 and 2030, which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.

Note: In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the aux arguments. For details see the subroutine descriptions in Part 2 of this book.

 For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

"Input-Argument Errors in Fortran" on page 119 and "Computational Errors in Fortran" on page 122 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in "Input-Argument Errors in Fortran" on page 119 and "Computational Errors in Fortran" on page 122 on each thread that calls ESSL. An example is shown in "Example of Handling Errors in a Multithreaded Application Program" on page 127.

# **Input-Argument Errors in Fortran**

To obtain corrected input-argument values in a Fortran program and to avert program termination for the optionally-recoverable input-argument errors 2015 and 2030, add the statements in the following steps your program. Steps 3 and 7 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

#### Step 1. Declare ENOTRM as External

EXTERNAL ENOTRM

This declares the ESSL error exit routine ENOTRM as an external reference in your program. This should be coded in the beginning of your program before any of the following statements.

### Step 2. Call EINFO for Initialization

CALL EINFO (0)

This calls the EINFO subroutine with one argument of value 0 to initialize the ESSL error option table. It is required only if you call ERRSET in your program. It is coded only once in the beginning of your program before any calls to ERRSET. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

### Step 3. Call ERRSAV

CALL ERRSAV (ierno, tabent)

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *tabent*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 7, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 3" on page 126, as the use is the same as for computational errors.

# Step 4. Call ERRSET

CALL ERRSET (ierno, inoal, inomes, itrace, iusadr, irange)

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (inoal)
- How many times each error message can be printed (inomes)
- The ESSL exit routine ENOTRM, to be invoked for the error indicated (iusadr)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015 or 2030. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the input-argument errors, see "Input-Argument Error Messages" on page 179. For a description of ERRSET, see Chapter 17 on page 957.

#### Step 5. Call ESSL

```
CALL name (arg-1,...,arg-n,*yyy,*zzz,...)
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- name specifies the ESSL subroutine.
- arg-1,..., arg-n are the input and output arguments.
- yyy, zzz, and any other statement numbers preceded by an "\*" are the Fortran statement numbers indicating where you want to branch when you get a nonzero return code. Each corresponds to a different ESSL value. Control goes to the corresponding statement number when a nonzero return code value is returned for the CALL statement. Return code values are described under "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

**Step 6. Perform the Desired Action:** These are the statements at statement number *yyy* or *zzz*, shown in the CALL statement in Step 5, and preceded by an "\*." The statement to which control is passed corresponds to the return code value for the error.

These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

#### Step 7. Call ERRSTR

```
CALL ERRSTR (ierno,tabent)
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *tabent*,

which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 3, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 3" on page 126, as the use is the same as for computational errors.

# **Example**

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```
C
                     DECLARE ENOTRM AS EXTERNAL
       EXTERNAL ENOTRM
C
                     INITIALIZE THE ESSL ERROR
C
                     OPTION TABLE
       CALL EINFO(0)
С
                     MAKE ERROR CODE 2015 A RECOVERABLE
C
                     ERROR AND SUPPRESS PRINTING ALL
С
                     ERROR MESSAGES FOR IT
       CALL ERRSET(2015,0,-1,0,ENOTRM,2015)
C
                     CALL ESSL ROUTINE SWLEV.
С
                     IF THE NAUX INPUT
С
                     ARGUMENT IS TOO SMALL, ERROR
С
                     2015 OCCURS. THE MINIMUM VALUE
C
                     REQUIRED IS STORED IN THE NAUX
С
                     INPUT ARGUMENT AND CONTROL GOES
C
                     TO LABEL 400.
       CALL SWLEV(X,INCX,U,INCU,Y,INCY,N,AUX,NAUX,*400)
```

C 400 .	DESIRED ACTION
•	

# Computational Errors in Fortran

To obtain information about an ESSL computational error in a Fortran program, add the statements in the following steps to your program. Steps 2 and 7 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

### Step 1. Call EINFO for Initialization

```
CALL EINFO (0)
```

This calls the EINFO subroutine with one argument of value 0 to initialize the ESSL error option table. It is required only if you call ERRSET in your program. It is coded only once in the beginning of your program before any calls to ERRSET. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

### Step 2. Call ERRSAV

```
CALL ERRSAV (ierno, tabent)
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number ierno in an 8-byte storage area, tabent, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 7, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53.

#### Step 3. Call ERRSET

```
CALL ERRSET (ierno, inoal, inomes, itrace, iusadr, irange)
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (ierno) or a range of errors (irange), you can specify:

How many times each error can occur before execution terminates (inoal)

How many times each error message can be printed (inomes)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, *ierno* should be set to one of the eligible values listed in Table 167 on page 960. To allow your program to continue after an error in the specified range occurs, *inoal* must be set to a value greater than 1. For ESSL, *iusadr* should be specified as either 0 or 1 in a 32-bit environment (0\_8 or 1\_8 in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the computational errors, see "Computational Error Messages" on page 187. For a description of ERRSET, see Chapter 17 on page 957.

### Step 4. Call ESSL

```
CALL name (arg-1,...,arg-n,*yyy,*zzz,...)
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- name specifies the ESSL subroutine.
- arg-1,..., arg-n are the input and output arguments.
- yyy, zzz, and any other statement numbers preceded by an "\*" are the Fortran
  statement numbers indicating where you want to branch when you get a
  nonzero return code. Each corresponds to a different ESSL value. Control goes
  to the corresponding statement number when a nonzero return code value is
  returned for the CALL statement. Return code values are described under
  "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

#### Step 5. Call EINFO for Information

```
nmbr CALL EINFO (icode,inf1)
-or-
nmbr CALL EINFO (icode,inf1,inf2)
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- nmbr is the statement number yyy, zzz, or any of the other statement numbers
  preceded by an "\*" in the CALL statement in Step 4, corresponding to the
  return code value for this error code.
- · icode is the error code of interest.
- inf1 and inf2 are the integer variables used to receive the information, where
  inf1 is assigned a value for all errors, and inf2 is assigned a value for some
  errors. For a description of EINFO, see "EINFO—ESSL Error
  Information-Handler Subroutine" on page 960.

Step 6. Check the Values in the Information Receivers: These statements check the values returned in the output argument information receivers, inf1 and inf2, which contain the information about the computational error.

### Step 7. Call ERRSTR

```
CALL ERRSTR (ierno, tabent)
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number ierno from an 8-byte storage area, tabent, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 2, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see " How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53.

# Example 1

This 32-bit environment example shows an error code 2104, which returns one piece of information: the index of the last diagonal with nonpositive value (I1).

```
C
                      INITIALIZE THE ESSL ERROR
С
                      OPTION TABLE
       CALL EINFO(0)
С
                      ALLOW 100 ERRORS FOR CODE 2104
       CALL ERRSET (2104, 100, 0, 0, 0, 2104)
С
                      CALL ESSL ROUTINE DPPF.
C
                      IF THE INPUT MATRIX IS NOT
С
                      POSITIVE DEFINITE, CONTROL GOES TO
С
                      LABEL 400
       IOPT=0
       CALL DPPF(APP,N,IOPT,*400)
```

```
CALL THE INFORMATION-HANDLER
С
                     ROUTINE FOR ERROR CODE 2104 TO
С
                     RETURN ONE PIECE OF INFORMATION
С
                     IN VARIABLE I1, THE INDEX OF THE
С
                     LAST NONPOSITIVE DIAGONAL FOUND
С
                     BY ROUTINE DPPF
400
       CALL EINFO (2104, I1)
```

# Example 2

This 32-bit environment example shows an error code 2103, which returns one piece of information: the index of the zero diagonal (I1) found by DGEF.

```
С
                      INITIALIZE THE ESSL ERROR
С
                      OPTION TABLE
       CALL EINFO(0)
С
                      ALLOW 100 ERRORS FOR CODE 2103
       CALL ERRSET(2103,100,0,0,0,2103)
С
                      CALL ESSL SUBROUTINE DGEF.
С
                      IF THE INPUT MATRIX IS
С
                      SINGULAR, CONTROL GOES TO
С
                      LABEL 400
       CALL DGEF(A, LDA, N, IPVT, *400)
```

```
CALL THE INFORMATION-HANDLER
С
                     ROUTINE FOR ERROR CODE 2103 TO
С
                     RETURN ONE PIECE OF INFORMATION
С
                     IN VARIABLE I1, THE INDEX OF THE
С
                     LAST ZERO DIAGONAL FOUND BY
С
                     SUBROUTINE DGEF
400
       CALL EINFO (2103, I1)
```

# Example 3

This 32-bit environment example shows an error code 2101, which returns two pieces of information: the eigenvalue (I1) that failed to converge after the indicated (I2) number of iterations. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2101 by this program.

```
С
                     DECLARE AN AREA TO SAVE THE
С
                     ERROR OPTION TABLE INFORMATION
С
                     FOR ERROR CODE 2101
       CHARACTER*8 SAV2101
С
                     INITIALIZE THE ESSL ERROR
С
                     OPTION TABLE
       CALL EINFO(0)
С
                     SAVE THE EXISTING ERROR OPTION
С
                     TABLE ENTRY FOR ERROR CODE 2101
       CALL ERRSAV (2101, SAV2101)
C
                     ALLOW 255 ERRORS FOR CODE 2101
       CALL ERRSET(2101,255,0,0,0,2101)
С
                     CALL ESSL SUBROUTINE DGEEV.
С
                     IF THE EIGENVALUE FAILED TO
C
                     CONVERGE, CONTROL GOES TO LABEL 400
       CALL DGEEV(IOPT,A,LDA,W,Z,LDZ,SELECT,N,AUX,NAUX,*400)
```

```
CALL THE INFORMATION-HANDLER
С
                     ROUTINE FOR ERROR CODE 2101 TO
С
                     RETURN TWO PIECES OF INFORMATION.
С
                     VARIABLE I1 CONTAINS THE EIGENVALUE
С
                     THAT FAILED TO CONVERGE. VARIABLE
С
                     12 CONTAINS THE NUMBER OF ITERATIONS.
400
       CALL EINFO (2101, I1, I2)
C
                     RESTORE THE PREVIOUS ERROR OPTION
С
                     TABLE ENTRY FOR ERROR CODE 2101.
С
                     ERROR PROCESSING RETURNS TO HOW IT
С
                     WAS BEFORE IT WAS ALTERED BY THE ABOVE
С
                     ERRSET STATEMENT.
       CALL ERRSTR(2101, SAV2101)
```

# **Example of Handling Errors in a Multithreaded Application Program**

This 32-bit environment example shows how to modify the MATINV\_EXAMPLE program in "Creating Multiple Threads and Calling ESSL from Your Fortran Program" on page 117 with calls to the ESSL error handling subroutines. The ESSL error handling subroutines are called from each thread to: initialize the error option table, save the current error option table values for input-argument error 2015 and computational error 2105, change the default values for errors 2015 and 2105, and then restore the original default values for errors 2015 and 2105.

```
program matinv example
       implicit none
!
!
  program to invert m nxn random matrices
       real(8), allocatable :: A(:,:,:), det(:,:), rcond(:)
       real(8)
                            :: dummy_aux, seed=1998, sd
       integer
                            :: rc, i, m=8, n=500, iopt=3, naux=0
       integer
                            :: inf1(8)
       character(8)
                            :: sav2015(8)
                            :: sav2105(8)
       character(8)
                            :: ENOTRM
       integer
```

```
external ENOTRM
! allocate storage
       allocate(A(n,n,m),stat=rc)
       call error exit(rc, "Allocation of matrix A")
       allocate(det(2,m),stat=rc)
       call error_exit(rc,"Allocation of det")
       allocate(rcond(m),stat=rc)
       call error exit(rc,"Allocation of rcond")
ļ
! Calculate inverses in parallel
!SMP$ parallel do private(i,sd), schedule(static),
!SMP$&
          share(n,m,a,iopt,rcond,det,dummy aux,naux,sav2015,sav2105,inf1)
       do i=1,m
Ţ
ļ
        initialize error handling
         call einfo(0)
!
!
        Save existing option table values for error 2015
         call errsav(2015, sav2015(i))
!
        Set Error 2015 to be non-recoverable so dgeicd will dynamically
        allocate the work area.
!
         call errset(2015,100,100,0,1,2015)
!
!
        Save existing option table values for error 2105
         call errsav(2105,sav2105(i))
!
!
        Set Error 2105 to be recoverable
         call errset(2105,100,100,0,ENOTRM,2105)
!
         sd = seed + 100*i
         call durand(sd,n*n,A(1,1,i))
         call dgeicd(A(1,1,i),n,n,iopt,rcond(i),det(1,i),
                     dummy aux, naux, *10, *20)
10
         goto 30
!
```

```
Catch singular matrix returned by dgeicd.
20
         CALL EINFO(2105, inf1(i))
         WRITE(*,*) 'ERROR: Zero pivot found at location ',inf1(i)
Ţ
1
        Restore the error option table entries
30
         continue
         call errstr(2015, SAV2015(i))
         call errstr(2105, SAV2105(i))
       enddo
       write(*,*)'Reciprocal condition numbers of the matrices are:'
       write(*,'(4E12.4)') rcond
!
!
!
       deallocate(A,stat=rc)
       call error exit(rc, "Deallocation of matrix A")
       deallocate(det,stat=rc)
       call error_exit(rc,"Deallocation of det")
       deallocate(rcond, stat=rc)
       call error exit(rc, "Deallocation of rcond")
       stop
       contains
         subroutine error exit(error code,string)
         character(*) :: string
         integer
                         :: error code
         if(error_code .eq. 0 ) return
         write(0,*)string,": failing return code was ",error code
         stop 1
         end subroutine error exit
       end
```

# **C Programs**

This section describes how to code your C program.

# Calling ESSL Subroutines and Functions in C

This section shows how to call ESSL subroutines and functions from your C program.

# **Before You Call ESSL**

Before you can call the ESSL subroutines from your C program, you must have the appropriate ESSL header file installed on your system. The ESSL header file allows you to code your function calls as described in this section. It contains entries for all the ESSL subroutines. The ESSL header file is distributed with the ESSL package. The ESSL header file to be used with the C compiler is named essl.h. You should check with your system support group to verify that the appropriate ESSL header file is installed.

In the beginning of your program, before you call any of the ESSL subroutines, you must code the following statement for the ESSL header file:

```
#include <essl.h>
```

If you are planning to create your own threads for the ESSL Thread-Safety or SMP Library, you must include the pthread.h header file as the first include file in your C program. For an example, see "Creating Multiple Threads and Calling ESSL from Your C Program" on page 134.

# **Coding the Calling Sequences**

In C programs, the ESSL subroutines, not returning a function value, are invoked with the following type of statement:

```
subroutine-name (argument-1, . . , argument-n);
```

An example of a calling sequence for SAXPY might be:

```
saxpy (5,a,x,incx,y,1);
```

The ESSL subroutines returning a function value are invoked with the following type of statement:

```
function-value-name=subroutine-name (argument-1, . . . , argument-n);
```

An example of invoking DASUM might be:

```
sum = dasum (n,x,incx);
```

See the C publications for details about how to code the function calls.

# **Passing Arguments in C**

This section describes how to pass arguments in your C program.

## About the Syntax Shown in This Book

The argument syntax shown in this book assumes that you have installed and are using the ESSL header file. For further details, see "Calling ESSL Subroutines and Functions in C" on page 129.

# **No Optional Arguments**

In the ESSL calling sequences for C, there are no optional arguments, as for some programming languages. You must code all the arguments listed in the syntax.

#### Arguments That Must Be Passed by Value

All scalar arguments that are not modified must be passed by value in the ESSL calling sequence. (This refers to input-only scalar arguments, such as *incx*, *m*, and *lda*.)

### **Arguments That Must Be Passed by Reference**

Following are the instances in which you pass your arguments by reference (as a pointer) in the ESSL calling sequence:

Arrays: Arguments that are arrays are passed by reference, as usual.

**Subroutine Names:** Some ESSL subroutines call a user-supplied subroutine. The name is part of the ESSL calling sequence. It must be passed by reference.

**Output Scalar Arguments:** When an output argument is a scalar data item, it must be passed by reference. This is true for all scalar data types: real, complex, and so forth. When this occurs, it is listed in the notes of each subroutine description in Part 2 of this book.

**Character Arguments:** Character arguments must be passed as strings, by reference. You specify the character, in upper- or lowercase, in the ESSL calling sequence with double quotation marks around it, as in "t". Following is an example of how you can call SGEADD, specifying the *transa* and *transb* arguments as strings *n* and *t*, respectively:

```
sgeadd (a,5,"n",b,3,"t",c,4,4,3);
```

Altered Arguments When Using Error Handling: If you use ESSL error handling in your C program, as described in "Handling Errors in Your C Program" on page 136, you must pass by reference all the arguments that can potentially be altered by ESSL error handling. This applies to all your ESSL call statements after the point where you code the #define statement, shown in step 1 in "Input-Argument Errors in C" on page 136 and in step 1 in "Computational Errors in C" on page 140. The two types of ESSL arguments are:

- · naux arguments for auxiliary storage
- *n* arguments for transform lengths

# Setting Up a User-Supplied Subroutine for ESSL in C

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in C, there are some coding rules you must follow for the *subf* subroutine:

- You can code the subf subroutine using only C or Fortran.
- You must declare *subf* as an external subroutine in your application program.
- You should code the *subf* subroutine to the specifications given in " Programming Considerations for the SUBF Subroutine" on page 920. For an example of coding a *subf* subroutine in C, see "Example 1" on page 931.

# Setting Up Scalar Data in C

Table 28 lists the scalar data types in C that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 28 (Page 1 of 2). Scalar Data Types in C Programs	
Terminology Used by ESSL	C Equivalent
Character item <sup>1</sup>	char *
'N', 'T', 'C' or 'n', 't', 'c'	"n", "t", "c"
Logical item	Specify it as described in "Setting Up
.TRUE., .FALSE.	Complex and Logical Data Types in C" on page 132.2

# Setting Up Complex and Logical Data Types in C

Complex and logical data types are not part of the C language; however, some ESSL subroutines require arguments of these data types.

#### Complex Data

ESSL provides identifiers, cmplx and dcmplx, for complex data types, defined in the ESSL header file, as well as two macro definitions, RE and IM, for handling the real and imaginary parts of complex numbers:

```
#ifndef CMPLX
#ifndef REIM
#define _REIM 1
#endif
typedef union { struct { float __re, __im;}
                __data; double __align;} cmplx;
#endif
#ifndef DCMPLX
#ifndef _REIM
#define _REIM 1
#endif
typedef union { struct { double __re, __im;}
                data; double align;} dcmplx;
#endif
#ifdef _REIM
#define RE(x) ((x). data. re)
#define IM(x) ((x).__data.__im)
#endif
```

<sup>1</sup> ESSL accepts character data in either upper- or lowercase in its calling sequences.

<sup>&</sup>lt;sup>2</sup> There are no equivalent data types for logical and complex data in C. These require special procedures. For details, see the referenced section.

<sup>3</sup> In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the iusadr argument for ERRSET.

<sup>&</sup>lt;sup>4</sup> Short- and long-precision numbers look the same in this book.

You must, therefore, code an include statement for the ESSL header file in the beginning of your program to use these definitions. For details, see "Calling ESSL Subroutines and Functions in C" on page 129.

Assuming you are using the ESSL header file, if you declare data items to be of type cmplx or dcmplx, you can pass them as short- and long-precision complex data to ESSL, respectively. You may want to write a CSET macro to initialize complex variables, using the RE and IM macros provided in the ESSL header file. Following is an example of how to use the CSET macro to initialize the complex variable alpha:

```
#include <essl.h>
#define CSET(x,a,b) (RE(x)=a, IM(x)=b)
main()
{
    cmplx alpha,t[3],s[5];
    .
    .
    CSET (alpha,2.0,3.0);
    caxpy (3,alpha,s,1,t,2);
    .
    .
}
```

If you choose to use your own definitions for complex data, instead of those provided in the ESSL header file, you can define \_CMPLX and \_DCMPLX in your program for short- and long-precision complex data, respectively, using the following #define statements. These statements are coded with your global declares in the front of your program and must be coded before the #include statement for the ESSL header file.

```
#define _CMPLX
#define DCMPLX
```

If you prefer to define your complex data at compile time, you can use the job processing procedures described in "Compiling" on page 163.

#### **Logical Data**

By coding the following simple macro definitions in your program, you can then use TRUE or FALSE in assigning values to or specifying any logical arguments passed to ESSL:

```
#define FALSE 0
#define TRUE 1
```

# **Setting Up Arrays in C**

C arrays are arranged in storage in row-major order. This means that the last subscript expression increases most rapidly, the next-to-the-last subscript expression increases less rapidly, and so forth, with the first subscript expression increasing least rapidly. ESSL subroutines require that arrays passed as arguments be in column-major order. This is the array storage convention used by Fortran, described in "Setting Up Arrays in Fortran" on page 112. To pass an array from your C program to ESSL, to have ESSL process the data correctly, and to get a

result that is in the proper form for your C program, you can do any of the following:

- · Build and process the matrix, logically transposed from the outset, and transpose the results as necessary.
- Before the ESSL call, transpose the input arrays. Then, following the ESSL call, transpose any arrays updated as output.
- If there are arguments in the ESSL calling sequence indicating whether the arrays are to be processed in normal or transposed form, such as the transa and transb arguments in the \_GEMM subroutines, use these arguments in combination with the matrix equivalence rules to avoid having to transpose your data in separate operations. For further detail, see "SGEMMS, DGEMMS, CGEMMS, and ZGEMMS—Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm" on page 405.

# Creating Multiple Threads and Calling ESSL from Your C Program

The example shown below shows how to create two threads, where each thread calls the ISAMAX subroutine. To use the AIX pthreads library, you must specify the pthread.h header file as the first include file in your program.

Be sure to compile this program with the cc r command.

```
#include <pthread.h>
#include <stdio.h>
#include <unistd.h>
#include <essl.h>
/* Create structure for argument list */
typedef struct {
 int
            n;
  float
            *Χ;
  int
        incx;
} arg list;
```

```
/* Define prototype for thread routine */
void *Thread(void *v);
int main()
 float sx1[9] = \{ 1., 2., 7., -8., -5., -10., -9., 10., 6. \};
 float sx2[8] = \{ 1.,12., 7., -8., -5., -10., -9., 19. \};
 pthread t first th;
 pthread_t second_th;
 int rc;
 arg_list a_l,b_l;
 /* Creating argument list for the first thread */
 a 1.n = 9;
 a_1.incx = 1;
 a 1.x = sx1;
 /* Creating argument list for the second thread */
 b 1.n = 8;
 b_1.incx = 1;
 b_1.x = sx2;
 /* Creating first thread which calls the ESSL subroutine ISAMAX */
 rc = pthread create(&first th, NULL, Thread, (void *) &a 1);
 if (rc) exit(-1);
 /* Creating second thread which calls the ESSL subroutine ISAMAX */
 rc = pthread_create(&second_th, NULL, Thread, (void *) &b_1);
 if (rc) exit(-1);
 sleep(1);
exit(0);
}
/* Thread routine which call ESSL routine ISAMAX */
void *Thread(void *v)
arg_list *al;
float *x;
 int n,incx;
 int i;
 al = (arg_list *)(v);
 x = al -> x;
 n = al -> n;
 incx = al->incx;
```

```
/* Calling the ESSL subroutine ISAMAX */
i = isamax(n,x,incx);
if (i == 8)
 printf("max for sx2 should be 8 = %d\n",i);
 printf("max for sx1 should be 6 = %d\n",i);
```

# Handling Errors in Your C Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

 For input-argument errors 2015 and 2030, which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.

Note: In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the aux arguments. For details see the subroutine descriptions in Part 2 of this book.

 For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

"Input-Argument Errors in C" and "Computational Errors in C" on page 140 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in "Input-Argument Errors in C" and "Computational Errors in C" on page 140 on each thread that calls ESSL.

### Input-Argument Errors in C

To obtain corrected input-argument values in a C program and to avert program termination for the optionally-recoverable input-argument errors 2015 and 2030, add the statements in the following steps to your program. Steps 4 and 8 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

#### Step 1. Code the Global Statements for ESSL Error Handling

```
/* Code two underscores */
/* before the letters ESVERR */
#define ESVERR
#include <essl.h>
      extern int enotrm();
```

These statements are coded with your global declares in the front of your program. The #define must be coded before the #include statement for the ESSL header

file. The extern statement declares the ESSL error exit routine ENOTRM as an external reference in your program. After the point where you code these statements in your program, you must pass by reference all ESSL calling sequence arguments that can potentially be altered by ESSL error handling. This applies to all your ESSL call statements. The two types of arguments are:

- naux arguments for auxiliary storage
- n arguments for transform lengths

#### Step 2. Declare the Variables

```
int (*iusadr) ();
int ierno,inoal,inomes,itrace,irange,irc,dummy;
char storarea[8];
```

This declares a pointer, *iusadr*, to be used for the ESSL error exit routine ENOTRM. Also included are declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

#### Step 3. Do Initialization for ESSL

```
iusadr = enotrm;
einfo (0,&dummy,&dummy);
```

The first statement sets the function pointer, *iusadr*, to ENOTRM, the ESSL error exit routine. The last statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960. These statements should be coded only once in the beginning of your program before calls to ERRSET.

### Step 4. Call ERRSAV

```
errsav (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 1" on page 143, as the use is the same as for computational errors.

### Step 5. Call ERRSET

```
errset (&ierno,&inoal,&inomes,&itrace,&iusadr,&irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- · How many times each error can occur before execution terminates (inoal)
- How many times each error message can be printed (*inomes*)
- The ESSL exit routine ENOTRM, to be invoked for the error indicated (iusadr)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015 or 2030. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the input-argument errors, see "Input-Argument Error Messages" on page 179. For a description of ERRSET, see Chapter 17 on page 957.

### Step 6. Call ESSL

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- name specifies the ESSL subroutine.
- arg1,...,argn are the input and output arguments. As explained in step 1, all
  arguments that can potentially be altered by error handling must be coded by
  reference.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.
- rc1, rc2, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C. The values can be 0, 1, 2, and so forth. Return code values are described under "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

**Step 7. Perform the Desired Action:** These are the statements following the test for each value of the return code, returned in *irc* in step 6. These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the

size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

#### Step 8. Call ERRSTR

```
errstr (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 1" on page 143, as the use is the same as for computational errors.

# Example 1

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```
/*INITIALIZE THE ESSL ERROR OPTION TABLE*/
einfo (0,&dummy,&dummy);
    /*MAKE ERROR CODE 2015 A RECOVERABLE ERROR AND
      SUPPRESS PRINTING ALL ERROR MESSAGES FOR IT*/
ierno = 2015;
inoal = 0;
inomes = -1;
itrace = 0;
irange = 2015;
errset (&ierno,&inoal,&inomes,&itrace,&iusadr,&irange);
    /*CALL ESSL SUBROUTINE SWLEV. NAUX IS PASSED BY
      REFERENCE. IF THE NAUX INPUT IS TOO SMALL,
      ERROR 2015 OCCURS. THE MINIMUM VALUE REQUIRED
      IS STORED IN THE NAUX INPUT ARGUMENT, AND THE
      RETURN CODE OF 1 IS SET IN IRC.*/
irc = swlev (x,incx,u,incu,y,incy,n,aux,&naux);
if irc == 1
     /*CHECK THE RESULTING INPUT ARGUMENT VALUE
       IN NAUX AND TAKE THE DESIRED ACTION*/
```

### Computational Errors in C

To obtain information about an ESSL computational error in a C program, add the statements in the following steps to your program. Steps 4 and 9 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see "EINFO-ESSL Error Information-Handler Subroutine" on page 960.

Step 1. Code the Global Statements for ESSL Error Handling

```
/* Code two underscores */
/* before the letters ESVERR */
#define __ESVERR
#include <essl.h>
```

These statements are coded with your global declares in the front of your program. The #define must be coded before the #include statement for the ESSL header file. After the point where you code these statements in your program, you must pass by reference all ESSL calling sequence arguments that can potentially be altered by ESSL error handling. This applies to all your ESSL call statements. The two types of arguments are:

- naux arguments for auxiliary storage
- n arguments for transform lengths

#### Step 2. Declare the Variables

```
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char storarea[8];
```

These statements include declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

## Step 3. Do Initialization for ESSL

```
einfo (0,&dummy,&dummy);
```

This statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960. These statements should be coded only once in the beginning of your program before calls to ERRSET.

#### Step 4. Call ERRSAV

```
errsav (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 1" on page 143.

### Step 5. Call ERRSET

```
errset (&ierno,&inoal,&inomes,&itrace,&iusadr,&irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (ierno) or a range of errors (irange), you can specify:

- How many times each error can occur before execution terminates (inoal)
- How many times each error message can be printed (inomes)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, ierno should be set to one of the eligible values listed in Table 167 on page 960. To allow your program to continue after an error in the specified range occurs, inoal must be set to a value greater than 1. For ESSL, iusadr should be specified as either 0 or 1 in a 32-bit environment (0l or 1l in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the computational errors, see "Computational Error Messages" on page 187. For a description of ERRSET, see Chapter 17 on page 957.

### Step 6. Call ESSL

```
irc = name (arg1, ..., argn);
if irc == rc1
if irc == rc2
```

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- name specifies the ESSL subroutine.
- arg1,...,argn are the input and output arguments. As explained in step 1, all arguments that can potentially be altered by error handling must be coded by reference.
- irc is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.
- rc1, rc2, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C. The values can be 0, 1, 2, and so forth. Return code values are described under "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

The statements following each test of the return code can perform any desired action. This includes calling EINFO for more information about the error, as described in step 7.

#### Step 7. Call EINFO for Information

```
einfo (ierno,&inf1,&inf2);
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- *ierno* is the error code of interest.
- inf1 and inf2 are the integer variables used to receive the information, where inf1 is assigned a value for all errors, and inf2 is assigned a value for some errors. You must specify both arguments, as there are no optional arguments for C. Both arguments must be passed by reference, because they are output scalar arguments. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

**Step 8. Check the Values in the Information Receivers:** These statements check the values returned in the output argument information receivers, *inf1* and *inf2*, which contain the information about the computational error.

#### Step 9. Call ERRSTR

```
errstr (&ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example 1."

#### Example 1

This 32-bit environment example shows an error code 2105, which returns one piece of information: the index of the pivot element (*i*) near zero, causing factorization to fail. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2105 by this program.

```
/*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define ESVERR
#include <essl.h>
            /*DECLARE THE VARIABLES*/
main ()
int ierno, inoal, inomes, itrace, iusadr, irange, irc;
int inf1,inf2,dummy;
char sav2105[8];
            /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
einfo (0,&dummy,&dummy);
            /*SAVE THE EXISTING ERROR OPTION TABLE ENTRY
              FOR ERROR CODE 2105*/
ierno = 2105;
errsav (&ierno,sav2105);
            /*MAKE ERROR CODES 2101 THROUGH 2105 RECOVERABLE
              ERRORS AND SUPPRESS PRINTING ALL ERROR MESSAGES
              FOR THEM. THIS SHOWS HOW YOU CODE THE
              ERRSET ARGUMENTS FOR A RANGE OF ERRORS. */
ierno = 2101;
inoal = 0;
inomes = 0; /*A DUMMY ARGUMENT*/
itrace = 0; /*A DUMMY ARGUMENT*/
iusadr = 0; /*A DUMMY ARGUMENT*/
irange = 2105
errset (&ierno,&inoal,&inomes,&itrace, &iusadr,&irange);
            /*CALL ESSL SUBROUTINE DGEICD. IF THE INPUT MATRIX
              IS SINGULAR OR NEARLY SINGULAR, ERROR 2105
              OCCURS. A RETURN CODE OF 2 IS SET IN IRC.*/
irc = dgeicd (a,lda,n,iopt,&rcond,det,aux,&naux);
if irc == 2
```

```
/*CALL THE INFORMATION-HANDLER ROUTINE FOR ERROR
              CODE 2105 TO RETURN ONE PIECE OF INFORMATION
              IN VARIABLE INF1, THE INDEX OF THE PIVOT ELEMENT
              NEAR ZERO, CAUSING FACTORIZATION TO FAIL.
              INF2 IS NOT USED, BUT MUST BE SPECIFIED.
              BOTH INF1 AND INF2 ARE PASSED BY REFERENCE,
              BECAUSE THEY ARE OUTPUT SCALAR ARGUMENTS.*/
   ierno = 2105;
   einfo (ierno,&inf1,&inf2);
            /*CHECK THE VALUE IN VARIABLE INF1 AND TAKE THE
              DESIRED ACTION*/
            /*RESTORE THE PREVIOUS ERROR OPTION TABLE ENTRY
              FOR ERROR CODE 2105. ERROR PROCESSING
              RETURNS TO HOW IT WAS BEFORE IT WAS ALTERED BY
              THE ABOVE ERRSAV STATEMENT*/
ierno = 2105;
errstr (&ierno, sav2105);
```

# C++ Programs

This section describes how to code your C++ program.

# Calling ESSL Subroutines and Functions in C++

This section shows how to call ESSL subroutines and functions from your C++ program.

#### Before You Call ESSL

Before you can call the ESSL subroutines from your C++ program, you must have the appropriate ESSL header file installed on your system. The ESSL header file allows you to code your function calls as described in this section. It contains entries for all the ESSL subroutines. The ESSL header file is distributed with the ESSL package. The ESSL header file to be used with the C++ compiler is named essl.h.

In the beginning of your program, before you call any of the ESSL subroutines, **you** must code the following statement for the ESSL header file:

```
#include <essl.h>
```

If you are creating your own threads for the ESSL Thread-Safe or SMP Library, you must include the pthread.h header file in your C++ program. For an example, see "Creating Multiple Threads and Calling ESSL from Your C++ Program" on page 150.

### **Coding the Calling Sequences**

In C++ programs, the ESSL subroutines, not returning a function value, are invoked with the following type of statement:

```
subroutine-name (argument-1, . . . , argument-n);
```

An example of a calling sequence for SAXPY might be:

```
saxpy (5,a,x,incx,y,1);
```

The ESSL subroutines returning a function value are invoked with the following type of statement:

```
function-value-name=subroutine-name (argument-1, . . . , argument-n);
```

An example of invoking DASUM might be:

```
sum = dasum (n,x,incx);
```

See the C++ publications for details about how to code the function calls.

### Passing Arguments in C++

This section describes how to pass arguments in your C++ program.

### **About the Syntax Shown in This Book**

The argument syntax shown in this book assumes that you have installed and are using the ESSL header file. For further details, see "Calling ESSL Subroutines and Functions in C++" on page 145.

#### No Optional Arguments

In the ESSL calling sequences for C++, there are no optional arguments, as for some programming languages. You must code all the arguments listed in the syntax.

#### **Arguments That Must Be Passed by Value**

All scalar arguments that are not modified must be passed by value in the ESSL calling sequence. (This refers to input-only scalar arguments, such as *incx*, *m*, and *lda*.)

#### **Arguments That Must Be Passed by Reference**

Following are the instances in which you pass your arguments by reference (as a pointer) in the ESSL calling sequence:

Arrays: Arguments that are arrays are passed by reference, as usual.

**Subroutine Names:** Some ESSL subroutines call a user-supplied subroutine. The name is part of the ESSL calling sequence. It must be passed by reference.

**Character Arguments:** Character arguments must be passed as strings, by reference. You specify the character, in upper- or lowercase, in the ESSL calling sequence with double quotation marks around it, as in "t". Following is an example

of how you can call SGEADD, specifying the *transa* and *transb* arguments as strings *n* and *t*, respectively:

sgeadd (a,5,"n",b,3,"t",c,4,4,3);

### Setting Up a User-Supplied Subroutine for ESSL in C++

Some ESSL numerical quadrature subroutines call a user-supplied subroutine, *subf*, identified in the ESSL calling sequence. If your program that calls the numerical quadrature subroutines is coded in C++, there are some coding rules you must follow for the *subf* subroutine:

- You can code the *subf* subroutine using only C, C++, or Fortran.
- You must declare *subf* as an external subroutine in your application program.
- You should code the *subf* subroutine to the specifications given in "
   Programming Considerations for the SUBF Subroutine" on page 920. For an
   example of coding a *subf* subroutine in C++, see "Example 1" on page 931.

### Setting Up Scalar Data in C++

Table 29 lists the scalar data types in C++ that are used for ESSL. Only those types and lengths used by ESSL are listed.

Table 29 (Page 1 of 2). Scalar Data Types in C++ Programs		
Terminology Used by ESSL	C++ Equivalent	
Character item <sup>1</sup>	char *	
'N', 'T', 'C' or 'n', 't', 'c'	"n", "t", "c"	
Logical item .TRUE., .FALSE.	Specify it as described in "Setting Up Short-Precision Complex Data Types and Logical Data Types in C++" on page 148.2	
32-bit environment integer	signed int	
12345, –12345		
64-bit environment integer <sup>3</sup>	long	
12345l, –12345l		
Short-precision real number <sup>4</sup>	float	
12.345		
Long-precision real number4	double	
12.345		
Short-precision complex number4	Specify it as described in "Setting Up	
(123.45, –54321.0)	Short-Precision Complex Data Types and Logical Data Types in C++" on page 148.2	
Long-precision complex number <sup>4</sup>	complex <sup>5</sup>	
(123.45, –54321.0)		

Table 29	(Page 2 of	<sup>:</sup> 2). Scalar Data	Types in C++	Programs
----------	------------	------------------------------	--------------	----------

#### Terminology Used by ESSL

C++ Equivalent

- 1 ESSL accepts character data in either upper- or lowercase in its calling sequences.
- <sup>2</sup> There are no equivalent data types for logical and short-precision complex data in C++. These require special procedures. For details, see the referenced section.
- <sup>3</sup> In accordance with the LP64 data model, all ESSL integer arguments remain 32-bits except for the **iusadr** argument for ERRSET.
- <sup>4</sup> Short- and long-precision numbers look the same in this book.
- <sup>5</sup> This data type is defined in file <complex.h> for C++.

# Setting Up Short-Precision Complex Data Types and Logical Data Types in C++

Short-precision complex data types and logical data types are not part of the C++ language; however, some ESSL subroutines require arguments of these data types.

### **Short-Precision Complex Data**

ESSL provides an identifier, cmplx, for the short-precision complex data type, defined in the ESSL header file, as well as two member functions, sreal and simag, for handling the real and imaginary parts of short-precision complex numbers:

You must, therefore, code an include statement for the ESSL header file in the beginning of your program to use these definitions. For details, see "Calling ESSL Subroutines and Functions in C++" on page 145.

Assuming you are using the ESSL header file, if you declare data items to be of type cmplx or complex, you can pass them as short- or long-precision complex data to ESSL, respectively. Following is an example of how you might code your program:

```
#include <complex.h>
#include <essl.h>
main()
{
    cmplx alpha,t[3],s[5];
    complex beta,td[3],sd[5];
    .
    .
    alpha = cmplx(2.0,3.0);
    caxpy (3,alpha,s,1,t,2);
    .
    beta = complex(2.0,3.0);
    zaxpy (3,beta,sd,1,td,2);
    .
    .
}
```

If you choose to use your own definition for short-precision complex data, instead of that provided in the ESSL header file, you can define \_CMPLX in your program, using the following #define statement. This statement is coded with your global declares in the front of your program and must be coded before the #include statement for the ESSL header file.

```
#define _CMPLX
```

If you prefer to define your short-precision complex data at compile time, you can use the job processing procedures described in "Compiling" on page 163.

#### **Logical Data**

By coding the following simple macro definitions in your program, you can then use TRUE or FALSE in assigning values to or specifying any logical arguments passed to ESSL:

```
#define FALSE 0
#define TRUE 1
```

# Setting Up Arrays in C++

C++ arrays are arranged in storage in row-major order. This means that the last subscript expression increases most rapidly, the next-to-the-last subscript expression increases less rapidly, and so forth, with the first subscript expression increasing least rapidly. ESSL subroutines require that arrays passed as arguments be in column-major order. This is the array storage convention used by Fortran, described in "Setting Up Arrays in Fortran" on page 112. To pass an array from your C++ program to ESSL, to have ESSL process the data correctly, and to get a result that is in the proper form for your C++ program, you can do any of the following:

- Build and process the matrix, logically transposed from the outset, and transpose the results as necessary.
- Before the ESSL call, transpose the input arrays. Then, following the ESSL call, transpose any arrays updated as output.

If there are arguments in the ESSL calling sequence indicating whether the
arrays are to be processed in normal or transposed form, such as the *transa*and *transb* arguments in the \_GEMM subroutines, use these arguments in
combination with the matrix equivalence rules to avoid having to transpose your
data in separate operations. For further detail, see "SGEMMS, DGEMMS,
CGEMMS, and ZGEMMS—Matrix Multiplication for General Matrices, Their
Transposes, or Conjugate Transposes Using Winograd's Variation of
Strassen's Algorithm" on page 405.

## Creating Multiple Threads and Calling ESSL from Your C++ Program

The example shown below shows how to create two threads, where each thread calls the ISAMAX subroutine. To use the AIX pthreads library, you must remember to code the pthread.h header file in your C++ program.

Be sure to compile this program with the x1C\_r command.

```
#include "essl.h"
#include <iostream.h>
/* Define prototype for thread routine */
void *Thread(void *v);
/* Define prototype for thread library routine, which is in C */
extern "C" {
#include <pthread.h>
#include <stdlib.h>
int pthread create(pthread t *tid, const pthread attr t *attr,
                   void *(*start routine)(void *), void *arg);
}
extern "Fortran" int isamax(const int &, float *, const int &);
/* Create structure for argument list */
struct arg_list {
 int
           n;
  float
          *X:
  int
       incx;
};
```

```
void main()
 float sx1[9] = \{ 1., 2., 7., -8., -5., -10., -9., 10., 6. \};
 float sx2[8] = \{ 1.,12., 7., -8., -5., -10., -9., 19. \};
 pthread_t first_th;
 pthread_t second_th;
 int rc;
 struct arg_list a_l,b_l;
 a_1.n = 9;
 a_1.incx = 1;
 a_1.x = sx1;
 b 1.n = 8;
 b_1.incx = 1;
 b 1.x = sx2;
 /* Creating argument list for first thread */
 rc = pthread_create(&first_th, NULL, Thread, (void *) &a_1);
 if (rc) exit(-1);
 /* Creating argument list for second thread */
 rc = pthread create(&second th, NULL, Thread, (void *) &b 1);
 if (rc) exit(-1);
 sleep(20);
exit(0);
/* Thread routine which calls the ESSL subroutine ISAMAX */
void* Thread(void *v)
struct arg_list *al;
float *t;
int n, incx;
 int i;
 al = (struct arg_list *)(v);
t = al->x;
n = al -> n;
 incx = al->incx;
```

```
/* Calling the ESSL subroutine ISAMAX */
i = isamax(n,t,incx);
if (i == 8)
 cout << "max for sx2 should be 8 = " << i << "\n";
 cout << "max for sx1 should be 6 = " << i << "\n";
return NULL;
```

# Handling Errors in Your C++ Program

ESSL provides you with flexibilities in handling both input-argument errors and computational errors:

• For input-argument errors 2015 and 2030, which are optionally-recoverable errors, ESSL allows you to obtain corrected input-argument values and react at run time.

Note: In the case where error 2015 is unrecoverable, you have the option of dynamic allocation for most of the aux arguments. For details see the subroutine descriptions in Part 2 of this book.

• For computational errors, ESSL provides a return code and additional information to help you analyze the problem in your program and react at run time.

"Input-Argument Errors in C++" and "Computational Errors in C++" on page 157 explain how to use these facilities by describing the additional statements you must code in your program.

For multithreaded application programs, if you want to initialize the error option table and change the default settings for input-argument and computational errors, you need to implement the steps shown in "Input-Argument Errors in C++" and "Computational Errors in C++" on page 157 on each thread that calls ESSL.

#### Input-Argument Errors in C++

To obtain corrected input-argument values in a C++ program and to avert program termination for the optionally-recoverable input-argument errors 2015 and 2030, add the statements in the following steps to your program. Steps 4 and 8 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary.

#### Step 1. Code the Global Statements for ESSL Error Handling

```
/* Code one underscore */
/* before the letters ESVERR */
#define ESVERR
#include <iostream.h>
#include <stdio.h>
#include <essl.h>
extern "Fortran" int enotrm(int &,int &);
```

These statements are coded with your global declares in the front of your program. The #define must be coded before the #include statements for the ESSL header file. The extern statement declares the ESSL error exit routine ENOTRM as an external reference in your program.

#### Step 2. Declare the Variables

```
int (*iusadr) (int &,int &);
int ierno,inoal,inomes,itrace,irange,irc,dummy;
char storarea[8];
```

This declares a pointer, *iusadr*, to be used for the ESSL error exit routine ENOTRM. Also included are declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

#### Step 3. Do Initialization for ESSL

```
iusadr = enotrm;
dummy = 0;
einfo (0,dummy,dummy);
```

The first statement sets the function pointer, *iusadr*, to ENOTRM, the ESSL error exit routine. The last statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960. These statements should be coded only once in the beginning of your program before calls to ERRSET.

#### Step 4. Call ERRSAV

```
errsav (ierno,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example" on page 159, as the use is the same as for computational errors.

#### Step 5. Call ERRSET

```
errset (ierno,inoal,inomes,itrace,iusadr,irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For optionally-recoverable ESSL input-argument errors, you need to call ERRSET only if you want to avoid terminating your program and you want the input arguments associated with this error to be assigned correct values in your program when the error occurs. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (inoal)
- How many times each error message can be printed (inomes)
- The ESSL exit routine ENOTRM, to be invoked for the error indicated (iusadr)

ERRSET must be called for each error code you want to indicate as being recoverable. For ESSL, *ierno* should have a value of 2015 or 2030. If you want to eliminate error messages, you should indicate a negative number for *inomes*; otherwise, you should specify 0 for this argument. All the other ERRSET arguments should be specified as 0.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the input-argument errors, see "Input-Argument Error Messages" on page 179. For a description of ERRSET, see Chapter 17 on page 957.

#### Step 6. Call ESSL

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

- name specifies the ESSL subroutine.
- arg1,...,argn are the input and output arguments.
- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.
- rc1, rc2, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C++. The values can be 0, 1, 2, and so forth. Return code values are described under "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

**Step 7. Perform the Desired Action:** These are the statements following the test for each value of the return code, returned in *irc* in step 6. These statements perform whatever action is desired when the recoverable error occurs. These statements may check the new values set in the input arguments to determine whether adequate program storage is available, and then decide whether to continue or terminate the program. Otherwise, these statements may check that the size of the working storage arrays or the length of the transform agrees with other data in the program. The program may also store this corrected input argument value for future reference.

#### Step 8. Call ERRSTR

```
errstr (ierno,storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example" on page 159, as the use is the same as for computational errors.

#### **Example**

This example shows an error code 2015, which resets the size of the work area *aux*, specified in *naux*, if the value specified is too small. It also indicates that no error messages should be issued.

```
/*DECLARE THE VARIABLES*/
main ()
int (*iusadr) (int &,int &);
int ierno,inoal,inomes,itrace,irc,dummy;
int naux;
    /*INITIALIZE THE POINTER TO THE ENOTRM ROUTINE*/
iusadr = enotrm;
    /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
dummy = 0;
einfo (0, dummy, dummy);
    /*MAKE ERROR CODE 2015 A RECOVERABLE ERROR AND
      SUPPRESS PRINTING ALL ERROR MESSAGES FOR IT*/
ierno = 2015;
inoal = 0;
inomes = -1;
itrace = 0;
irange = 2015;
errset (ierno,inoal,inomes,itrace,iusadr,irange);
    /*CALL ESSL SUBROUTINE SWLEV. NAUX IS PASSED BY
      REFERENCE. IF THE NAUX INPUT IS TOO SMALL,
      ERROR 2015 OCCURS. THE MINIMUM VALUE REQUIRED
      IS STORED IN THE NAUX INPUT ARGUMENT, AND THE
      RETURN CODE OF 1 IS SET IN IRC.*/
irc = swlev (x,incx,u,incu,y,incy,n,aux,naux);
if irc == 1
     /*CHECK THE RESULTING INPUT ARGUMENT VALUE
       IN NAUX AND TAKE THE DESIRED ACTION*/
}
```

### Computational Errors in C++

To obtain information about an ESSL computational error in a C++ program, add the statements in the following steps to your program. Steps 4 and 9 for ERRSAV and ERRSTR, respectively, are optional. Adding these steps makes the effect of the call to ERRSET temporary. For a list of those computational errors that return information and to which these steps apply, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

#### Step 1. Code the Global Statements for ESSL Error Handling

```
/* Code one underscore */
/* before the letters ESVERR */
#define _ESVERR
#include <iostream.h>
#include <stdio.h>
#include <essl.h>
```

These statements are coded with your global declares in the front of your program. The #define must be coded before the #include statement for the ESSL header file.

#### Step 2. Declare the Variables

```
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char storarea[8];
```

These statements include declares for the variables used by the ESSL and Fortran error-handling subroutines. Note that *storarea* must be 8 characters long. These should be coded in the beginning of your program before any of the following statements.

#### Step 3. Do Initialization for ESSL

```
dummy = 0;
einfo (0,dummy,dummy);
```

The last statement calls the EINFO subroutine to initialize the ESSL error option table, where *dummy* is a declared integer and is a placeholder. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960. These statements should be coded only once in the beginning of your program before calls to ERRSET.

#### Step 4. Call ERRSAV

```
errsav (ierno,storarea);
```

(This is an optional step.) This calls the ERRSAV subroutine, which stores the error option table entry for error number *ierno* in an 8-byte storage area, *storarea*, which is accessible to your program. ERRSAV must be called for each entry you want to save. This step is used, along with step 8, for ERRSTR. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example" on page 159.

#### Step 5. Call ERRSET

```
errset (ierno,inoal,inomes,itrace,iusadr,irange);
```

This calls the ERRSET subroutine, which allows you to dynamically modify the action taken when an error occurs. For ESSL computational errors, you need to call ERRSET only if you want to change the default values in the ESSL error option table. For one error (*ierno*) or a range of errors (*irange*), you can specify:

- How many times each error can occur before execution terminates (inoal)
- How many times each error message can be printed (inomes)

ERRSET must be called for each error code for which you want to change the default values. For ESSL, *ierno* should be set to one of the eligible values listed in Table 167 on page 960. To allow your program to continue after an error in the specified range occurs, *inoal* must be set to a value greater than 1. For ESSL, *iusadr* should be specified as either 0 or 1 in a 32-bit environment (0I or 1I in a 64-bit environment), so a user exit is not taken.

For a list of the default values set in the ESSL error option table, see Table 26 on page 51. For a description of the computational errors, see "Computational Error Messages" on page 187. For a description of ERRSET, see Chapter 17 on page 957.

#### Step 6. Call ESSL

This calls the ESSL subroutine and specifies a branch on one or more return code values, where:

name specifies the ESSL subroutine.

- *irc* is the integer variable containing the return code resulting from the computation performed by the ESSL subroutine.
- rc1, rc2, and so forth are the possible return code values that can be passed back from the ESSL subroutine to C++. The values can be 0, 1, 2, and so forth. Return code values are described under "Error Conditions" in each ESSL subroutine description in Part 2 of this book.

The statements following each test of the return code can perform any desired action. This includes calling EINFO for more information about the error, as described in step 7.

#### Step 7. Call EINFO for Information

```
einfo (ierno,inf1,inf2);
```

This calls the EINFO subroutine, which returns information about certain computational errors, where:

- *ierno* is the error code of interest.
- inf1 and inf2 are the integer variables used to receive the information, where inf1 is assigned a value for all errors, and inf2 is assigned a value for some errors. You must specify both arguments, as there are no optional arguments for C. For a description of EINFO, see "EINFO—ESSL Error Information-Handler Subroutine" on page 960.

**Step 8. Check the Values in the Information Receivers:** These statements check the values returned in the output argument information receivers, *inf1* and *inf2*, which contain the information about the computational error.

#### Step 9. Call ERRSTR

```
errstr (ierno, storarea);
```

(This is an optional step.) This calls the ERRSTR subroutine, which stores an entry in the error option table for error number *ierno* from an 8-byte storage area, *storarea*, which is accessible to your program. ERRSTR must be called for each entry you want to store. This step is used, along with step 4, for ERRSAV. For information on whether you should use ERRSAV and ERRSTR, see "How Can You Control Error Handling in Large Applications by Saving and Restoring Entries in the Error Option Table?" on page 53. For an example, see "Example."

#### Example

This 32-bit environment example shows an error code 2105, which returns one piece of information: the index of the pivot element (*i*) near zero, causing factorization to fail. It uses ERRSAV and ERRSTR to insulate the effects of the error handling for error 2105 by this program.

```
/*GLOBAL STATEMENTS FOR ESSL ERROR HANDLING*/
#define ESVERR
#include <essl.h>
#include <iostream.h>
#include <stdio.h>
            /*DECLARE THE VARIABLES*/
main ()
int ierno,inoal,inomes,itrace,iusadr,irange,irc;
int inf1,inf2,dummy;
char sav2105[8];
            /*INITIALIZE THE ESSL ERROR OPTION TABLE*/
dummy = 0;
einfo (0, dummy, dummy);
            /*SAVE THE EXISTING ERROR OPTION TABLE ENTRY
              FOR ERROR CODE 2105*/
ierno = 2105;
errsav (ierno, sav2105);
            /*MAKE ERROR CODES 2101 THROUGH 2105 RECOVERABLE
              ERRORS AND SUPPRESS PRINTING ALL ERROR MESSAGES
              FOR THEM. THIS SHOWS HOW YOU CODE THE
              ERRSET ARGUMENTS FOR A RANGE OF ERRORS. */
ierno = 2101;
inoal = 0;
inomes = 0; /*A DUMMY ARGUMENT*/
itrace = 0; /*A DUMMY ARGUMENT*/
iusadr = 0; /*A DUMMY ARGUMENT*/
irange = 2105
errset (ierno, inoal, inomes, itrace, iusadr, irange);
            /*CALL ESSL SUBROUTINE DGEICD. IF THE INPUT MATRIX
              IS SINGULAR OR NEARLY SINGULAR, ERROR 2105
              OCCURS. A RETURN CODE OF 2 IS SET IN IRC.*/
irc = dgeicd (a,lda,n,iopt,rcond,det,aux,naux);
if irc == 2
```

```
/*CALL THE INFORMATION-HANDLER ROUTINE FOR ERROR
              CODE 2105 TO RETURN ONE PIECE OF INFORMATION
              IN VARIABLE INF1, THE INDEX OF THE PIVOT ELEMENT
              NEAR ZERO, CAUSING FACTORIZATION TO FAIL.
              INF2 IS NOT USED, BUT MUST BE SPECIFIED.
              BOTH INF1 AND INF2 ARE PASSED BY REFERENCE,
              BECAUSE THEY ARE OUTPUT SCALAR ARGUMENTS.*/
   ierno = 2105;
   einfo (ierno, inf1, inf2);
            /*CHECK THE VALUE IN VARIABLE INF1 AND TAKE THE
              DESIRED ACTION*/
            /*RESTORE THE PREVIOUS ERROR OPTION TABLE ENTRY
              FOR ERROR CODE 2105. ERROR PROCESSING
              RETURNS TO HOW IT WAS BEFORE IT WAS ALTERED BY
              THE ABOVE ERRSAV STATEMENT*/
ierno = 2105;
errstr (ierno, sav2105);
```

# **PL/I Programs**

If you are using ESSL with PL/I Set for AIX, Version 1, see the PL/I publications for details on calling subroutines and functions.

# **Chapter 5. Processing Your Program**

This chapter provides information on how to process your program. It contains processing procedures that apply to Fortran, C, and C++ programs using ESSL. It describes **only the ESSL-specific changes** you need to make to your job setup procedures. For complete examples of job setup procedures, see your programming language's programming guide.

#### Notes:

- For the ESSL SMP Library, you can use the XL Fortran XLSMPOPTS environment variable to specify options which affect SMP execution. For details, see the Fortran publications.
- 2. If you are using either the ESSL POWER2 Library or the ESSL Thread-Safe POWER2 Library, you must be running on a RS/6000 POWER2 processor.

# **Compiling**

This section describes how to compile your program.

### **General Procedures**

You can use any procedures you are currently using for compiling your program. ESSL requires no changes to the compile-time setup procedures for C or C++ programs, because the ESSL header file, essl.h, which is used for C and C++ programs, is installed in the /usr/include directory.

ESSL supports the XL Fortran compile-time option **-qextname**. For details, see the Fortran manuals.

You must use only the allowable compilers or assemblers listed in Table 2 on page 8.

## Using Your Own Complex Data Definitions in C Programs

If you want to specify your own definitions for short- and long-precision complex data, add -D\_CMPLX and -D\_DCMPLX, respectively, to your compile command, as shown here:

	ESSL Library Name	Command
	SMP -or-	cc_r -c0 -D_CMPLX -D_DCMPLX <i>xyz</i> .c
	Thread-Safe -or-	
	Thread-Safe POWER2	
	POWER2 -or-	cc -c0 -D_CMPLX -D_DCMPLX <i>xyz</i> .c
	POWER	

where *xyz.c* is the name of your C program. Otherwise, you automatically use the definitions of short- and long-precision complex data provided in the ESSL header file.

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### Using Your Own Short Complex Data Definitions in C++ Programs

If you want to specify your own definition for short-precision complex data, add -D\_CMPLX to your command, as shown here:

	ESSL Library Name	Command
1	SMP -or-	xlC_r -c0 -D_CMPLX xyz.C -qnocinc=/usr/include/essl
1	Thread-Safe <i>-or-</i>	
	Thread-Safe POWER2	
Ι	POWER2 -or-	x1C -c0 -D_CMPLX xyz.C -qnocinc=/usr/include/ess1
	POWER	

where *xyz*.C is the name of your C++ program. Otherwise, you automatically use the definition of short-precision complex data provided in the ESSL header file.

## **Compiling and Linking**

You can use any procedures you are currently using to link or run your program, as long as you make the necessary modifications for ESSL. This section describes these modifications. For details on the complete procedures, see your operating system and programming language manuals.

### 64-bit environment

The ESSL libraries for AIX 4.3.2 which support a 64-bit environment are:

- The ESSL POWER Library
- The ESSL Thread-Safe Library
- The ESSL SMP Library

64-bit environment applications can be created on any AIX 4.3.2 system, but can run only on 64-bit hardware.

If you are accessing ESSL from a 64-bit environment program, you must add the **-q64** compiler option. This compiler option is language independent.

1	ESSL Library Name	Command
1	SMP	xlf_r -0 -qnosave -q64 <i>xyz</i> .f -lesslsmp
1	Thread-Safe	cc_r -0 -q64 <i>xyz</i> .c -less1_r
1	POWER	x1C -0 -q64 xyz.C -less1

where *xyz*.f is the name of your Fortran program, *xyz*.c is the name of your C program, and *xyz*.C is the name of your C++ program.

# **Fortran Programs**

If you are accessing ESSL from a Fortran program and want to compile and link in one step, you can use the following command:

ESSL Library Name	Command
SMP	xlf_r -0 -qnosave <i>xyz</i> .f -lesslsmp
Thread-Safe	xlf_r -0 -qnosave <i>xyz</i> .f -lessl_r
Thread-Safe POWER2	xlf_r -0 -qnosave <i>xyz</i> .f -lesslp2_r
POWER2	xlf -0 xyz.f -lesslp2
POWER	xlf -0 xyz.f -lessl

where xyz.f is the name of your Fortran program.

If you want to compile and link your Fortran program in separate steps, you can use the following commands:

ESSL Library Name	Command
SMP	<pre>xlf_r -0 -c -qnosave xyz.f xlf_r xyz.o -lesslsmp</pre>
Thread-Safe	xlf_r -0 -c -qnosave xyz.f xlf_r xyz.o -lessl_r
Thread-Safe POWER2	xlf_r -0 -c -qnosave <i>xyz</i> .f xlf_r <i>xyz</i> .o -lesslp2_r
POWER2	xlf -0 -c xyz.f xlf xyz.o -lesslp2
POWER	xlf -0 -c xyz.f xlf xyz.o -lessl

where *xyz*.f is the name of your Fortran program, and *xyz*.0 is the name of your object file.

# **C Programs**

If you are accessing ESSL from a C program and want to compile and link in one step, you can use the following command:

ESSL Library Name	Command
SMP	cc_r -0 xyz.c -lesslsmp
Thread-Safe	cc_r -0 <i>xyz</i> .c -lessl_r
Thread-Safe POWER2	cc_r -0 <i>xyz</i> .c -lesslp2_r
POWER2	cc -0 <i>xyz</i> .c -less1p2
POWER	cc -0 xyz.c -less1

where xyz.c is the name of your C program.

If you want to compile and link your C program in separate steps, you can use the following commands:

ESSL Library Name	Command
SMP	cc_r -c0 xyz.c cc_r xyz.o -lesslsmp
Thread-Safe	cc_r -c0 <i>xyz.</i> c cc_r <i>xyz.</i> o -lessl_r
Thread-Safe POWER2	cc_r -c0 <i>xyz</i> .c cc_r <i>xyz</i> .o -lesslp2_r
POWER2	cc -c0 xyz.c cc xyz.o -lesslp2
POWER	cc -c0 xyz.c cc xyz.o -lessl

where xyz.c is the name of your C program and xyz.o is the name of your object file

In the above cases, you automatically use the definitions of short- and long-precision complex data provided in the ESSL header file. If you prefer to specify your own definitions for short- and long-precision complex data, add -D\_CMPLX and -D\_DCMPLX, respectively, to your commands, as shown here:

ESSL Library Name	Command
SMP	cc_r -0 -D_CMPLX -D_DCMPLX xyz.c -less1smp
Thread-Safe	cc_r -O -D_CMPLX -D_DCMPLX xyz.c -lessl_r
Thread-Safe POWER2	cc_r -O -D_CMPLX -D_DCMPLX <i>xyz</i> .c -lesslp2_r
POWER2	cc -O -D_CMPLX -D_DCMPLX xyz.c -less1p2
POWER	cc -O -D_CMPLX -D_DCMPLX xyz.c -lessl

# C++ Programs

If you are accessing ESSL from a C++ program and want to compile and link in one step, you can use the following command:

ESSL Library Name	Command
SMP	xlC_r -0 xyz.C -lesslsmp -qnocinc=/usr/include/essl
Thread-Safe	xlC_r -0 xyz.C -lessl_r -qnocinc=/usr/include/essl
Thread-Safe POWER2	xlC_r -0 xyz.C -lesslp2_r -qnocinc=/usr/include/essl
POWER2	x1C -0 xyz.C -less1p2 -qnocinc=/usr/include/ess1
POWER	xlC -0 xyz.C -lessl -qnocinc=/usr/include/essl

where xyz.C is the name of your C++ program.

If you want to compile and link your C++ program in separate steps, you can use the following commands:

ESSL Library Name	Command	
SMP	xlC_r -c0 xyz.C -qnocinc=/usr/include/essl xlC_r xyz.o -lesslsmp	

ESSL Library Name	Command
Thread-Safe	xlC_r -c0 xyz.C -qnocinc=/usr/include/essl xlC_r xyz.o -lessl_r
Thread-Safe POWER2	xlC_r -c0 xyz.C -qnocinc=/usr/include/essl xlC_r xyz.o -lesslp2_r
POWER2	x1C -c0 xyz.C -qnocinc=/usr/include/essl x1C xyz.o -lesslp2
POWER	x1C -c0 xyz.C -qnocinc=/usr/include/essl x1C xyz.o -lessl

where xyz.C is the name of your C++ program, and xyz.o is the name of your object file.

In the above cases, you automatically use the definition of short-precision complex data provided in the ESSL header file. If you prefer to specify your own definition for short-precision complex data, add -D\_CMPLX to your commands, as shown here:

ESSL Library Name	Command
SMP	x1C_r -0 -D_CMPLX xyz.C -less1smp -qnocinc=/usr/include/ess1
Thread-Safe	x1C_r -0 -D_CMPLX xyz.C -less1_r -qnocinc=/usr/include/ess1
Thread-Safe POWER2	x1C_r -0 -D_CMPLX xyz.C -less1p2_r -qnocinc=/usr/include/ess1
POWER2	x1C -O -D_CMPLX xyz.C -less1p2 -qnocinc=/usr/include/ess1
POWER	x1C -O -D_CMPLX xyz.C -less1 -qnocinc=/usr/include/ess1

1

# **Chapter 6. Migrating Your Programs**

This chapter explains many aspects of migrating your application programs to use the ESSL subroutines. It covers:

- Migrating ESSL Version 3 programs to Version 3 Release 1.1
- Migrating ESSL Version 2 programs to Version 3
- Planning for future migration
- Migrating between RS/6000 processors
- · Migrating from other libraries to ESSL

# Migrating ESSL Version 3 Programs to Version 3 Release 1.1

This section describes all the aspects of migrating your ESSL Version 3 application programs to Version 3 Release 1.1.

**Note:** For a list of the new features added in ESSL Version 3 Release 1.1, see "What's New for ESSL for AIX" on page xxxiii.

### **ESSL Subroutines**

The calling sequences for the subroutines in ESSL Version 3 and ESSL Version 3 Release 1.1 are identical.

Distinct libraries are provided for AIX 4.2.1 and AIX 4.3.2

- For AIX 4.2.1, the ESSL Thread-Safe Library, the ESSL Thread-Safe POWER2 Library, and the ESSL SMP Library were built using the pthreads draft 7 supplied on AIX 4.2.1. (This is the same as ESSL 3.1)
- For AIX 4.3.2, the ESSL Thread-Safe Library, the ESSL Thread-Safe
   POWER2 Library, and the ESSL SMP Library were built using the pthreads
   library that conforms to the IEEE POSIX 1003.1-1996 specification supplied on
   AIX 4.3.

Threaded applications built using ESSL 3.1 will continue to run with ESSL 3.1.1.

If you are migrating to a 64-bit environment you may need to make changes to your call to **ERRSET**. See "ERRSET—ESSL ERRSET Subroutine for ESSL" on page 964.

# Migrating ESSL Version 2 Programs to Version 3

This section describes all the aspects of migrating your ESSL Version 2 application programs to Version 3.

**Note:** For a list of the new features and subroutines added in ESSL Version 3, see "Changes for ESSL Version 3" on page xxxiii.

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### **ESSL Subroutines**

The calling sequences for the subroutines in ESSL Version 2 and ESSL Version 3 are identical. This includes the new ESSL SMP and Thread-Safe Libraries that are included in the ESSL Version 3 product. You do not have to change your existing application programs that call ESSL subroutines when migrating to the ESSL Version 3 product. You must, however, re-link your application program. Therefore, you can simply re-link your existing programs to take advantage of the the increased performance of using the ESSL SMP Library on the SMP processors.

For the \_GEF and \_GEFCD subroutines, the first column of the matrix  $\boldsymbol{L}$  with the corresponding  $\boldsymbol{U}_{ii} = 0$  diagonal element is identified in a computational error message. Previously, the last column was identified. You do not have to make any modifications to your existing application programs that call these subroutines.

### **ESSL Messages**

The text of message format has changed. **ESV** has been removed from the message text. For details on the new format, see "Message Format" on page 178.

Some input-argument and computational error message numbers have been changed. The old message numbers can still be used when calling ERRSET, however, you should migrate to the new message numbers. The following describes which error messages have been modified:

Old Error Message Number	New Error Message Number
2074	2608
2123	2609
2128	2700

# **Planning for Future Migration**

With respect to planning for the future, if working storage does not need to persist after the subroutine call, you should use dynamic allocation. Otherwise, you should use the processor-independent formulas or simple formulas for calculating the values for the *naux* arguments in the ESSL calling sequences. Two things may occur that could cause the minimum values of *naux*, returned by ESSL error handling, to increase in the future:

- If changes are made to the ESSL subroutines to improve performance
- If changes are necessary to support future processors

The formulas allow you to specify your auxiliary storage large enough to accommodate any future improvements to ESSL and any future processors. If you do not provide, at least, these amounts of storage, your program may not run in the future.

You should use the following rule of thumb: To protect your application from having to be recoded in the future because of possible increased requirements for auxiliary storage, use dynamic allocation if possible. If the working storage must persists after the subroutine call, then you should provide as much storage as possible in your current application. In determining the right amount to specify, you should weigh your storage constraints against the inconvenience of making future

changes, then specify what you think is best. If possible, you should provide this larger amount of storage to prevent future migration problems.

### Migrating between RS/6000 Processors

This section describes all the aspects of migrating your ESSL application programs (back and forth) between the RS/6000 PowerPC, POWER, POWER2, and POWER3 processors.

### **Auxiliary Storage**

The minimum amount of auxiliary storage returned by ESSL error handling may vary among the RS/6000 processors for the following subroutines: all the Fourier transform subroutines, SCONF, SCORF, and SACORF. Therefore, to guarantee that your application programs always migrate from any platform to any other platform, you should use the processor independent formulas to determine the amount of auxiliary storage to use.

### **Bitwise-Identical Results**

Because of hardware and ESSL design differences, the results you obtain when migrating from one ESSL Library to another may not be bitwise identical. The results, however, are mathematically equivalent.

### Migrating from Other Libraries to ESSL

This section describes some general aspects of moving from an IBM or non-IBM engineering and scientific library to ESSL.

## Migrating from ESSL/370

There is a high degree of compatibility between ESSL/370 and ESSL for AIX. However you may need to make some coding changes for certain subroutines. See the *Engineering and Scientific Subroutine Library Version 2.2 Guide and Reference* for details.

## Migrating from Another IBM Subroutine Library

If you are migrating from other IBM library products—such as Subroutine Library—Mathematics (SL MATH) or Scientific Subroutine Package (SSP), which have some functions similar to ESSL—the ESSL calling sequences differ from the calling sequences you are currently using. Your program must be modified to add the ESSL calling sequences and make the other ESSL-related coding changes.

If you are migrating from the Basic Linear Algebra Subroutine Library provided with the RS/6000 basic operating system, your calling sequences do not need to be changed.

# **Migrating from LAPACK**

ESSL contains a few subroutines that conform to the LAPACK interface (see Appendix B on page APB-1). If you are using these subroutines, no coding changes are needed to migrate to ESSL.

Additionally, you may be interested in using the Call Conversion Interface (CCI) that is available with LAPACK. The CCI substitutes a call to an ESSL subroutine in place of an LAPACK subroutine whenever an ESSL subroutine provides either functional or near-functional equivalence. Using the CCI allows LAPACK users to obtain the optimized performance of ESSL for an additional subset of LAPACK subroutines. For details, see reference [40].

### Migrating from a Non-IBM Subroutine Library

If you are using a non-IBM library, ESSL may provide subroutines corresponding to those you are currently using. You may choose to migrate your program to benefit from the increased performance offered by the ESSL subroutines. In this case, you may have to recode your program to use the ESSL calling sequences, because the names and arguments used by ESSL may be different from those used by the non-IBM library. On the other hand, if you are using any of the standard Level 1, 2, and 3 BLAS or LAPACK routines that correspond to ESSL subroutines, you do not need to recode the calling sequences. The ESSL calling sequences are the same as the public domain code.

# **Chapter 7. Handling Problems**

This chapter provides the following information for your use when dealing with errors:

- · How to obtain IBM support.
- What to do about NLS (National Language Support) problems.
- A description of the different types of errors that can occur in ESSL. It explains
  what happens when an error occurs and, in some instances, how you can use
  error handling to obtain further information.
- All of the ESSL error messages are categorized into the different error types.
   There is also a description of the error message format.

### Where to Find More Information About Errors

Specific errors associated with each ESSL subroutine are listed under "Error Conditions" in each subroutine description in Part 3 of this book.

### **Getting Help from IBM Support**

Should you require help from IBM in resolving an ESSL problem, report it and provide the following information, if available and appropriate.

- 1. Your customer number
- 2. The ESSL program number:
  - 5765-C42

This is important information that speeds up the correct routing of your call.

3. The version and release of the operating system that you are running on. To get this information on AIX, enter the following command:

oslevel

4. The names and versions of key products being run. To get this information on AIX, enter the following command:

where the appropriate values of *product* for AIX Version 4 are listed in Table 30.

Table 30. Product File Set Names when Using AIX Version 4		
Product File Sets	Descriptive Name	
essl.*	ESSL	
xlfrte	XL Fortran Run-Time Environment	
xlhpf.rte	XL HPF Run-Time Environment	
xlsmp.rte	SMP Run-Time Environment	
xlfcmp	XL Fortran Compiler	
vac.C	C for AIX Compiler	
ibmcxx.cmp	IBM C, C++ Version 3.6 Compilers	

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- 5. The message that is returned when an error is detected.
- Any error message relating to core dumps.
- 7. The compiler listings, including compiler options in effect, and any run-time listings produced
- 8. Program changes made in comparison with a previous successful run
- 9. A small test case demonstrating the problem using the minimum number of statements and variables, including input data

Consult your IBM Service representative for more assistance.

### **National Language Support**

For National Language Support (NLS), all ESSL subroutines display messages located in externalized message catalogs. English versions of the message catalogs are shipped with the IBM Engineering and Scientific Subroutine Library for AIX product, but your site maybe using its own translated message catalogs. The AIX environment variable **NLSPATH** is used by the various ESSL subroutines to find the appropriate message catalog. NLSPATH specifies a list of directories to search for message catalogs. The directories are searched, in the order listed, to locate the message catalog. In resolving the path to the message catalog, NLSPATH is affected by the value of the environment variables LC\_MESSAGES and LANG. If you get an error saying that a message catalog is not found and want the default message catalog, enter the following:

```
export NLSPATH = /usr/lib/nls/msg/%L/%N
export LANG = C
```

The ESSL message catalogs are in English, and are located in the following directories:

```
/usr/lib/nls/msq/C
/usr/lib/nls/msg/En US
/usr/lib/nls/msg/en_US
```

If your site is using its own translations of the message catalogs, consult your system administrator for the appropriate value of NLSPATH or LANG. For additional information on NLS and message catalogs, see IBM AIX Version 4 for RISC System/6000 General Programming Concepts.

If ESSL cannot successfully find a message, ESSL returns message 2799, indicating which message could not be located. Message 2799 is described in "Miscellaneous Error Messages" on page 178.

# **Dealing with Errors**

At run time, you can encounter a number of different types of errors that are specifically related to the use of the ESSL subroutines:

- Program exceptions
- Input-argument errors (2001-2099) and (2801-2899)
- Computational errors (2100-2199)

- Resource errors (2401-2499)
- Informational and Attention messages (2600-2699)
- Miscellaneous errors (2700-2799)

### **Program Exceptions**

The program exceptions you can encounter in ESSL are described in the RS/6000 architecture manuals. For details, see:

- ANSI/IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Standard 754-1985.
- RS/6000 POWERstation and POWERserver Hardware Technical Reference Information—General Architectures.

### **ESSL Input-Argument Error Messages**

If you receive an error message in the form 2538-20*nn*, you have an input-argument error in the calling sequence for an ESSL subroutine. Your program terminated at this point unless you did one of the following:

- Specified the ESSL user exit routine, ENOTRM, with ERRSET to determine the correct input argument values in your program for the optionally-recoverable ESSL errors 2015 or 2030. For details on how to do this, see Chapter 4 on page 111.
- Reset the number of allowable errors (2099) during ESSL installation or using ERRSET in your program. This is not recommended for input-argument errors.

**Note:** For many of the ESSL subroutines requiring auxiliary storage, you can avoid program termination due to error 2015 by allowing ESSL to dynamically allocate auxiliary storage for you. You do this by setting naux = 0 and making error 2015 unrecoverable. For details on which aux arguments allow dynamic allocation and how to specify them, see the subroutine descriptions in Part 2 of this book.

The name of the ESSL subroutine detecting the error is listed as part of the message. The argument number(s) involved in the error appears in the message text. See "Input-Argument Error Messages" on page 179 for a complete description of the information contained in each message and for an indication of which messages correspond to optionally-recoverable errors. Regardless of whether the name in the message is a user-callable ESSL subroutine or an internal ESSL routine, the message-text and its unique parts apply to the user-callable ESSL subroutine. Return code values are described under "Error Conditions" for each ESSL subroutine in Part 2 of this book.

You may get more than one error message, because most of the arguments are checked by ESSL for possible errors during each call to the subroutine. The ESSL subroutine returns as many messages as there are errors detected. As a result, fewer runs are necessary to diagnose your program.

Fix the error(s), recompile, relink, and rerun your program.

### **ESSL Computational Error Messages**

If you receive an error message in the form 2538-21*nn*, you have a computational error in the ESSL subroutine. A computational error is any error occurring in the ESSL subroutine while using the computational data (that is, scalar and array data). The name of the ESSL subroutine detecting the error is listed as part of the message. Regardless of whether the name in the message is a user-callable ESSL subroutine or an internal ESSL routine, the message-text and its unique parts apply to the user-callable ESSL subroutine. A nonzero return code is returned when the ESSL subroutine encounters a computational error. See "Computational Error Messages" on page 187 for a complete description of the information in each message. Return code values are described under "Error Conditions" for each ESSL subroutine in Part 2 of this book.

Your program terminates for some computational errors unless you have called ERRSET to reset the number of allowable errors for that particular error, and the number has not been exceeded. A message is issued for each computational error. You should use the message to determine where the error occurred in your program.

If you called ERRSET and you have not reached the limit of errors you had set, you can check the return code. If it is not 0, you should call the EINFO subroutine to obtain information about the data involved in the error. EINFO provides the same information provided in the messages; however, it is provided to your program so your program can check the information during run time. Depending on what you want to do, you may choose to continue processing or terminate your program after the error occurs. For information on how to make these changes in your program to reset the number of allowable errors, how to diagnose the error, and how to decide whether to continue or terminate your program, see Chapter 4 on page 111.

If you are unable to solve the problem, report it and provide the following information, if available and appropriate:

- The message number and the module that detected an error
- The system dump, system error code, and system log of this job
- The compiler listings, including compiler options in effect, and any run-time listings produced
- Program changes made in comparison with a previous successful run
- A small test case demonstrating the problem using the minimum number of statements and variables, including input data
- A brief description of the problem

# **ESSL** Resource Error Messages

If you receive a message in the form 2538-24*nn*, it means that ESSL issued a resource error message.

A resource error occurs when a buffer storage allocation request fails in a ESSL subroutine. In general, the ESSL subroutines allocate internal auxiliary storage dynamically as needed. Without sufficient storage, the subroutine cannot complete the computation.

When a buffer storage allocation request fails, a resource error message is issued, and the application program is terminated. You need to reduce the memory constraint on the system or increase the amount of memory available before rerunning the application program.

The following ways may reduce memory constraints:

- Investigate the load of your process and run in a more dedicated environment.
- Increase your processor's paging space.
- Select a machine with more memory.
- Consider specifying the -bmaxdata binder option when linking your program. For details see the Fortran publications.
- Check the setting of your user ID's user limit (ulimit). (see the IBM AIX Version 4 Commands Reference).

### **ESSL Informational and Attention Messages**

If you receive a message in the form 2538-26*nn*, it means that ESSL issued an informational or attention message.

### **Informational Messages**

When you receive an informational message, check your application to determine why the condition was detected.

### **ESSL Attention Messages**

An attention message is issued to describe a condition that occurred. ESSL is able to continue processing, but performance may be degraded.

One condition that may produce an attention message is when enough work area was available to continue processing, but was not the amount initially requested. ESSL does not terminate your application program, but performance may be degraded. If you want to reduce the memory constraint on the system or increase the amount of memory available to eliminate the attention message, see the suggestions in "ESSL Resource Error Messages" on page 176. For a list of subroutines that may generate this type of attention message, see Table 31.

```
Table 31 (Page 1 of 2). ESSL Subroutines

Subroutine Names

Matrix-Vector Linear Algebra Subprograms:
   _GEMV, _GER, _SPMV, _SYMV, _SPR, _SYR, _SPR2, _SYR2
   _GERC, _GERU, _HPMV, _HEMV, _HPR, _HER, _HPR2, _HER2
   _SBMV, _TBMV, SGBMV, DGBMV, CGBMV
   _TPMV
   _TRMV

Matrix Operations:
   _GEMM, _GEMUL
   _SYMM, _SYR2K, _TRMM
   _HEMM, _HER2K
```

```
Table 31 (Page 2 of 2). ESSL Subroutines

Subroutine Names

Dense Linear Algebraic Equations:
   _POF, _POICD, _PPICD
   _GEICD, _TPI, _TRI
   _TRSM, _TPSV
   _TRSV

Banded Linear Algebraic Equations:
   STBSV, DTBSV

Linear Least Squares:
   _GESVS

Fourier Transforms:
   _CFT, _CFT3
   _RCFT, _RCFT3
   _CRFT, _CRFT3
```

### Miscellaneous Error Messages

If you receive a message in the form 2538-27*nn*, it means that ESSL issued a miscellaneous error message.

A miscellaneous error is an error that does not fall under any other categories.

When ESSL detects a miscellaneous error, you receive an error message with information on how to proceed and your application program is terminated.

## Messages

This section explains the conventions used for the ESSL messages and lists all the ESSL messages. For a description of each of the four types of ESSL messages, see "Dealing with Errors" on page 174.

## **Message Conventions**

This section describes the message conventions for the ESSL product.

### **About Upper- and Lowercase**

The literals, such as, 'N', 'T', 'U', and so forth, appear in the messages in this book in uppercase; however, they may be specified in your ESSL calling sequence in either upper- or lowercase, for example, 'n', 't', and 'u'.

### Message Format

The ESSL messages are issued in your output in the following format:

```
rtn-name : 2538-mmnn
message-text
```

Figure 10. Message Format

The parts of the ESSL message are as follows:

rtn-name gives the name of the ESSL subroutine that encountered the

error.

is the ESSL component identification number.

*mm* indicates the type of ESSL error message:

20—Input-argument error message 21—Computational error message 24—Resource error message

26—Information and attention message 27—Miscellaneous error message

*nn* is the message identification number.

message-text describes the nature of the error. Where one of several possible message-texts can be issued for a particular ESSL error, they are listed in this book with an "or" between them. The possible unique

parts are:

 The argument number of each argument involved in the error is included in the message description as (ARG NO. \_ )

 Additional information about the error is included in the message. The placement of this information is shown in the messages as (\_)

## **Input-Argument Error Messages**

RTN NAME: 2538-2001

The number of elements (ARG NO. \_) in a vector must be greater than or equal to zero.

RTN NAME: 2538-2002

The stride (ARG NO. ) for a vector must be nonzero.

RTN NAME : 2538-2003

The number of rows (ARG NO.  $\_$ ) in a matrix must be greater than or equal to zero.

RTN NAME: 2538-2004

The number of columns (ARG NO.  $\_$ ) in a matrix must be greater than or equal to zero.

RTN\_NAME : 2538-2005

The size of the leading dimension (ARG NO. \_) of an array must be greater than zero.

RTN NAME: 2538-2006

The number of rows (ARG NO. \_) of a matrix must be less than or equal to the size of the leading dimension (ARG NO. \_) of its array.

RTN NAME: 2538-2007

The degree of a polynomial (ARG NO. \_) must be greater than or equal to zero.

RTN NAME: 2538-2008

The number of elements (ARG NO.  $\_$ ) to be scanned must be greater than or equal to 2.

```
RTN NAME: 2538-2009
The number of elements (ARG NO. _) in a vector to be processed must be
greater than or equal to 3.
RTN NAME : 2538-2010
The transform length (ARG NO. ) must be a power of 2.
RTN NAME : 2538-2011
The number of points used in the interpolation (ARG NO. ) must be
greater than or equal to zero and less than or equal to \overline{\mbox{the number of data}}
points (ARG NO. ).
RTN NAME: 2538-2012
The transform length (ARG NO. ) must be less than or equal to ( ).
RTN NAME: 2538-2013
The transform length (ARG NO. ) must be greater than or equal to ( ).
RTN NAME: 2538-2014
The routine must be initialized with the present value of (ARG NO. _).
RTN NAME: 2538-2015
The number of elements (ARG NO. ) in a work array must be greater than
or equal to ().
RTN NAME: 2538-2016
The form (ARG NO. ) of a matrix must be 'N' or 'T'.
The form (ARG NO. ) of a matrix must be 'N', 'T', or 'C'.
The form (ARG NO. _) of a matrix must be 'N' or 'C'.
RTN NAME: 2538-2017
The dimension (ARG NO. ) of the matrices must be greater than or equal to zero.
RTN NAME : 2538-2018
The matrix form is specified by (ARG NO. ); therefore, the leading
dimension (ARG NO. ) of its array must be greater than or equal to the
number of its rows (ARG NO. ).
RTN NAME : 2538-2019
The number of sequences (ARG NO. ) must be greater than zero.
RTN NAME: 2538-2020
(ARG NO. ) must be nonzero.
RTN NAME : 2538-2021
The storage control switch (ARG NO. _) must be 1, 2, 3, or 4.
RTN NAME : 2538-2022
(ARG NO. _) must be less than (_).
RTN NAME: 2538-2023
The outer loop increment (ARG NO. ) must be greater than or equal to zero.
RTN NAME : 2538-2024
The stride (ARG NO. _) for a vector must be greater than or equal to zero.
```

```
RTN NAME: 2538-2025
The stride (ARG NO. _) for a vector must be greater than zero.
RTN NAME: 2538-2026
The stride (ARG NO. _) for a vector must be greater than or equal to (_).
RTN NAME: 2538-2027
The order (ARG NO. ) of a matrix must be greater than or equal to zero.
RTN NAME : 2538-2028
The job option argument (ARG NO. ) must be 0, 1, or 2.
The job option argument (ARG NO. \_) must be 0, 1, 2, or 3.
The job option argument (ARG NO. \_) must be 0, 1, 2, 10, 11, or 12.
The job option argument (ARG NO. ) must be 0, 1, 10, or 11.
The job option argument (ARG NO. ) must be 0, 1, 20, or 21.
The job option argument (ARG NO. ) must be 0, 1, 10, 11, 20, 21, 30,
or 31.
   or
The job option argument (ARG NO. _) must be 0, 1, 2, 3, or 4.
RTN NAME: 2538-2029
The job option argument (ARG NO. \_) must be 0 or 1.
RTN_NAME : 2538-2030
The transform length (ARG NO. ) is not an allowed value. The next higher
allowed value is (_).
RTN NAME: 2538-2031
The resulting convolution length obtained from ARG NO. 10 = (),
ARG NO.11 = (), ARG NO.13 = (), and ARG NO.14 = ()
must be less than ().
RTN NAME : 2538-2032
The size of the leading dimension (ARG NO. ) of the matrix must be greater
than or equal to (_), the bandwidth constraint.
RTN NAME: 2538-2033
The lower bandwidth (ARG NO. ) must be greater than or equal to zero.
RTN NAME: 2538-2034
The upper bandwidth (ARG NO. _) must be greater than or equal to zero.
RTN NAME : 2538-2035
The half-band bandwidth (ARG NO. _) must be greater than or equal to zero.
RTN NAME: 2538-2036
The lower bandwidth (ARG NO. ) must be less than the order (ARG NO. )
of the matrix.
RTN NAME : 2538-2037
The upper bandwidth (ARG NO. ) must be less than the order (ARG NO. )
of the matrix.
```

```
RTN NAME: 2538-2038
The half-band bandwidth (ARG NO. ) must be less than the order (ARG NO. )
of the matrix.
RTN NAME: 2538-2039
(ARG NO. ) must be greater than zero.
RTN NAME : 2538-2040
Insufficient storage allocated for positive definite solve.
() additional bytes required.
RTN NAME : 2538-2041
The resulting correlation length obtained from ARG NO. 8 = () and
ARG NO. 10 = () must be less than ().
RTN NAME: 2538-2042
(ARG NO. ) must be greater than or equal to zero.
RTN NAME: 2538-2043
(ARG NO. _) must be greater than (_).
RTN NAME: 2538-2044
The number of initialized coefficients (ARG NO. ) cannot exceed the size
of the coefficient vector (ARG NO. _).
RTN NAME: 2538-2045
The order specified (ARG NO. _) is not supported for this quadrature method.
The nearest supported order is ( ).
RTN NAME: 2538-2046
The scaling parameter (ARG NO. ) must be greater than zero for this
quadrature method.
RTN NAME: 2538-2047
The scaling parameter (ARG NO. ) must be nonzero for this quadrature
method.
RTN_NAME : 2538-2048
The sum of (ARG NO. ) and (ARG NO. ) must be nonzero for this quadrature
method.
RTN NAME: 2538-2049
The number of data points (ARG NO. ) must be greater than one in order
to perform numerical quadrature.
RTN NAME: 2538-2050
The number of columns specified for the arrays to store the matrix in
compressed matrix mode (ARG NO. _) must be greater than or equal to (_).
RTN NAME : 2538-2051
The number of columns (ARG NO. ) specified for the matrix used to store
the sparse matrix in compressed mode must be greater than zero.
RTN NAME: 2538-2052
The total number of non-zero elements of the input sparse matrix stored by
rows, obtained from element (_) of the row pointers array (ARG NO. _),
must be greater than or equal to zero.
```

```
The number of non-zero elements in row ( ) obtained from the row pointer
array (ARG NO. ) is less than zero.
RTN NAME: 2538-2054
The number of diagonals (ARG NO. _) specified for the matrix used to store the
sparse matrix in compressed diagonal mode must be greater than zero.
RTN NAME: 2538-2055
Element ( ) of the vector used to store the diagonal numbers (ARG NO. )
is incompatible with the order of the sparse matrix (ARG NO. ).
RTN NAME: 2538-2056
The matrix is singular because the number of non-zero entries (ARG NO. )
is zero.
RTN NAME: 2538-2057
Element ( ) in the integer parameter vector (ARG NO. ) must be greater than
or equal to zero.
RTN NAME: 2538-2058
Element () in the integer parameter vector (ARG NO. ) must be (),(), or ().
RTN NAME: 2538-2059
Element (_) in the real parameter vector (ARG NO. ) must be greater than zero.
RTN_NAME : 2538-2060
The size of the leading dimension (ARG NO. ) of an array must be greater
than or equal to the maximum of (ARG NO. _) and (ARG NO. _).
RTN_NAME : 2538-2061
Parameter (ARG NO. _), which specifies the number of columns of the input
sparse matrix (ARG NO. _ and ARG NO. _) must be greater than or equal to (_).
RTN NAME: 2538-2062
The number of random numbers generated (ARG NO. ) must be even and
greater than or equal to zero.
RTN NAME : 2538-2063
SIDE (ARG NO. ), which specifies whether the triangular input matrix
(ARG NO. _) appears on the left or right of the other input matrix, must
be 'L' or 'R'.
RTN NAME: 2538-2064
UPLO (ARG NO. ), which specifies whether an input matrix (ARG NO. )
is upper or lower triangular, must be 'U' or 'L'.
RTN NAME : 2538-2065
DIAG (ARG NO. _), which specifies whether an input matrix (ARG NO. _)
is unit triangular, must be 'U' or 'N'.
RTN NAME: 2538-2066
Given the value which has been assigned to SIDE (ARG NO. ), the leading
dimension (ARG NO. ) for the triangular input matrix must be greater
than or equal to (ARG NO. _).
```

RTN NAME : 2538-2053

```
RTN NAME: 2538-2067
TRANSA (ARG NO. _) specifies whether an input matrix (ARG NO. _), its transpose,
or its conjugate transpose should be used. TRANSA must be 'N', 'T', or 'C'.
RTN NAME: 2538-2068
The size of the leading dimension (ARG NO. ) of an array must be greater
than or equal to zero.
RTN NAME: 2538-2069
The vector section size of the scalar library (ARG NO. ) must be 128 or 256.
RTN NAME: 2538-2070
Element (\_) in (ARG NO. \_) must be 0 or 1.
Element ( ) in (ARG NO. ) must be greater than zero.
Element ( ) in (ARG NO. ) must be greater than or equal to zero.
Element ( ) in (ARG NO. ) must be greater than or equal to zero and
less than or equal to 1.
Element (_) in (ARG NO. _) must be greater than the preceding element.
Element (_) in (ARG NO. _) must be greater than or equal to 1 and
less than or equal to n.
  or
Element ( ) in (ARG NO. ) must be -1 or 1.
Element (_) in (ARG NO. _) must be nonzero.
Element (_) in (ARG NO. _) must be 0, 1, 2, 10, or 11.
Element (_) in (ARG NO. _) must be 0, 1, 2, 10, 11, 100, 102, or 110.
Element ( ) in (ARG NO. ) must be 0.
Element ( ) in (ARG NO. ) must be 1.
Element ( ) in (ARG NO. ) must be 0, 1, 2, 10, 11, 100, 101, 102,
110, or 111.
  or
Element ( ) in (ARG NO. ) must be 1, 2, 3, or 4.
Element (_) in (ARG NO. _) must be 1, 2, 3, 4, or 5.
RTN NAME : 2538-2071
The number of eigenvalues (ARG NO. ) must be less than or equal to the
order of the matrix (ARG NO. ).
RTN NAME: 2538-2072
The work area (ARG NO. ) does not contain a valid vector seed. The
routine must be called with a nonzero value of ISEED (ARG NO. ).
RTN NAME: 2538-2073
(ARG NO. _) must be a double precision whole number greater than or equal
to 1.0 and less than 2147483647.0.
```

```
RTN NAME: 2538-2074
Performance can be improved by using a larger work array. For best performance,
specify the number of elements (ARG NO. ) in the work array to be greater
than or equal to ( ).
RTN NAME : 2538-2075
The data type parameter (ARG NO. _) must be 'S', 'D', 'C', or 'Z'.
RTN NAME: 2538-2076
(ARG NO. ) must be greater than or equal to ( ) and smaller than ( ).
RTN NAME: 2538-2077
The matrix is singular. Column (_) is empty in the matrix specified by
(ARG NO. ), (ARG NO. ), and (ARG NO. ).
RTN NAME: 2538-2078
The matrix is singular. Row ( ) is empty in the matrix specified by
(ARG NO. ), (ARG NO. ), and (ARG NO. ).
RTN NAME: 2538-2079
The matrix, specified by (ARG NO. _), (ARG NO. _), and (ARG NO. _),
contains at least one duplicate column index in row (_).
RTN NAME: 2538-2080
Element ( ) in (ARG NO. ) must be greater than or equal to ( )
and less than or equal to ().
Element ( ) in (ARG NO. ) must be greater than or equal to ( ) and
less than or equal to (ARG NO. _).
Element (_) in (ARG NO. _) must be greater than or equal to element (_)
and less than or equal to ().
Element ( ) in (ARG NO. ) must be zero or must be greater than or
equal to ().
RTN NAME: 2538-2081
Element (_) in (ARG NO. _) must be less than or equal to (_).
RTN NAME: 2538-2082
Element (_) in (ARG NO. _) may cause incorrect or misleading results.
A nonzero number with absolute value less than or equal to 1 is recommended.
Element ( ) in (ARG NO. ) may cause incorrect or misleading results.
A positive number less than or equal to 1 is recommended.
RTN NAME : 2538-2083
The pivot tolerance (element (_) in (ARG NO. _)) may cause incorrect
or misleading results. A number greater than or equal to 0 and less than or
equal to 1 is recommended.
RTN NAME: 2538-2084
The dimension (ARG NO. _) of the array (ARG NO. _) must be greater than or
equal to ().
RTN NAME : 2538-2085
The number of steps after which the generalized minimum residual method is
restarted, element ( ) in (ARG NO. ), must be greater than 0.
```

```
RTN NAME: 2538-2086
The acceleration parameter, element ( ) in (ARG NO. ), must be greater than \theta
when using the SSOR preconditioner.
RTN NAME: 2538-2087
STOR (ARG NO. _), which specifies the storage variation used to represent
the input sparse matrix, must be 'G', 'L', or 'U'.
RTN NAME: 2538-2088
INIT (ARG NO. _), which specifies the type of computation to be performed,
must be 'I', or 'S'.
RTN NAME: 2538-2089
Element (_) in (ARG NO. _) must be greater than or equal to (_).
Element ( ) in (ARG NO. ) must be greater than or equal to element ( ).
RTN NAME : 2538-2090
For level (), the number of grid points for dimension () must be
an odd number greater than 1.
RTN NAME: 2538-2091
Since the mesh spacing (ARG NO. _) here is not constant, the second order
prolongation method must be used. That is, element ( ) of (ARG NO. )
must be ().
RTN NAME: 2538-2092
The index into (ARG NO. _) is out of range.
This index is element (\_,\_) of (ARG NO. \_).
RTN NAME : 2538-2093
The index into (ARG NO. _) is out of range.
This index is element ( , , ) of (ARG NO. ).
RTN NAME: 2538-2094
For dimension (_) on level (_), the mesh spacing must be changed to
a positive value.
RTN NAME : 2538-2095
Excess space in (ARG NO. _) has been decreased and may be inadequate.
To avoid this, specify the coarse level matrix as the final item in this
argument.
RTN NAME: 2538-2096
For level (_), the matrix type, solver, and preconditioner are incompatible.
RTN NAME : 2538-2097
The solver requested for level ( ) requires a square matrix.
Elements (\_,\_,\_) and (\_,\_,\_) in (ARG NO. \_) must be equal.
RTN NAME: 2538-2098
Element (_,_) of (ARG NO. _) must be greater than or equal to (_).
RTN NAME : 2538-2099
End of input argument error reporting. For more information, refer to
Engineering and Scientific Subroutine Library Guide and Reference (SA22-7272).
```

### **Computational Error Messages**

RTN NAME : 2538-2100 The computed index of a vector is out of the range ( ) to ( ). RTN NAME : 2538-2101 Eigenvalue (\_) failed to converge after (\_) iterations. RTN NAME: 2538-2102 Eigenvector ( ) failed to converge after ( ) iterations. RTN NAME : 2538-2103 The matrix (ARG NO. \_) is singular. Zero diagonal element ( ) has been detected. RTN NAME : 2538-2104 The matrix (ARG NO. \_) is not positive definite. The last diagonal element with nonpositive value is (). RTN NAME: 2538-2105 Factorization failed due to near zero pivot number ( ). RTN NAME : 2538-2106 Vector boundary misalignment detected in ESSL scalar library. RTN NAME: 2538-2107 Singular value (\_) failed to converge after (\_) iterations. RTN NAME: 2538-2108 The matrix specified by (ARG NO. \_) and (ARG NO. \_) is not definite because the diagonal is not of constant sign. RTN NAME: 2538-2109 The matrix specified by (ARG NO. ) and (ARG NO. ) is not definite and the iterative process is stopped at iteration number (). RTN NAME : 2538-2110 The maximum allowed number of iterations, element number ( ) of (ARG NO. ), were performed but the iterative process did not converge to a solution according to the stopping procedure. RTN NAME : 2538-2111 The factorization matrix (ARG NO. ) is not consistent with the sparse matrix specified by (ARG NO. \_) and (ARG NO. \_). RTN NAME : 2538-2112 The incomplete factorization of the sparse matrix specified by (ARG NO. ) and (ARG NO. ) is not stable. RTN NAME : 2538-2113 Unexpected nonzero vector mask detected in ESSL scalar routine. Contact your IBM Service Representative. RTN NAME: 2538-2114 Eigenvalue (\_) failed to converge after (\_) iterations.

```
RTN NAME: 2538-2115
The matrix (ARG NO. _) is not positive definite.
The leading minor of order ( ) has a nonpositive determinant.
RTN NAME: 2538-2116
The matrix specified by (ARG NO. ) and (ARG NO. ) is singular.
RTN NAME : 2538-2117
The pivot element in column ( ) is smaller than the first element in
(ARG NO. ).
RTN NAME: 2538-2118
The pivot element in row (_) is smaller than the first element in
(ARG NO. ).
RTN NAME: 2538-2119
The storage space, specified by (ARG NO. ), is insufficient.
RTN NAME : 2538-2120
The matrix is singular. The last row processed in the matrix was row ( ).
RTN NAME : 2538-2121
The matrix is singular. the last column processed was column ( ).
RTN NAME : 2538-2122
The factorization failed. No pivot element was found in the active submatrix.
RTN NAME : 2538-2123
Performance can be improved by specifying a larger value for (ARG NO. _).
( ) compressions were performed.
RTN NAME : 2538-2124
The data contained in AUX1, (ARG NO. _), was computed for a different
algorithm.
RTN NAME : 2538-2125
This subroutine initializes part of the ESSL run-time environment. It may
be called only once, at the beginning of the run. It must be called before
any ESSL computational routines are called.
RTN NAME : 2538-2126
The pivot value at row (_) is not acceptable based on pivot criteria
((ARG NO. ) and (ARG NO. )). No fixup was applicable to this pivot.
The matrix (ARG NO. _) may be singular or not definite.
RTN NAME : 2538-2127
The pivot value at row ( ) was replaced with element ( ) in
(ARG NO. _). The matrix (ARG NO. _) may be singular or not definite.
RTN NAME : 2538-2128
Internal ESSL error. contact your IBM service representative.
RTN NAME: 2538-2129
The matrix specified by (ARG NO. _), (ARG NO. _), and (ARG NO. _)
is not definite because the diagonal is not of constant sign or some diagonal
element is zero.
```

RTN NAME : 2538-2130

The incomplete factorization of the sparse matrix specified by (ARG NO. \_), (ARG NO. ), and (ARG NO. ) is not stable.

RTN NAME : 2538-2131

The matrix specified by (ARG NO. \_), (ARG NO. \_), and (ARG NO. \_) is singular.

RTN NAME : 2538-2132

Element (\_) in (ARG NO. \_) indicates that factorization was done on a previous call. The data passed is not the result of a prior valid factorization.

RTN NAME: 2538-2133

An error occurred on level (\_), in the user-supplied subroutine specified by (ARG NO. ).

RTN NAME: 2538-2134

The data contained in (ARG NO.  $\_$ ) is not consistent with the sparse matrix specified by (ARG NO. ), (ARG NO. ), and (ARG NO. ).

RTN NAME : 2538-2135

For level (\_), loss of orthogonality occurred in a minimum residual solver because the input matrix (element (\_,\_) of (ARG NO. \_)) is inappropriate. Choose one of the other non-symmetric solvers.

RTN NAME : 2538-2136

For level (), the main diagonal element for row () of a matrix is 0.

RTN NAME : 2538-2137

This subroutine may be called only once in the beginning of the program.

RTN\_NAME : 2538-2138

An error was detected while attempting to open the ESSLPARM file. A default ESSL processor family number of (\_) will be assumed. This may not be the best choice for optimal performance. Be sure that you have defined the interface to ESSLPARM correctly for the run. If you have, contact ESSL system installation personnel.

RTN NAME : 2538-2139

An error was detected while attempting to close the ESSLPARM file. An ESSL processor family number of  $(\_)$  was assigned.

RTN NAME: 2538-2140

An input/output error was detected while attempting to read line (\_) of the ESSLPARM file. A default ESSL process or family number of (\_) will be assumed. This may not be the best choice for optimal performance. Be sure that you have defined the interface to ESSLPARM correctly for the run. If you have, contact ESSL system installation personnel.

RTN\_NAME : 2538-2141

The end of file marker on line (\_) of the ESSLPARM file was reached before a valid specification for the ESSL processor family number was read. A default ESSL processor family number of (\_) will be assumed. This may not be the best choice for optimal performance. Be sure that you have defined the interface to ESSLPARM correctly for the run. If you have, contact ESSL system installation personnel.

RTN NAME : 2538-2142

A syntax error was detected on line (\_), column (\_), of the ESSLPARM

file. No valid specification for the ESSL processor family number was read. A default ESSL processor family number of (\_) will be assumed. This may not be the best choice for optimal performance. Contact ESSL system installation personnel.

RTN NAME : 2538-2143

The processor family number (\_) on line (\_) of the ESSLPARM file is not in the allowable range. Please specify a processor family number greater than or equal to (\_) and less than or equal to (\_). A default ESSL processor family number of ( ) will be assumed. This may not be the best choice for optimal performance. Contact ESSL system installation personnel.

RTN NAME: 2538-2144

This subroutine must be called before any computational ESSL routines are called.

RTN NAME : 2538-2145

The input matrix (ARG NO. ) is singular. The first diagonal element found to be exactly 0, was in column ().

RTN NAME: 2538-2146

The input matrix (ARG NO. \_) is singular. The first diagonal element found to be exactly 0, was in column ().

RTN NAME : 2538-2199

End of computational error reporting. For more information, refer to Engineering and Scientific Subroutine Library Guide and Reference (SA22-7272).

## Resource Error Messages

RTN NAME: 2538-2400

An internal buffer allocation has failed due to insufficient memory.

## Informational and Attention Error Messages

RTN NAME : 2538-2600

Performance may be degraded due to limited buffer space availability.

RTN NAME : 2538-2601

Execution terminating due to error count for error number ( )

Message summary: Message number - Count

RTN NAME : 2538-2602

User error corrective routine entered.

User corrective action taken. Execution continuing.

RTN NAME : 2538-2603

Standard corrective action taken. Execution continuing.

RTN NAME : 2538-2604

Execution terminating due to error count for error number .

RTN NAME : 2538-2605

Message summary:

RTN NAME : 2538-2606

Serial execution is taking place since the input array is equal

to the output array and either:

```
INC2X (ARG NO. _) is not equal to 2 times INC2Y (ARG NO. _) or INC3X (ARG NO. _) is not equal to 2 times INC3Y (ARG NO. _).

RTN_NAME : 2538-2607

Serial execution is taking place since the input array is equal to the output array and either:

INC2X (ARG NO. _) is not equal to INC2Y (ARG NO. _) or INC3X (ARG NO. _) is not equal to INC3Y (ARG NO. _).

RTN_NAME : 2538-2608

Performance may be improved by using a larger work array. For best performance, specify the number of elements (ARG NO. _) in the work array to be greater than or equal to (_).

RTN_NAME : 2538-2609

Performance may be improved by specifying a larger value for (ARG NO. _).

(_) compressions were performed.
```

## Miscellaneous Error Messages

RTN\_NAME : 2538-2700

Internal ESSL error number (\_).

Contact your IBM service representative.

RTN\_NAME : 2538-2703

Internal ESSL error: message number requested (\_) is outside of the valid range. Contact your IBM service representative.

## Part 2. Reference Information

This part of the book is organized into ten areas, providing reference information for coding the ESSL calling sequences. It is organized as follows:

- Linear Algebra Subprograms
- Matrix Operations
- Linear Algebraic Equations
- Eigensystem Analysis
- Fourier Transforms, Convolutions and Correlations, and Related Computations
- Sorting and Searching
- Interpolation
- Numerical Quadrature
- Random Number Generation
- Utilities

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## **Chapter 8. Linear Algebra Subprograms**

The linear algebra subprograms, provided in four areas, are described in this chapter.

## **Overview of the Linear Algebra Subprograms**

This section describes the subprograms in each of the four linear algebra subprogram areas:

- Vector-scalar linear algebra subprograms (Table 32)
- Sparse vector-scalar linear algebra subprograms (Table 33)
- Matrix-vector linear algebra subprograms (Table 34)
- Sparse matrix-vector linear algebra subprograms (Table 35)

#### Notes:

- The term subprograms is used to be consistent with the Basic Linear Algebra Subprograms (BLAS), because many of these subprograms correspond to the BLAS.
- 2. Some of the linear algebra subprograms were designed in accordance with the Level 1 and Level 2 BLAS de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program.

## Vector-Scalar Linear Algebra Subprograms

The vector-scalar linear algebra subprograms include a subset of the standard set of Level 1 BLAS. For details on the BLAS, see reference [73]. The remainder of the vector-scalar linear algebra subprograms are commonly used computations provided for your applications. Both real and complex versions of the subprograms are provided.

Table 32 (Page 1 of 2). List of Vector-Scalar Linear Algebra Subprograms			
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX†■ ICAMAX†■	IDAMAX†■ IZAMAX†■	201
Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value	ISAMIN†	IDAMIN†	204
Position of the First or Last Occurrence of the Vector Element Having Maximum Value	ISMAX†	IDMAX†	207
Position of the First or Last Occurrence of the Vector Element Having Minimum Value	ISMIN†	IDMIN†	210
Sum of the Magnitudes of the Elements in a Vector	SASUM†• SCASUM†•	DASUM†• DZASUM†•	213
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY CAXPY	DAXPY• ZAXPY•	216

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Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Copy a Vector	SCOPY*	DCOPY ZCOPY	219
Dot Product of Two Vectors	SDOT† CDOTU† CDOTC†	DDOT† ZDOTU† ZDOTC†	222
Compute SAXPY or DAXPY N Times	SNAXPY	DNAXPY	226
Compute Special Dot Products N Times	SNDOT	DNDOT	231
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2† SCNRM2†	DNRM2†  DZNRM2†	236
Euclidean Length of a Vector with No Scaling of Input	SNORM2† CNORM2†	DNORM2† ZNORM2†	239
Construct a Givens Plane Rotation	SROTG* CROTG*	DROTG* ZROTG*	242
Apply a Plane Rotation	SROT* CROT* CSROT*	DROT• ZROT• ZDROT•	249
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL* CSCAL* CSSCAL*	DSCAL* ZSCAL* ZDSCAL*	253
Interchange the Elements of Two Vectors	SSWAP• CSWAP•	DSWAP■ ZSWAP■	256
Add a Vector X to a Vector Y and Store in a Vector Z	SVEA CVEA	DVEA ZVEA	259
Subtract a Vector Y from a Vector X and Store in a Vector Z	SVES CVES	DVES ZVES	263
Multiply a Vector X by a Vector Y and Store in a Vector Z	SVEM CVEM	DVEM ZVEM	267
Multiply a Vector X by a Scalar and Store in a Vector Y	SYAX CYAX CSYAX	DYAX ZYAX ZDYAX	271
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z	SZAXPY CZAXPY	DZAXPY ZZAXPY	274

<sup>†</sup> This subprogram is invoked as a function in a Fortran program.

## **Sparse Vector-Scalar Linear Algebra Subprograms**

The sparse vector-scalar linear algebra subprograms operate on sparse vectors using optimized storage techniques; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the vector-scalar subprograms. These subprograms represent a subset of the sparse extensions to the Level 1 BLAS described in reference [29]. Both real and complex versions of the subprograms are provided.

<sup>■</sup> Level 1 BLAS

Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode	SSCTR CSCTR	DSCTR ZSCTR	279
Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode	SGTHR CGTHR	DGTHR ZGTHR	282
Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y	SGTHRZ CGTHRZ	DGTHRZ ZGTHRZ	285
Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y	SAXPYI CAXPYI	DAXPYI ZAXPYI	288
Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode	SDOTI† CDOTCI† CDOTUI†	DDOTI† ZDOTCI† ZDOTUI†	291

## **Matrix-Vector Linear Algebra Subprograms**

The matrix-vector linear algebra subprograms operate on a higher-level data structure—matrix-vector rather than vector-scalar—using optimized algorithms to improve performance. These subprograms represent a subset of the Level 2 BLAS described in references [34] and [35]. Both real and complex versions of the subprograms are provided.

Table 34 (Page 1 of 2). List of Matrix-Vector Linear Algebra Subprograms			
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV CGEMV SGEMX SGEMTX	DGEMV ZGEMV DGEMX DGEMTX	296
Rank-One Update of a General Matrix	SGER CGERUCCGERC	DGER ZGERU ZGERC	307
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV CHPMV SSYMV CHEMV SSLMX§	DSPMV4 ZHPMV4 DSYMV4 ZHEMV4 DSLMX§	315
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR CHPR SSYR CHER SSLR18	DSPR ZHPR DSYR ZHER DSLR1	323

Table 34 (Page 2 of 2). List of Matrix-Vector Linear Algebra Subpr  Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	Page
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR24 CHPR24 SSYR24 CHER24 SSLR2§	DSPR24 ZHPR24 DSYR24 ZHER24 DSLR28	331
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV◀ CGBMV◀	DGBMV◀ ZGBMV◀	340
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV⁴ CHBMV⁴	DSBMV⁴ ZHBMV⁴	347
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STRMV CTRMV STPMV CTPMV	DTRMV• ZTRMV• DTPMV• ZTPMV•	352
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV◀ CTBMV◀	DTBMV◀ ZTBMV◀	358

<sup>◆</sup> Level 2 BLAS

## **Sparse Matrix-Vector Linear Algebra Subprograms**

The sparse matrix-vector linear algebra subprograms operate on sparse matrices using optimized storage techniques; that is, only the nonzero elements of the vector are stored. These subprograms provide similar functions to the matrix-vector subprograms.

Table 35. List of Sparse Matrix-Vector Linear Algebra Subprograms		
Descriptive Name	Long- Precision Subprogram	Page
Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode	DSMMX	365
Transpose a Sparse Matrix in Compressed-Matrix Storage Mode	DSMTM	368
Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode	DSDMX	372

#### **Use Considerations**

If your program uses a sparse matrix stored by rows, as defined in "Storage-by-Rows" on page 99, you should first convert your sparse matrix to compressed-matrix storage mode by using the subroutine DSRSM on page 979. DSRSM converts a matrix to compressed-matrix storage mode. To convert your sparse matrix to compressed-diagonal storage mode, you need to perform this conversion in your application program before calling the ESSL subroutine.

<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.

## **Performance and Accuracy Considerations**

- 1. In ESSL, the SSCAL and DSCAL subroutines provide the fastest way to zero out contiguous (stride 1) arrays, by specifying incx = 1 and  $\alpha = 0$ .
- Where possible, use the matrix-vector linear algebra subprograms, rather than the vector-scalar, to optimize performance. Because data is presented in matrices rather than vectors, multiple operations can be performed by a single ESSL subprogram.
- 3. Where possible, use subprograms that do multiple computations, such as SNDOT and SNAXPY, rather than individual computations, such as SDOT and SAXPY. You get better performance.
- Many of the short-precision subprograms provide increased accuracy by accumulating results in long precision. This is noted in the functional description of each subprogram.
- 5. In some of the subprograms, because implementation techniques vary to optimize performance, accuracy of the results may vary for different array sizes. In the subprograms in which this occurs, a general description of the implementation techniques is given in the functional description for each subprogram.
- 6. To select the sparse matrix subroutine that gives you the best performance, you must consider the layout of the data in your matrix. From this, you can determine the most efficient storage mode for your sparse matrix. ESSL provides two versions of each of its sparse matrix-vector subroutines that you can use. One operates on sparse matrices stored in compressed-matrix storage mode, and the other operates on sparse matrices stored in compressed-diagonal storage mode. These two storage modes are described in "Sparse Matrix" on page 92.
  - Compressed-matrix storage mode is generally applicable. It should be used when each row of the matrix contains approximately the same number of nonzero elements. However, if the matrix has a special form—that is, where the nonzero elements are concentrated along a few diagonals—compressed-diagonal storage mode gives improved performance.
- 7. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

## **Vector-Scalar Subprograms**

This section contains the vector-scalar subprogram descriptions.

# ISAMAX, IDAMAX, ICAMAX, and IZAMAX—Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude

ISAMAX and IDAMAX find the position *i* of the first or last occurrence of a vector element having the maximum absolute value. ICAMAX and IZAMAX find the position *i* of the first or last occurrence of a vector element having the largest sum of the absolute values of the real and imaginary parts of the vector elements.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $\mathbf{x}$ . Regardless of the stride, the position i is always relative to the location specified in the calling sequence for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ).

Table 36. Data Types	
x	Subprogram
Short-precision real	ISAMAX
Long-precision real	IDAMAX
Short-precision complex	ICAMAX
Long-precision complex	IZAMAX

#### Syntax

Fortran	ISAMAX   IDAMAX   ICAMAX   IZAMAX (n, x, incx)
C and C++	isamax   idamax   icamax   izamax (n, x, incx);
PL/I	ISAMAX   IDAMAX   ICAMAX   IZAMAX (n, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

X

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 36. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the position *i* of the element in the array, where:

If  $incx \ge 0$ , i is the position of the first occurrence.

If incx < 0, i is the position of the last occurrence.

Returned as: a fullword integer;  $0 \le i \le n$ .

**Note:** Declare the ISAMAX, IDAMAX, ICAMAX, and IZAMAX functions in your program as returning a fullword integer value.

**Function:** ISAMAX and IDAMAX find the first element  $x_k$ , where k is defined as the smallest index k, such that:

$$|x_k| = \max\{|x_j| \text{ for } j = 1, n\}$$

ICAMAX and IZAMAX find the first element  $x_k$ , where k is defined as the smallest index k, such that:

$$|a_k| + |b_k| = \max\{|a_j| + |b_j| \text{ for } j = 1, n\}$$
  
where  $x_k = (a_k, b_k)$ 

By specifying a positive or negative stride for vector  $\mathbf{x}$ , the first or last occurrence, respectively, is found in the array. The position i, returned as the value of the function, is always figured relative to the location specified in the calling sequence for vector **x** (in argument x). Therefore, depending on the stride specified for incx, i has the following values:

For 
$$incx \ge 0$$
,  $i = k$   
For  $incx < 0$ ,  $i = n-k+1$ 

See reference [73]. The result is returned as a function value. If n is 0, then 0 is returned as the value of the function.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

**Example 3:** This example shows a vector, **x**, with a stride of 0.

Function Reference and Input

$$\begin{bmatrix} N & X & INCX \\ | & | & | \\ IMAX = ISAMAX(9, X, 0) \end{bmatrix}$$
 $X = (1.0, ..., ..., ..., ..., ...)$ 
 $Output$ 
 $IMAX = 1$ 

**Example 4:** This example shows a vector,  $\mathbf{x}$ , with a negative stride. Processing begins at element X(15), which is 2.0.

Function Reference and Input

**Example 5:** This example shows a vector, **x**, containing complex numbers and having a stride of 1.

Function Reference and Input

= 2

IMAX

# ISAMIN and IDAMIN—Position of the First or Last Occurrence of the Vector Element Having Minimum Absolute Value

These subprograms find the position *i* of the first or last occurrence of a vector element having the minimum absolute value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $\mathbf{x}$ . Regardless of the stride, the position i is always relative to the location specified in the calling sequence for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ).

Table 37. Data Types	
x	Subprogram
Short-precision real	ISAMIN
Long-precision real	IDAMIN

#### Syntax

Fortran	ISAMIN   IDAMIN (n, x, incx)
C and C++	isamin   idamin (n, x, incx);
PL/I	ISAMIN   IDAMIN (n, x, incx);

#### On Entry

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

x is the vector x of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 37. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the position *i* of the element in the array, where:

If  $incx \ge 0$ , i is the position of the first occurrence.

If incx < 0, i is the position of the last occurrence.

Returned as: a fullword integer;  $0 \le i \le n$ .

**Note:** Declare the ISAMIN and IDAMIN functions in your program as returning a fullword integer value.

**Function:** These subprograms find the first element  $x_k$ , where k is defined as the smallest index k, such that:

$$|x_k| = \min\{|x_j| \text{ for } j = 1, n\}$$

By specifying a positive or negative stride for vector  $\mathbf{x}$ , the first or last occurrence, respectively, is found in the array. The position i, returned as the value of the

function, is always figured relative to the location specified in the calling sequence for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ). Therefore, depending on the stride specified for *incx*, i has the following values:

For 
$$incx \ge 0$$
,  $i = k$   
For  $incx < 0$ ,  $i = n-k+1$ 

See reference [73]. The result is returned as a function value. If n is 0, then 0 is returned as the value of the function.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with a positive stride and two elements with the minimum absolute value. The position of the first occurrence is returned.

**Example 4:** This example shows a vector, **x**, with a negative stride and two elements with the minimum absolute value. The position of the last occurrence is returned. Processing begins at element X(7), which is 1.0.

## ISMAX and IDMAX—Position of the First or Last Occurrence of the Vector Element Having the Maximum Value

These subprograms find the position *i* of the first or last occurrence of a vector element having the maximum value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $\mathbf{x}$ . Regardless of the stride, the position i is always relative to the location specified in the calling sequence for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ).

Table 38. Data Types	
x	Subprogram
Short-precision real	ISMAX
Long-precision real	IDMAX

#### Syntax

Fortran	ISMAX   IDMAX (n, x, incx)
C and C++	ismax   idmax (n, x, incx);
PL/I	ISMAX   IDMAX (n, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length  $1+(n-1)|inc\mathbf{x}|$ , containing numbers of the data type indicated in Table 38.

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the position *i* of the element in the array, where:

If  $incx \ge 0$ , i is the position of the first occurrence.

If incx < 0, i is the position of the last occurrence.

Returned as: a fullword integer;  $0 \le i \le n$ .

**Note:** Declare the ISMAX and IDMAX functions in your program as returning a fullword integer value.

**Function:** These subprograms find the first element  $x_k$ , where k is defined as the smallest index k, such that:

$$x_k = \max\{x_i \text{ for } j = 1, n\}$$

By specifying a positive or negative stride for vector  $\mathbf{x}$ , the first or last occurrence, respectively, is found in the array. The position i, returned as the value of the function, is always figured relative to the location specified in the calling sequence

for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ). Therefore, depending on the stride specified for incx, i has the following values:

For 
$$incx \ge 0$$
,  $i = k$   
For  $incx < 0$ ,  $i = n-k+1$ 

See reference [73]. The result is returned as a function value. If n is 0, then 0 is returned as the value of the function.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

IMAX

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with a positive stride and two elements with the maximum value. The position of the first occurrence is returned.

**Example 4:** This example shows a vector,  $\mathbf{x}$ , with a negative stride and two elements with the maximum value. The position of the last occurrence is returned. Processing begins at element X(7), which is 1.0.

## ISMIN and IDMIN—Position of the First or Last Occurrence of the Vector Element Having Minimum Value

These subprograms find the position *i* of the first or last occurrence of a vector element having the minimum value.

You get the position of the first or last occurrence of an element by specifying positive or negative stride, respectively, for vector  $\mathbf{x}$ . Regardless of the stride, the position i is always relative to the location specified in the calling sequence for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ).

Table 39. Data Types	
x	Subprogram
Short-precision real	ISMIN
Long-precision real	IDMIN

#### Syntax

Fortran	ISMIN   IDMIN (n, x, incx)
C and C++	ismin   idmin (n, x, incx);
PL/I	ISMIN   IDMIN (n, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length  $1+(n-1)|inc\mathbf{x}|$ , containing numbers of the data type indicated in Table 39.  $inc\mathbf{x}$ 

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the position *i* of the element in the array, where:

If  $incx \ge 0$ , i is the position of the first occurrence.

If incx < 0, i is the position of the last occurrence.

Returned as: a fullword integer;  $0 \le i \le n$ .

**Note:** Declare the ISMIN and IDMIN functions in your program as returning a fullword integer value.

**Function:** These subprograms find the first element  $x_k$ , where k is defined as the smallest index k, such that:

$$x_k = \min\{x_i \text{ for } j = 1, n\}$$

By specifying a positive or negative stride for vector  $\mathbf{x}$ , the first or last occurrence, respectively, is found in the array. The position i, returned as the value of the function, is always figured relative to the location specified in the calling sequence

for vector  $\mathbf{x}$  (in argument  $\mathbf{x}$ ). Therefore, depending on the stride specified for incx, i has the following values:

For 
$$incx \ge 0$$
,  $i = k$   
For  $incx < 0$ ,  $i = n-k+1$ 

See reference [73]. The result is returned as a function value. If n is 0, then 0 is returned as the value of the function.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with a positive stride and two elements with the minimum value. The position of the first occurrence is returned. Processing begins at element X(7), which is 1.0.

**Example 4:** This example shows a vector, **x**, with a negative stride and two elements with the minimum value. The position of the last occurrence is returned. Processing begins at element X(7), which is 1.0.

## SASUM, DASUM, SCASUM, and DZASUM—Sum of the Magnitudes of the Elements in a Vector

SASUM and DASUM compute the sum of the absolute values of the elements in vector  $\mathbf{x}$ . SCASUM and DZASUM compute the sum of the absolute values of the real and imaginary parts of the elements in vector  $\mathbf{x}$ .

Table 40. Data Types		
x	Result	Subprogram
Short-precision real	Short-precision real	SASUM
Long-precision real	Long-precision real	DASUM
Short-precision complex	Short-precision real	SCASUM
Long-precision complex	Long-precision real	DZASUM

#### Syntax

Fortran	SASUM   DASUM   SCASUM   DZASUM (n, x, incx)
C and C++	sasum   dasum   scasum   dzasum (n, x, incx);
PL/I	SASUM   DASUM   SCASUM   DZASUM (n, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

X

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 40. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the result of the summation. Returned as: a number of the data type indicated in Table 40.

**Note:** Declare this function in your program as returning a value of the type indicated in Table 40.

**Function:** SASUM and DASUM compute the sum of the absolute values of the elements of x, which is expressed as follows:

$$\sum_{i=1}^{n} |x_i| = |x_1| + |x_2| + \dots + |x_n|$$

SCASUM and DZASUM compute the sum of the absolute values of the real and imaginary parts of the elements of x, which is expressed as follows:

$$\sum_{i=1}^{n} (|a_i| + |b_i|) = (|a_1| + |b_1|) + (|a_2| + |b_2|) + \dots + (|a_n| + |b_n|)$$
where  $x_i = (a_i, b_i)$ 

See reference [73]. The result is returned as a function value. If n is 0, then 0.0 is returned as the value of the function. For SASUM and SCASUM, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with negative stride. Processing begins at element X(7), which is -4.0.

**Example 4:** This example shows a vector,  $\mathbf{x}$ , with a stride of 0. The result in SUMM is  $n\mathbf{x}_1$ .

Function Reference and Input

**Example 5:** This example shows a vector, **x**, containing complex numbers and having a stride of 1.

Function Reference and Input

Output

SUMM = 55.0

## SAXPY, DAXPY, CAXPY, and ZAXPY—Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $\textbf{\textit{x}}$  and  $\textbf{\textit{y}}$ :

$$y \leftarrow y + \alpha x$$

Table 41. Data Types	
alpha, <b>x</b> , <b>y</b>	Subprogram
Short-precision real	SAXPY
Long-precision real	DAXPY
Short-precision complex	CAXPY
Long-precision complex	ZAXPY

#### Syntax

Fortran	CALL SAXPY   DAXPY   CAXPY   ZAXPY (n, alpha, x, incx, y, incy)
C and C++ saxpy   daxpy   caxpy   zaxpy (n, alpha, x, incx, y, incy);	
PL/I	CALL SAXPY   DAXPY   CAXPY   ZAXPY (n, alpha, x, incx, y, incy);

#### On Entry

n

is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

#### alpha

is the scalar *alpha*. Specified as: a number of the data type indicated in Table 41.

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length  $1+(n-1)|inc\mathbf{x}|$ , containing numbers of the data type indicated in Table 41.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

У

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 41.

is the stride for vector y. Specified as: a fullword integer. It can have any value.

#### On Return

У

is the vector  $\mathbf{y}$ , containing the results of the computation  $\mathbf{y}+\alpha\mathbf{x}$ . Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 41.

#### **Notes**

1. If you specify the same vector for **x** and **y**, *incx* and *incy* must be equal; otherwise, results are unpredictable.

2. If you specify different vectors for **x** and **y**, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [73]. If *alpha* or *n* is zero, no computation is performed. For CAXPY, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x** and **y** with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is 1.0.

Call Statement and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with 0 stride. Vector  $\mathbf{x}$  is treated like a vector of length n, all of whose elements are the same as the single element in  $\mathbf{x}$ .

Example 4: This example shows how SAXPY can be used to compute a scalar value. In this case, vectors x and y contain scalar values and the strides for both vectors are 0. The number of elements to be processed, n, is 1.

#### Call Statement and Input

**Example 5:** This example shows how to use CAXPY, where vectors **x** and **y** contain complex numbers. In this case, vectors  $\mathbf{x}$  and  $\mathbf{y}$  have positive strides.

#### SCOPY, DCOPY, CCOPY, and ZCOPY—Copy a Vector

These subprograms copy vector  $\boldsymbol{x}$  to another vector,  $\boldsymbol{y}$ :

$$y \leftarrow x$$

Table 42. Data Types	
<i>x</i> , <i>y</i>	Subprogram
Short-precision real	SCOPY
Long-precision real	DCOPY
Short-precision complex	CCOPY
Long-precision complex	ZCOPY

#### Syntax

Fortran	CALL SCOPY   DCOPY   CCOPY   ZCOPY (n, x, incx, y, incy)
C and C++	scopy   dcopy   ccopy   zcopy (n, x, incx, y, incy);
PL/I	CALL SCOPY   DCOPY   CCOPY   ZCOPY (n, x, incx, y, incy);

#### On Entry

is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

X

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 42. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

y See "On Return."

incy

is the stride for vector y. Specified as: a fullword integer. It can have any value.

#### On Return

У

is the vector  $\mathbf{y}$  of length n. Returned as: a one-dimensional array of (at least) length  $1+(n-1)|inc\mathbf{y}|$ , containing numbers of the data type indicated in Table 42.

#### Notes

- 1. If you specify the same vector for  $\mathbf{x}$  and  $\mathbf{y}$ , incx and incy must be equal; otherwise, results are unpredictable.
- 2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{y}$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The copy is expressed as follows:

$$\begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

See reference [73]. If n is 0, no copy is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows input vector **x** and output vector **y** with positive strides.

Call Statement and Input

**Example 2:** This example shows how to obtain a reverse copy of the input vector  $\mathbf{x}$  by specifying strides with the same absolute value, but with opposite signs, for input vector  $\mathbf{x}$  and output vector  $\mathbf{y}$ . For  $\mathbf{y}$ , which has a negative stride, results are stored beginning at element Y(5).

Call Statement and Input

**Example 3:** This example shows an input vector,  $\mathbf{x}$ , with 0 stride. Vector  $\mathbf{x}$  is treated like a vector of length n, all of whose elements are the same as the single element in  $\mathbf{x}$ . This is a technique for replicating an element of a vector.

Output

$$Y = (13.0, 13.0, 13.0, 13.0, 13.0)$$

**Example 4:** This example shows input vector  $\mathbf{x}$  and output vector  $\mathbf{y}$ , containing complex numbers and having positive strides.

### SDOT, DDOT, CDOTU, ZDOTU, CDOTC, and ZDOTC—Dot **Product of Two Vectors**

SDOT, DDOT, CDOTU, and ZDOTU compute the dot product of vectors **x** and **y**:

 $x \bullet y$ 

CDOTC and ZDOTC compute the dot product of the complex conjugate of vector  $\boldsymbol{x}$ with vector y:

 $\bar{x} \bullet y$ 

Table 43. Data Types	
x, y, Result	Subprogram
Short-precision real	SDOT
Long-precision real	DDOT
Short-precision complex	CDOTU and CDOTC
Long-precision complex	ZDOTU and ZDOTC

#### Syntax

Fortran	SDOT   DDOT   CDOTU   ZDOTC   ZDOTC (n, x, incx, y, incy)
C and C++	sdot   ddot   cdotu   zdotu   cdotc   zdotc (n, x, incx, y, incy);
PL/I	SDOT   DDOT   CDOTU   ZDOTU   CDOTC   ZDOTC (n, x, incx, y, incy);

#### On Entry

n is the number of elements in vectors **x** and **y**. Specified as: a fullword integer;

Х is the vector **x** of length *n*. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 43. incx

is the stride for vector x. Specified as: a fullword integer. It can have any value.

is the vector **y** of length *n*. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 43.

is the stride for vector y. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the result of the dot product computation. Returned as: a number of the data type indicated in Table 43.

Note: Declare this function in your program as returning a value of the data type indicated in Table 43.

**Function:** SDOT, DDOT, CDOTU, and ZDOTU compute the dot product of the vectors  $\mathbf{x}$  and  $\mathbf{y}$ , which is expressed as follows:

$$x \bullet y = x_1 y_1 + x_2 y_2 + ... + x_n y_n$$

CDOTC and ZDOTC compute the dot product of the complex conjugate of vector  $\mathbf{x}$  with vector  $\mathbf{y}$ , which is expressed as follows:

$$\overline{x} \bullet y = \overline{x}_1 y_1 + \overline{x}_2 y_2 + \dots + \overline{x}_n y_n$$

See reference [73]. The result is returned as a function value. If n is 0, then zero is returned as the value of the function.

For SDOT, CDOTU, and CDOTC, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows how to compute the dot product of two vectors,  $\mathbf{x}$  and  $\mathbf{y}$ , having strides of 1.

Function Reference and Input

**Example 2:** This example shows how to compute the dot product of a vector,  $\mathbf{x}$ , with a stride of 1, and a vector,  $\mathbf{y}$ , with a stride greater than 1.

**Example 3:** This example shows how to compute the dot product of a vector,  $\mathbf{x}$ , with a negative stride, and a vector,  $\mathbf{y}$ , with a stride greater than 1. For  $\mathbf{x}$ , processing begins at element X(5), which is 5.0.

Function Reference and Input

**Example 4:** This example shows how to compute the dot product of a vector,  $\mathbf{x}$ , with a stride of 0, and a vector,  $\mathbf{y}$ , with a stride of 1. The result in DOTT is  $x_1(y_1+...+y_p)$ .

Function Reference and Input

**Example 5:** This example shows how to compute the dot product of two vectors,  $\mathbf{x}$  and  $\mathbf{y}$ , with strides of 0. The result in D0TT is  $nx_1y_1$ .

Function Reference and Input

**Example 6:** This example shows how to compute the dot product of two vectors,  $\mathbf{x}$  and  $\mathbf{y}$ , containing complex numbers, where  $\mathbf{x}$  has a stride of 1, and  $\mathbf{y}$  has a stride greater than 1.

**Example 7:** This example shows how to compute the dot product of the conjugate of a vector,  $\mathbf{x}$ , with vector  $\mathbf{y}$ , both containing complex numbers, where  $\mathbf{x}$  has a stride of 1, and  $\mathbf{y}$  has a stride greater than 1.

```
N X INCX Y INCY
| | | | | | |
DOTT = CDOTC(3, X, 1, Y, 2)

X = ((1.0, 2.0), (3.0, -4.0), (-5.0, 6.0))
Y = ((10.0, 9.0), ., (-6.0, 5.0), ., (2.0, 1.0))

Output

DOTT = ((10.0 - 18.0 - 10.0) + (18.0 - 20.0 + 6.0), (9.0 + 15.0 - 5.0) - (20.0 + 24.0 + 12.0))
= (-14.0, -37.0)
```

#### **SNAXPY and DNAXPY—Compute SAXPY or DAXPY N Times**

These subprograms compute SAXPY or DAXPY, respectively, *n* times:

$$\mathbf{y}_i \leftarrow \mathbf{y}_i + \alpha_i \mathbf{x}_i$$
 for  $i = 1, n$ 

where each  $\alpha_i$  is a scalar value, contained in the vector  $\mathbf{a}$ , and each  $\mathbf{x}_i$  and  $\mathbf{y}_i$  are vectors, contained in vectors (or matrices)  $\mathbf{x}$  and  $\mathbf{y}$ , respectively. For an explanation of the SAXPY and DAXPY computations, see "SAXPY, DAXPY, CAXPY, and ZAXPY—Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y" on page 216.

Table 44. Data Types	
a, x, y	Subprogram
Short-precision real	SNAXPY
Long-precision real	DNAXPY

#### Syntax

Fortran	CALL SNAXPY   DNAXPY (n, m, a, inca, x, incxi, incxo, y, incyi, incyo)
C and C++ snaxpy   dnaxpy (n, m, a, inca, x, incxi, incxo, y, incyi, incyo);	
PL/I	CALL SNAXPY   DNAXPY (n, m, a, inca, x, incxi, incxo, y, incyi, incyo);

#### On Entry

n

is the number of SAXPY or DAXPY computations to be performed and the number of elements in vector  $\mathbf{a}$ . Specified as: a fullword integer;  $n \ge 0$ .

n

is the number of elements in vectors  $\mathbf{x}_i$  and  $\mathbf{y}_i$  for each SAXPY or DAXPY computation. Specified as: a fullword integer;  $m \ge 0$ .

а

is the vector  $\boldsymbol{a}$  of length n, containing the scalar values  $\alpha_i$ , used in each computation of  $\boldsymbol{y}_i + \alpha_i \boldsymbol{x}_i$ . Specified as: a one-dimensional array of (at least) length 1+(n-1)|inca|, containing numbers of the data type indicated in Table 44.

inca

is the stride for vector a. Specified as: a fullword integer. It can have any value.

Х

is the vector (or matrix)  $\mathbf{x}$ , containing the  $\mathbf{x}_i$  vectors of length m, used in the n computations of  $\mathbf{y}_i + \alpha_i \mathbf{x}_i$ . Specified as: a one- or two-dimensional array of (at least) length (1+(n-1)(incxo)) + (m-1)[incxi], containing numbers of the data type indicated in Table 44.

incxi

is the stride for x in the inner loop—that is, the stride identifying the elements in each vector  $x_i$ . Specified as: a fullword integer. It can have any value.

incxo

is the stride for x in the outer loop—that is, the stride identifying each vector  $x_i$  in x. Specified as: a fullword integer;  $incxo \ge 0$ .

У

is the vector (or matrix)  $\mathbf{y}$ , containing the  $\mathbf{y}_i$  vectors of length m, used in the n computations of  $\mathbf{y}_i + \alpha_i \mathbf{x}_i$ . Specified as: a one- or two-dimensional array of (at least) length (1+(n-1)(incyo)) + (m-1)|incyi|, containing numbers of the data type indicated in Table 44.

incyi

is the stride for y in the inner loop—that is, the stride identifying the elements in each vector  $y_i$  in y. Specified as: a fullword integer; incyi > 0 or incyi < 0. incyo

is the stride for y in the outer loop—that is, the stride identifying each vector  $y_i$  in y. Specified as: a fullword integer;  $incyo \ge 0$ .

#### On Return

V

is the vector (or matrix)  $\mathbf{y}$ , containing the  $\mathbf{y}_i$  vectors of length m, which contain the results of the n SAXPY or DAXPY computations,  $\mathbf{y}_i + \alpha_i \mathbf{x}_i$  for i = 1, n. Returned as: a one- or two-dimensional array, containing numbers of the data type indicated in Table 44 on page 226.

**Note:** Vector **y** must have no common elements with vector **a** or vector **x**; otherwise, results are unpredictable. See "Concepts" on page 55.

Function: The SAXPY or DAXPY computations:

$$y \leftarrow y + \alpha x$$

are performed *n* times. This is expressed as follows:

$$\mathbf{y}_i \leftarrow \mathbf{y}_i + \alpha_i \mathbf{x}_i$$
 for  $i = 1, n$ 

where each  $\alpha_i$  is a scalar value, contained in the vector  $\mathbf{a}$ , and each  $\mathbf{x}_i$  and  $\mathbf{y}_i$  are vectors, contained in vectors (or matrices)  $\mathbf{x}$  and  $\mathbf{y}$ , respectively.

Each computation of SAXPY or DAXPY on page 216 uses the length of the  $x_i$  and  $y_i$  vectors, m, for its input argument, n. It also uses the strides for the inner loop, *incxi* and *incyi*, for its parameters *incx* and *incy*, respectively. See "Function" on page 217 for a description of how the computation is done.

The outer loop of the SNAXPY or DNAXPY computation uses the strides of *inca*, *incxo*, and *incyo* to locate the elements in  $\boldsymbol{a}$  and vectors in  $\boldsymbol{x}$  and  $\boldsymbol{y}$  for each i-th computation. These are:

```
For i = 1, n:

\alpha_{((i-1)inca+1)} for inca \ge 0

\alpha_{((i-n)inca+1)} for inca < 0

X_{((i-1)incxo+1)}

Y_{((i-1)incyo+1)}
```

If m or n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. n < 02. m < 0
- 3. *incxo* < 0
- 4. incyi = 0
- 5. incyo < 0

**Example 1:** This example shows vectors, contained in matrices, with the stride of the inner loops *incxi* and *incyi* equal to 1.

#### Call Statement and Input

$$A = (3.0, 2.0, 4.0)$$

#### Output

$$Y = \begin{bmatrix} 7.0 & 9.0 & 15.0 \\ 9.0 & 8.0 & 20.0 \\ 11.0 & 7.0 & 10.0 \\ 13.0 & 6.0 & 5.0 \\ & & & & \end{bmatrix}$$

**Example 2:** This example shows vectors, contained in matrices, with a stride of the inner loop *incxi* greater than 1.

$$X = \begin{bmatrix} 1.0 & 4.0 & 3.0 \\ . & . & . \\ 2.0 & 3.0 & 4.0 \\ . & . & . \\ 3.0 & 2.0 & 2.0 \\ . & . & . \\ 4.0 & 1.0 & 1.0 \\ . & . & . \\ . & . & . \end{bmatrix}$$

Output

Y =(same as output Y in Example 1)

**Example 3:** This example shows vectors, contained in matrices, with a negative stride, *incyi*, for the inner loop.

Call Statement and Input

$$A = (3.0, 2.0, 4.0)$$

Output

$$Y = \begin{bmatrix} 13.0 & 6.0 & 5.0 \\ 11.0 & 7.0 & 10.0 \\ 9.0 & 8.0 & 20.0 \\ 7.0 & 9.0 & 15.0 \\ & & & & & \end{bmatrix}$$

**Example 4:** This example shows vectors, contained in matrices, with a negative stride, *inca*, for vector  $\boldsymbol{a}$ . For vector  $\boldsymbol{a}$ , processing begins at element A(5), which is 3.0.

Call Statement and Input

$$Y = \begin{bmatrix} 4.0 & 1.0 & 3.0 \\ 3.0 & 2.0 & 4.0 \\ 2.0 & 3.0 & 2.0 \\ 1.0 & 4.0 & 1.0 \\ & & & & & & \end{bmatrix}$$

Output

Y =(same as output Y in Example 1)

#### **SNDOT and DNDOT—Compute Special Dot Products N Times**

These subprograms compute one of the following special dot products *n* times:

 $s_i \leftarrow \mathbf{x}_i \bullet \mathbf{y}_i$  Store positive dot product  $s_i \leftarrow -\mathbf{x}_i \bullet \mathbf{y}_i$  Store negative dot product  $s_i \leftarrow s_i + \mathbf{x}_i \bullet \mathbf{y}_i$  Accumulate positive dot product  $s_i \leftarrow s_i - \mathbf{x}_i \bullet \mathbf{y}_i$  Accumulate negative dot product for i = 1, n

where each  $s_i$  is an element in vector s, and each  $x_i$  and  $y_i$  are vectors contained in vectors (or matrices) s and s, respectively.

Table 45. Data Types	
s, x, y	Subprogram
Short-precision real	SNDOT
Long-precision real	DNDOT

#### Syntax

Fortran	CALL SNDOT   DNDOT (n, m, s, incs, isw, x, incxi, incxo, y, incyi, incyo)
C and C++	sndot   dndot (n, m, s, incs, isw, x, incxi, incxo, y, incyi, incyo);
PL/I	CALL SNDOT   DNDOT (n, m, s, incs, isw, x, incxi, incxo, y, incyi, incyo);

#### On Entry

n

is the number of dot product computations to be performed and the number of elements in the vector  $\mathbf{s}$ . Specified as: a fullword integer;  $n \ge 0$ .

m

is the number of elements in vectors  $\mathbf{x}_i$  and  $\mathbf{y}_i$  for each dot product computation. Specified as: a fullword integer;  $m \ge 0$ .

s

is the vector  $\mathbf{s}$ , containing the n scalar values  $\mathbf{s}_i$ , where: If  $i\mathbf{s}w = 1$  or 2,  $\mathbf{s}_i$  is not used in the computation (no input value specified.)

If isw = 3 or 4,  $s_i$  is used in the computation (input value specified.)

Specified as: a one-dimensional array of (at least) length 1+(n-1)|incs|, containing numbers of the data type indicated in Table 45.

incs

is the stride for vector  $\mathbf{s}$ . Specified as: a fullword integer; incs > 0 or incs < 0. isw

indicates the type of computation to perform, depending on the value specified:

If 
$$isw = 1$$
,  $s_i \leftarrow \mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 2$ ,  $s_i \leftarrow -\mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 3$ ,  $s_i \leftarrow s_i + \mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 4$ ,  $s_i \leftarrow s_i - \mathbf{x}_i \cdot \mathbf{y}_i$   
where  $i = 1$ ,  $n$ 

Specified as: a fullword integer. Its value must be 1, 2, 3, or 4.

Х is the vector (or matrix)  $\mathbf{x}$ , containing the  $\mathbf{x}_i$  vectors of length m, used in the ndot product computations. Specified as: a one- or two-dimensional array of (at least) length (1+(n-1)(incxo))+(m-1)[incxi], containing numbers of the data type indicated in Table 45.

#### incxi

is the stride for x in the inner loop—that is, the stride identifying the elements in each vector  $\mathbf{x}_i$ . Specified as: a fullword integer. It can have any value.

#### incxo

is the stride for x in the outer loop—that is, the stride identifying each vector  $x_i$ in x. Specified as: a fullword integer;  $incxo \ge 0$ .

V is the vector (or matrix)  $\mathbf{y}$ , containing the  $\mathbf{y}_i$  vectors of length m, used in the ndot product computations. Specified as: a one- or two-dimensional array of (at least) length (1+(n-1)(incyo)) + (m-1)[incyi], containing numbers of the data type indicated in Table 45 on page 231.

#### incvi

is the stride for y in the inner loop—that is, the stride identifying the elements in each vector  $\mathbf{y}_i$ . Specified as: a fullword integer. It can have any value.

is the stride for y in the outer loop—that is, the stride identifying each vector  $y_i$ in y. Specified as: a fullword integer;  $incyo \ge 0$ .

#### On Return

is the vector **s** of length *n*, containing the results of the *n* dot product computations. The type of dot product computation depends of the value specified for isw.

If 
$$isw = 1$$
,  $s_i \leftarrow \mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 2$ ,  $s_i \leftarrow -\mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 3$ ,  $s_i \leftarrow s_i + \mathbf{x}_i \cdot \mathbf{y}_i$   
If  $isw = 4$ ,  $s_i \leftarrow s_i - \mathbf{x}_i \cdot \mathbf{y}_i$   
where  $i = 1$ ,  $n$ 

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 45 on page 231.

**Function:** The four possible computations that can be performed by these subprograms are:

$$s_i \leftarrow \mathbf{x}_i \bullet \mathbf{y}_i$$
 Store positive dot product  $s_i \leftarrow -\mathbf{x}_i \bullet \mathbf{y}_i$  Store negative dot product  $s_i \leftarrow s_i + \mathbf{x}_i \bullet \mathbf{y}_i$  Accumulate positive dot product  $s_i \leftarrow s_i - \mathbf{x}_i \bullet \mathbf{y}_i$  Accumulate negative dot product for  $i = 1, n$ 

where each  $s_i$  is a scalar element in the vector **s** of length n, and each of the  $n \mathbf{x}_i$ and  $y_i$  vectors of length m are contained in vectors (or matrices) x and y, respectively. Each computation uses the dot product, which is expressed:

$$\mathbf{X}_{i} \bullet \mathbf{y}_{i} = u_{1}v_{1} + u_{2}v_{2} + ... + u_{m}v_{m}$$

where  $u_i$  and  $v_i$  are elements of  $\mathbf{x}_i$  and  $\mathbf{y}_i$ , respectively. To find the elements for the computation, it uses:

- The strides for the inner loops, *incxi* and *incyi*, to locate the elements in vectors  $\mathbf{x}_i$  and  $\mathbf{y}_i$ , respectively.
- The strides for the outer loops, incs, incxo, and incyo, to locate the element s<sub>i</sub> in vector s and the vectors x<sub>i</sub> and y<sub>i</sub> in vectors (or matrices) x and y, respectively.

If m or n is 0, no computation is performed. For SNDOT, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2. m < 0
- 3. incs = 0
- 4. isw < 1 or isw > 4
- 5. incxo < 0
- 6. incyo < 0

**Example 1:** This example shows a store positive dot product computation using vectors with positive strides.

Call Statement and Input

$$X = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 3.0 & 4.0 \\ 3.0 & 4.0 & 5.0 \\ 4.0 & 5.0 & 6.0 \end{bmatrix}$$

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ 3.0 & 2.0 & 1.0 \\ 2.0 & 1.0 & 4.0 \\ 1.0 & 4.0 & 3.0 \end{bmatrix}$$

Output

$$S = (20.0, 36.0, 48.0)$$

**Example 2:** This example shows a store negative dot product computation using vectors with positive and negative strides.

#### Call Statement and Input

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ 3.0 & 2.0 & 1.0 \\ 2.0 & 1.0 & 4.0 \\ 1.0 & 4.0 & 3.0 \\ & & & & \\ & & & & \\ & & & & & \\ \end{bmatrix}$$

#### Output

$$S = (-42.0, -34.0, -30.0)$$

**Example 3:** This example shows an accumulative positive dot product using vectors with positive and negative strides.

$$S = (2.0, 5.0, 8.0)$$

$$Y = \begin{bmatrix} 4.0 & 3.0 & 2.0 \\ . & . & . \\ 3.0 & 2.0 & 1.0 \\ . & . & . \\ 2.0 & 1.0 & 4.0 \\ . & . & . \\ 1.0 & 4.0 & 3.0 \\ . & . & . \\ . & . & . \end{bmatrix}$$

#### Output

$$S = (32.0, 39.0, 50.0)$$

**Example 4:** This example shows an accumulative negative dot product using vectors with positive and negative strides.

#### Call Statement and Input

#### Output

$$S = (-45.0, -30.0, -11.0)$$

# SNRM2, DNRM2, SCNRM2, and DZNRM2—Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow

These subprograms compute the Euclidean length ( $I_2$  norm) of vector  $\mathbf{x}$ , with scaling of input to avoid destructive underflow and overflow.

Table 46. Data Types		
x	Result	Subprogram
Short-precision real	Short-precision real	SNRM2
Long-precision real	Long-precision real	DNRM2
Short-precision complex	Short-precision real	SCNRM2
Long-precision complex	Long-precision real	DZNRM2

**Note:** If there is a possibility that your data will cause the computation to overflow or underflow, you should use these subroutines instead of SNORM2, DNORM2, CNORM2, and ZNORM2, because the intermediate computational results may exceed the maximum or minimum limits of the machine. "Notes" on page 239 explains how to estimate whether your data will cause an overflow or underflow.

#### **Syntax**

Fortran	SNRM2   DNRM2   SCNRM2   DZNRM2 (n, x, incx)	
C and C++	C and C++ snrm2   dnrm2   scnrm2   dznrm2 (n, x, incx);	
PL/I	SNRM2   DNRM2   SCNRM2   DZNRM2 (n, x, incx);	

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

is the vector  $\mathbf{x}$  of length n, whose Euclidean length is to be computed. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 46.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the Euclidean length ( $l_2$  norm) of the vector  $\mathbf{x}$ . Returned as: a number of the data type indicated in Table 46.

**Note:** Declare this function in your program as returning a value of the data type indicated in Table 46.

**Function:** The Euclidean length ( $l_2$  norm) of vector  $\mathbf{x}$  is expressed as follows, with scaling of input to avoid destructive underflow and overflow:

$$\sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2}$$

See reference [73]. The result is returned as the function value. If *n* is 0, then 0.0 is returned as the value of the function.

For SNRM2 and SCNRM2, the sum of the squares of the absolute values of the elements is accumulated in long precision. The square root of this long-precision sum is then computed and, if necessary, is unscaled.

Although these subroutines eliminate destructive underflow, nondestructive underflows may occur if the input elements differ greatly in magnitude. This does not affect accuracy, but it degrades performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

*Important Information About the Following Examples:* Workstations use workstation architecture precisions: ANSI/IEEE 32-bit and 64-bit binary floating-point format. The ranges are:

For short-precision: 3.37×10<sup>-38</sup> to 3.37×10<sup>38</sup>
 For long-precision: 1.67×10<sup>-308</sup> to 1.67×10<sup>308</sup>

**Example 1:** This example shows a vector, **x**, whose elements must be scaled to prevent overflow.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, whose elements must be scaled to prevent destructive underflow.

Function Reference and Input

= 0.1469D+201

Output

**DNORM** 

DNORM = 0.21590D-200

**Example 3:** This example shows a vector, **x**, with a stride of 0. The result in SNORM is:

$$\sqrt{nx_1^2}$$

Function Reference and Input

**Example 4:** This example shows a vector,  $\mathbf{x}$ , containing complex numbers, and whose elements must be scaled to prevent overflow.

Function Reference and Input

**Example 5:** This example shows a vector, **x**, containing complex numbers, and whose elements must be scaled to prevent destructive underflow.

## SNORM2, DNORM2, CNORM2, and ZNORM2—Euclidean Length of a Vector with No Scaling of Input

These subprograms compute the euclidean length ( $l_2$  norm) of vector  $\boldsymbol{x}$  with no scaling of input.

Table 47. Data Types		
x	Result	Subprogram
Short-precision real	Short-precision real	SNORM2
Long-precision real	Long-precision real	DNORM2
Short-precision complex	Short-precision real	CNORM2
Long-precision complex	Long-precision real	ZNORM2

#### Syntax

Fortran	SNORM2   DNORM2   CNORM2   ZNORM2 (n, x, incx)
C and C++	snorm2   dnorm2   cnorm2   znorm2 (n, x, incx);
PL/I	SNORM2   DNORM2   CNORM2   ZNORM2 (n, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

Χ

is the vector  $\mathbf{x}$  of length n, whose euclidean length is to be computed. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 47.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

#### Function value

is the euclidean length ( $l_2$  norm) of the vector  $\mathbf{x}$ . Returned as: a number of the data type indicated in Table 47.

#### Notes

- This subroutine does not underflow or overflow if the values of the elements in vector x conform to the following conditions. If these conditions are violated, overflow or destructive underflow may occur:
  - For short-precision numbers:

Any valid short-precision number.

For long-precision numbers:

$$|x_i| = 0$$
 or  $0.10010E-145 < |x_i| < 0.13408E+155$  for  $i = 1$ ,  $n$ 

2. Declare this function in your program as returning a value of the data type indicated in Table 47.

**Function:** The euclidean length ( $l_2$  norm) of vector  $\mathbf{x}$  is expressed as follows with no scaling of input:

#### SNORM2, DNORM2, CNORM2, and ZNORM2

$$\sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2}$$

See reference [73]. The result is returned as the function value. If n is 0, then 0.0 is returned as the value of the function.

For SNORM2 and CNORM2, the sum of the squares of the absolute values of the elements is accumulated in long-precision. The square root of this long-precision sum is then computed.

This subroutine should not be used if the values in vector  $\mathbf{x}$  do not conform to the restriction given in "Notes" on page 239.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Function Reference and Input

**Example 2:** This example shows a vector, **x**, with a stride greater than 1.

Function Reference and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with a stride of 0. The result in SNORM is:

$$\sqrt{nx_1^2}$$

#### SNORM2, DNORM2, CNORM2, and ZNORM2

**Example 4:** This example shows a vector,  $\mathbf{x}$ , containing complex numbers and having a stride of 1.

#### SROTG, DROTG, CROTG, and ZROTG—Construct a Givens **Plane Rotation**

SROTG and DROTG construct a real Givens plane rotation, and CROTG and ZROTG construct a complex Givens plane rotation. The computations use rotational elimination parameters a and b. Values are returned for r, as well as the cosine c and the sine s of the angle of rotation. SROTG and DROTG also return a value for z.

**Note:** Throughout this description, the symbols r and z are used to represent two of the output values returned for this computation. It is important to note that the values for r and z are actually returned in the input-output arguments a and b, respectively, overwriting the original values passed in a and b.

Table 48. Data Types			
a, b, r, s	С	Z	Subprogram
Short-precision real	Short-precision real	Short-precision real	SROTG
Long-precision real	Long-precision real	Long-precision real	DROTG
Short-precision complex	Short-precision real	(No value returned)	CROTG
Long-precision complex	Long-precision real	(No value returned)	ZROTG

#### **Syntax**

Fortran	CALL SROTG   DROTG   CROTG   ZROTG (a, b, c, s)	
C and C++	srotg   drotg   crotg   zrotg (a, b, c, s);	
PL/I	CALL SROTG   DROTG   CROTG   ZROTG (a, b, c, s);	

#### On Entry

а

is the rotational elimination parameter a. Specified as: a number of the data type indicated in Table 48.

is the rotational elimination parameter b. Specified as: a number of the data type indicated in Table 48.

See "On Return."

See "On Return."

#### On Return

а

is the value computed for r.

For SROTG and DROTG:

$$r = \sigma \sqrt{a^2 + b^2}$$

where:

$$\sigma = SIGN(a) \text{ if } |a| > |b|$$

$$\sigma = SIGN(b)$$
 if  $|a| \le |b|$ 

For CROTG and ZROTG:

$$r = \psi \sqrt{|a|^2 + |b|^2} \quad \text{if } |a| \neq 0$$

$$r = b \quad \text{if } |a| = 0$$

where:

b

С

s

$$\psi = a/|a|$$

Returned as: a number of the data type indicated in Table 48 on page 242.

is the value computed for z.

For SROTG and DROTG:

$$z = s$$
 if  $|a| > |b|$ 

$$z = 1/c$$
 if  $|a| \le |b|$  and  $c \ne 0$  and  $r \ne 0$ 

$$z = 1$$
 if  $|a| \le |b|$  and  $c = 0$  and  $r \ne 0$ 

$$z = 0$$
 if  $r = 0$ 

For CROTG and ZROTG: no value is returned, and the input value is not changed.

Returned as: a number of the data type indicated in Table 48 on page 242.

is the cosine *c* of the angle of (Givens) rotation. For SROTG and DROTG:

$$c = a/r$$
 if  $r \neq 0$ 

$$c = 1$$
 if  $r = 0$ 

For CROTG and ZROTG:

$$c = \frac{|a|}{\sqrt{|a|^2 + |b|^2}}$$
 if  $|a| \neq 0$ 

$$c = 0$$
 if  $|a| = 0$ 

Returned as: a number of the data type indicated in Table 48 on page 242.

is the sine *s* of the angle of (Givens) rotation.

For SROTG and DROTG:

$$s = b/r$$
 if  $r \neq 0$ 

$$s = 0$$
 if  $r = 0$ 

For CROTG and ZROTG:

$$s = \frac{\psi \overline{b}}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$s = (1.0, 0.0)$$
 if  $|a| = 0$ 

where  $\psi = a/|a|$ 

Returned as: a number of the data type indicated in Table 48 on page 242.

**Note:** In your C program, arguments a, b, c, and s must be passed by reference.

#### **Function**

SROTG and DROTG: A real Givens plane rotation is constructed for values a and b by computing values for r, c, s, and z, where:

$$r = \sigma \sqrt{a^2 + b^2}$$

where:

$$\sigma = SIGN(a)$$
 if  $|a| > |b|$   
 $\sigma = SIGN(b)$  if  $|a| \le |b|$ 

$$c = a/r$$
 if  $r \neq 0$ 

$$c = 1$$
 if  $r = 0$ 

$$s = b/r$$
 if  $r \neq 0$ 

$$s = 0$$
 if  $r = 0$ 

$$z = s$$
 if  $|a| > |b|$ 

$$z = 1/c$$
 if  $|a| \le |b|$  and  $c \ne 0$  and  $r \ne 0$ 

$$z = 1$$
 if  $|a| \le |b|$  and  $c = 0$  and  $r \ne 0$ 

$$z = 0$$
 if  $r = 0$ 

See reference [73].

Following are some important points about the computation:

1. The numbers for *c*, *s*, and *r* satisfy:

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

2. Where necessary, scaling is used to avoid overflow and destructive underflow in the computation of *r*, which is expressed as follows:

$$r = \sigma(|a|+|b|) \sqrt{\left(\frac{a}{|a|+|b|}\right)^2 + \left(\frac{b}{|a|+|b|}\right)^2}$$

3.  $\sigma$  is not essential to the computation of a Givens rotation matrix, but its use permits later stable reconstruction of c and s from just one stored number, z. See reference [85]. c and s are reconstructed from z as follows:

For 
$$z = 1$$
,  $c = 0$  and  $s = 1$   
For  $|z| < 1$ ,  $c = \sqrt{1 - z^2}$  and  $s = z$   
For  $|z| > 1$ ,  $c = 1/z$  and  $s = \sqrt{1 - c^2}$ 

CROTG and ZROTG: A complex Givens plane rotation is constructed for values a and b by computing values for r, c, and s, where:

$$r = \psi \sqrt{|a|^2 + |b|^2} \quad \text{if } |a| \neq 0$$

$$r = b \quad \text{if } |a| = 0$$

where:

$$\psi = a/|a|$$

$$c = \frac{|a|}{\sqrt{|a|^2 + |b|^2}}$$
 if  $|a| \neq 0$ 

$$c = 0$$
 if  $|a| = 0$ 

$$s = \frac{\psi \overline{b}}{\sqrt{|a|^2 + |b|^2}} \quad \text{if } |a| \neq 0$$

$$s = (1.0, 0.0)$$
 if  $|a| = 0$ 

See reference [73].

Following are some important points about the computation:

1. The numbers for *c*, *s*, and *r* satisfy:

$$\begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$

2. Where necessary, scaling is used to avoid overflow and destructive underflow in the computation of *r*, which is expressed as follows:

$$r = \psi\left(|a| + |b|\right)\sqrt{\left|\frac{a}{|a| + |b|}\right|^2 + \left|\frac{b}{|a| + |b|}\right|^2}$$

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: None

**Example 1:** This example shows the construction of a real Givens plane rotation, where r is 0.

Call Statement and Input

#### Output

A = 0.0 B = 0.0 C = 1.0 S = 0.0

**Example 2:** This example shows the construction of a real Givens plane rotation, where c is 0.

Call Statement and Input

#### Output

A = 2.0 B = 1.0 C = 0.0 S = 1.0

**Example 3:** This example shows the construction of a real Givens plane rotation, where |b| > |a|.

#### Output

$$A = -10.0$$

B = 
$$-1.66\overline{6}$$

$$C = -0.6$$

S = 0.8

**Example 4:** This example shows the construction of a real Givens plane rotation, where |a| > |b|.

Call Statement and Input

#### Output

$$A = 10.0$$

$$B = 0.6$$

$$C = 0.8$$

$$S = 0.6$$

**Example 5:** This example shows the construction of a complex Givens plane rotation, where |a| = 0.

Call Statement and Input

$$A = (0.0, 0.0)$$

B = 
$$(1.0, 0.0)$$

#### Output

$$A = (1.0, 0.0)$$

$$C = 0.0$$

$$S = (1.0, 0.0)$$

**Example 6:** This example shows the construction of a complex Givens plane rotation, where  $|a| \neq 0$ .

Call Statement and Input

$$A = (3.0, 4.0)$$

$$B = (4.0, 6.0)$$

Output

```
= (5.26, 7.02)
= 0.57
= (0.82, -0.05)
```

## SROT, DROT, CROT, ZROT, CSROT, and ZDROT—Apply a Plane Rotation

SROT and DROT apply a real plane rotation to real vectors; CROT and ZROT apply a complex plane rotation to complex vectors; and CSROT and ZDROT apply a real plane rotation to complex vectors. The plane rotation is applied to n points, where the points to be rotated are contained in vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and where the cosine and sine of the angle of rotation are  $\mathbf{c}$  and  $\mathbf{s}$ , respectively.

Table 49. Data Types			
<i>x</i> , <i>y</i>	С	s	Subprogram
Short-precision real	Short-precision real	Short-precision real	SROT
Long-precision real	Long-precision real	Long-precision real	DROT
Short-precision complex	Short-precision real	Short-precision complex	CROT
Long-precision complex	Long-precision real	Long-precision complex	ZROT
Short-precision complex	Short-precision real	Short-precision real	CSROT
Long-precision complex	Long-precision real	Long-precision real	ZDROT

#### Syntax

Fortran	CALL SROT   DROT   CROT   ZROT   CSROT   ZDROT (n, x, incx, y, incy, c, s)	
C and C++	srot   drot   crot   zrot   csrot   zdrot (n, x, incx, y, incy, c, s);	
PL/I	CALL SROT   DROT   CROT   ZROT   CSROT   ZDROT (n, x, incx, y, incy, c, s);	

#### On Entry

n

is the number of points to be rotated—that is, the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

is the vector  $\mathbf{x}$  of length n, containing the  $x_i$  coordinates of the points to be rotated. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 49.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

is the vector  $\mathbf{y}$  of length n, containing the  $y_i$  coordinates of the points to be rotated. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 49.

incy

is the stride for vector **y**. Specified as: a fullword integer. It can have any value.

the cosine, *c*, of the angle of rotation. Specified as: a number of the data type indicated in Table 49.

the sine, *s*, of the angle of rotation. Specified as: a number of the data type indicated in Table 49.

#### On Return

#### SROT, DROT, CROT, ZROT, CSROT, and ZDROT

х

is the vector  $\mathbf{x}$  of length n, containing the rotated  $x_i$  coordinates, where:

$$x_i \leftarrow cx_i + sy_i$$
 for  $i = 1$ ,

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 49 on page 249.

У

is the vector  $\mathbf{y}$  of length n, containing the rotated  $y_i$  coordinates, where:

For SROT, DROT, CSROT, and ZDROT:

$$y_i \leftarrow -sx_i + cy_i$$
 for  $i = 1, n$ 

For CROT and ZROT:

$$y_i \leftarrow -\bar{s}x_i + cy_i$$
 for  $i = 1, n$ 

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 49 on page 249.

**Note:** The vectors **x** and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** Applying a plane rotation to n points, where the points to be rotated are contained in vectors  $\mathbf{x}$  and  $\mathbf{y}$ , is expressed as follows, where c and s are the cosine and sine of the angle of rotation, respectively. For SROT, DROT, CSROT, and ZDROT:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, n$$

For CROT and ZROT:

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} \leftarrow \begin{bmatrix} c & s \\ -\overline{s} & c \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \text{for } i = 1, n$$

See references [54] and [73]. No computation is performed if n is 0 or if c is 1.0 and s is zero. For SROT, CROT, and CSROT, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows how to apply a real plane rotation to real vectors  $\mathbf{x}$  and  $\mathbf{y}$  having positive strides.

#### Output

$$X = (-0.366, -0.732, -1.098, -1.464, -1.830)$$
  
 $Y = (-1.366, -2.732, -4.098, -5.464, -6.830)$ 

**Example 2:** This example shows how to apply a real plane rotation to real vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite sign.

Call Statement and Input

#### Output

**Example 3:** This example shows how scalar values in vectors  $\mathbf{x}$  and  $\mathbf{y}$  can be processed by specifying 0 strides and the number of elements to be processed, n, equal to 1.

Call Statement and Input

Output

#### SROT, DROT, CROT, ZROT, CSROT, and ZDROT

```
= (-0.366)
= (-1.366)
```

**Example 4:** This example shows how to apply a complex plane rotation to complex vectors **x** and **y** having positive strides.

Call Statement and Input

**Example 5:** This example shows how to apply a real plane rotation to complex vectors **x** and **y** having positive strides.

Call Statement and Input

Output

```
= ((-0.366, 5.330), (-0.732, 4.964), (-1.098, 4.598))
Υ
        = ((-1.366, 0.768), . , (-2.732, -0.598), . ,
            (-4.098, -1.964))
```

## SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, and ZDSCAL—Multiply a Vector X by a Scalar and Store in the Vector X

These subprograms perform the following computation, using the scalar  $\alpha$  and the vector  $\mathbf{x}$ :

$$\mathbf{x} \leftarrow \alpha \mathbf{x}$$

Table 50. Data Types		
α	x	Subprogram
Short-precision real	Short-precision real	SSCAL
Long-precision real	Long-precision real	DSCAL
Short-precision complex	Short-precision complex	CSCAL
Long-precision complex	Long-precision complex	ZSCAL
Short-precision real	Short-precision complex	CSSCAL
Long-precision real	Long-precision complex	ZDSCAL

#### **Syntax**

Fortran	CALL SSCAL   DSCAL   CSCAL   CSSCAL   ZDSCAL (n, alpha, x, incx)
C and C++	sscal   dscal   cscal   cscal   cscal   zdscal (n, alpha, x, incx);
PL/I	CALL SSCAL   DSCAL   CSCAL   CSSCAL   ZDSCAL (n, alpha, x, incx);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 0$ . alpha

is the scalar  $\alpha$ . Specified as: a number of the data type indicated in Table 50.

Χ

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 50. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

#### On Return

х

is the vector  $\mathbf{x}$  of length n, containing the result of the computation  $\alpha \mathbf{x}$ . Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 50.

**Note:** The fastest way in ESSL to zero out contiguous (stride 1) arrays is to call SSCAL or DSCAL, specifying incx = 1 and  $\alpha = 0$ .

**Function:** The computation is expressed as follows:

#### SSCAL, DSCAL, CSCAL, ZSCAL, CSSCAL, and ZDSCAL

$$\begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \leftarrow \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [73]. If *n* is 0, no computation is performed. For CSCAL, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a vector, **x**, with a stride of 1.

Call Statement and Input

**Example 2:** This example shows vector, **x**, with a stride greater than 1.

Call Statement and Input

**Example 3:** This example illustrates that when the strides for two similar computations (Example 1 and Example 3) have the same absolute value but have opposite signs, the output is the same. This example is the same as Example 1, except the stride for x is negative (-1). For performance reasons, it is better to specify the positive stride. For x, processing begins at element X(5), which is 5.0, and results are stored beginning at the same element.

Output

$$X = (2.0, 4.0, 6.0, 8.0, 10.0)$$

**Example 4:** This example shows how SSCAL can be used to compute a scalar value. In this case, input vector  $\mathbf{x}$  contains a scalar value, and the stride is 0. The number of elements to be processed, n, is 1.

Call Statement and Input

**Example 5:** This example shows a scalar,  $\alpha$ , and a vector,  $\mathbf{x}$ , containing complex numbers, where vector  $\mathbf{x}$  has a stride of 1.

Call Statement and Input

**Example 6:** This example shows a scalar,  $\alpha$ , containing a real number, and a vector,  $\mathbf{x}$ , containing complex numbers, where vector  $\mathbf{x}$  has a stride of 1.

## SSWAP, DSWAP, CSWAP, and ZSWAP—Interchange the Elements of Two Vectors

These subprograms interchange the elements of vectors  $\mathbf{x}$  and  $\mathbf{y}$ :

$$y \longleftrightarrow x$$

Table 51. Data Types	
x, y	Subprogram
Short-precision real	SSWAP
Long-precision real	DSWAP
Short-precision complex	CSWAP
Long-precision complex	ZSWAP

#### Syntax

Fortran	CALL SSWAP   DSWAP   CSWAP   ZSWAP (n, x, incx, y, incy)
C and C++	sswap   dswap   cswap   zswap (n, x, incx, y, incy);
PL/I	CALL SSWAP   DSWAP   CSWAP   ZSWAP (n, x, incx, y, incy);

#### On Entry

*n* is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 51. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 51. incy

is the stride for vector **y**. Specified as: a fullword integer. It can have any value.

#### On Return

is the vector **x** of length *n*, containing the elements that were swapped from vector **y**. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 51.

is the vector **y** of length *n*, containing the elements that were swapped from vector **x**. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 51.

#### **Notes**

1. If you specify the same vector for **x** and **y**, then *incx* and *incy* must be equal; otherwise, results are unpredictable.

2. If you specify different vectors for **x** and **y**, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The elements of vectors **x** and **y** are interchanged as follows:

$$\begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_n \end{bmatrix} \longleftrightarrow \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

See reference [73]. If n is 0, no elements are interchanged.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x** and **y** with positive strides.

Call Statement and Input

**Example 2:** This example shows how to obtain output vectors  $\mathbf{x}$  and  $\mathbf{y}$  that are reverse copies of the input vectors  $\mathbf{y}$  and  $\mathbf{x}$ . You must specify strides with the same absolute value, but with opposite signs. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is -5.0, and the results of the swap are stored beginning at the same element.

Example 3: This example shows how SSWAP can be used to interchange scalar values in vectors  $\mathbf{x}$  and  $\mathbf{y}$  by specifying 0 strides and the number of elements to be processed as 1.

#### Call Statement and Input

**Example 4:** This example shows vectors **x** and **y**, containing complex numbers and having positive strides.

## SVEA, DVEA, CVEA, and ZVEA—Add a Vector X to a Vector Y and Store in a Vector Z

These subprograms perform the following computation, using vectors x, y, and z:

$$z \leftarrow x + y$$

Table 52. Data Types	
x, y, z	Subprogram
Short-precision real	SVEA
Long-precision real	DVEA
Short-precision complex	CVEA
Long-precision complex	ZVEA

#### Syntax

Fortran	CALL SVEA   DVEA   CVEA   ZVEA (n, x, incx, y, incy, z, incz)
C and C++	svea   dvea   cvea   zvea (n, x, incx, y, incy, z, incz);
PL/I	CALL SVEA   DVEA   CVEA   ZVEA (n, x, incx, y, incy, z, incz);

#### On Entry

n

is the number of elements in vectors x, y, and z. Specified as: a fullword integer;  $n \ge 0$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 52. incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

У

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length  $1+(n-1)|inc\mathbf{y}|$ , containing numbers of the data type indicated in Table 52.  $inc\mathbf{y}$ 

is the stride for vector **y**. Specified as: a fullword integer. It can have any value.

2

See "On Return."

incz

is the stride for vector z. Specified as: a fullword integer. It can have any value.

#### On Return

Z

is the vector  $\mathbf{z}$  of length n, containing the result of the computation. Returned as: a one-dimensional array of (at least) length 1+(n-1)|incz|, containing numbers of the data type indicated in Table 52.

#### **Notes**

1. If you specify the same vector for **x** and **z**, then *incx* and *incz* must be equal; otherwise, results are unpredictable. The same is true for **y** and **z**.

2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{z}$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $\mathbf{y}$  and  $\mathbf{z}$ . See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix}$$

If n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x**, **y**, and **z**, with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite sign, and an output vector  $\mathbf{z}$  having a positive stride. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is 1.0.

Call Statement and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with 0 stride and a vector,  $\mathbf{z}$ , with negative stride.  $\mathbf{x}$  is treated like a vector of length  $\mathbf{n}$ , all of whose elements are the same as the single element in  $\mathbf{x}$ . For vector  $\mathbf{z}$ , results are stored beginning in element  $\mathbf{z}(5)$ .

Call Statement and Input

**Example 4:** This example shows a vector, y, with 0 stride. y is treated like a vector of length n, all of whose elements are the same as the single element in y.

Call Statement and Input

**Example 5:** This example shows the output vector,  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has positive stride, and the vector  $\mathbf{y}$  has 0 stride. The number of elements to be processed, n, is greater than 1.

Call Statement and Input

**Example 6:** This example shows the output vector  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has 0 stride, and the vector  $\mathbf{y}$  has negative stride. The number of elements to be processed, n, is greater than 1.

Call Statement and Input

Output

$$Z = (6.0)$$

Example 7: This example shows how SVEA can be used to compute a scalar value. In this case, vectors  $\mathbf{x}$  and  $\mathbf{y}$  contain scalar values. The strides of all vectors, x, y, and z, are 0. The number of elements to be processed, n, is 1.

Call Statement and Input

**Example 8:** This example shows vectors **x** and **y**, containing complex numbers and having positive strides.

## SVES, DVES, CVES, and ZVES—Subtract a Vector Y from a Vector X and Store in a Vector Z

These subprograms perform the following computation, using vectors  $\boldsymbol{x}$ ,  $\boldsymbol{y}$ , and  $\boldsymbol{z}$ :

$$z \leftarrow x - y$$

Table 53. Data Types	
x, y, z	Subprogram
Short-precision real	SVES
Long-precision real	DVES
Short-precision complex	CVES
Long-precision complex	ZVES

#### Syntax

Fortran	CALL SVES   DVES   CVES   ZVES (n, x, incx, y, incy, z, incz)
C and C++	sves   dves   cves   zves (n, x, incx, y, incy, z, incz);
PL/I	CALL SVES   DVES   CVES   ZVES (n, x, incx, y, incy, z, incz);

#### On Entry

n

is the number of elements in vectors x, y, and z. Specified as: a fullword integer;  $n \ge 0$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 53.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

У

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 53. incy

is the stride for vector y. Specified as: a fullword integer. It can have any value.

2

See On Return.

incz

is the stride for vector z. Specified as: a fullword integer. It can have any value.

#### On Return

Z

is the vector  $\mathbf{z}$  of length n, containing the result of the computation. Returned as: a one-dimensional array of (at least) length 1+(n-1)|incz|, containing numbers of the data type indicated in Table 53.

#### **Notes**

1. If you specify the same vector for **x** and **z**, then *incx* and *incz* must be equal; otherwise, results are unpredictable. The same is true for **y** and **z**.

2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{z}$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $\mathbf{y}$  and  $\mathbf{z}$ . See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} - \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix}$$

If n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x**, **y**, and **z**, with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite sign, and an output vector  $\mathbf{z}$  having a positive stride. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is 1.0.

Call Statement and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with 0 stride, and a vector,  $\mathbf{z}$ , with negative stride.  $\mathbf{x}$  is treated like a vector of length  $\mathbf{n}$ , all of whose elements are the same as the single element in  $\mathbf{x}$ . For vector  $\mathbf{z}$ , results are stored beginning in element  $\mathbf{z}(5)$ .

Call Statement and Input

**Example 4:** This example shows a vector, y, with 0 stride. y is treated like a vector of length n, all of whose elements are the same as the single element in y.

Call Statement and Input

**Example 5:** This example shows the output vector  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has positive stride, and the vector  $\mathbf{y}$  has 0 stride. The number of elements to be processed, n, is greater than 1.

Call Statement and Input

**Example 6:** This example shows the output vector  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has 0 stride, and the vector  $\mathbf{y}$  has negative stride. The number of elements to be processed, n, is greater than 1.

Call Statement and Input

Output

$$Z = (-4.0)$$

**Example 7:** This example shows how SVES can be used to compute a scalar value. In this case, vectors  $\mathbf{x}$  and  $\mathbf{y}$  contain scalar values. The strides of all vectors,  $\mathbf{x}$ ,  $\mathbf{y}$ , and  $\mathbf{z}$ , are 0. The number of elements to be processed, n, is 1.

Call Statement and Input

**Example 8:** This example shows vectors **x** and **y**, containing complex numbers and having positive strides.

## SVEM, DVEM, CVEM, and ZVEM—Multiply a Vector X by a Vector Y and Store in a Vector Z

These subprograms perform the following computation, using vectors  $\boldsymbol{x}$ ,  $\boldsymbol{y}$ , and  $\boldsymbol{z}$ :

$$z \leftarrow xy$$

Table 54. Data Types	
x, y, z	Subprogram
Short-precision real	SVEM
Long-precision real	DVEM
Short-precision complex	CVEM
Long-precision complex	ZVEM

#### Syntax

Fortran	CALL SVEM   DVEM   CVEM   ZVEM (n, x, incx, y, incy, z, incz)
C and C++	svem   dvem   cvem   zvem (n, x, incx, y, incy, z, incz);
PL/I	CALL SVEM   DVEM   CVEM   ZVEM (n, x, incx, y, incy, z, incz);

#### On Entry

n

is the number of elements in vectors  $\mathbf{x}$ ,  $\mathbf{y}$ , and  $\mathbf{z}$ . Specified as: a fullword integer;  $n \ge 0$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 54.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

У

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 54. incy

is the stride for vector y. Specified as: a fullword integer. It can have any value.

2

See "On Return."

incz

is the stride for vector z. Specified as: a fullword integer. It can have any value.

#### On Return

z

is the vector  $\mathbf{z}$  of length n, containing the result of the computation. Returned as: a one-dimensional array of (at least) length 1+(n-1)|incz|, containing numbers of the data type indicated in Table 54.

#### Notes

1. If you specify the same vector for **x** and **z**, then *incx* and *incz* must be equal; otherwise, results are unpredictable. The same is true for **y** and **z**.

2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{z}$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $\mathbf{y}$  and  $\mathbf{z}$ . See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$z_i \leftarrow x_i y_i$$
 for  $i = 1, n$ 

If *n* is 0, no computation is performed. For CVEM, intermediate results are accumulated in long precision (short-precision Multiply followed by a long-precision Add), with the final result truncated to short precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x**, **y**, and **z**, with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite sign, and an output vector  $\mathbf{z}$  having a positive stride. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is 1.0.

Call Statement and Input

**Example 3:** This example shows a vector,  $\mathbf{x}$ , with 0 stride, and a vector,  $\mathbf{z}$ , with negative stride.  $\mathbf{x}$  is treated like a vector of length  $\mathbf{n}$ , all of whose elements are the same as the single element in  $\mathbf{x}$ . For vector  $\mathbf{z}$ , results are stored beginning in element  $\mathbf{Z}(5)$ .

**Example 4:** This example shows a vector, y, with 0 stride. y is treated like a vector of length n, all of whose elements are the same as the single element in y.

Call Statement and Input

**Example 5:** This example shows the output vector,  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has positive stride, and the vector  $\mathbf{y}$  has 0 stride. The number of elements to be processed, n, is greater than 1.

Call Statement and Input

**Example 6:** This example shows the output vector  $\mathbf{z}$ , with 0 stride, where the vector  $\mathbf{x}$  has 0 stride, and the vector  $\mathbf{y}$  has negative stride. The number of elements to be processed,  $\mathbf{n}$ , is greater than 1.

Example 7: This example shows how SVEM can be used to compute a scalar value. In this case, vectors  $\mathbf{x}$  and  $\mathbf{y}$  contain scalar values. The strides of all vectors,  $\boldsymbol{x}$ ,  $\boldsymbol{y}$ , and  $\boldsymbol{z}$ , are 0. The number of elements to be processed,  $\boldsymbol{n}$ , is 1.

Call Statement and Input

**Example 8:** This example shows vectors **x** and **y**, containing complex numbers and having positive strides.

## SYAX, DYAX, CYAX, ZYAX, CSYAX, and ZDYAX—Multiply a Vector X by a Scalar and Store in a Vector Y

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $\textbf{\textit{x}}$  and  $\textbf{\textit{y}}$ :

$$y \leftarrow \alpha x$$

Table 55. Data Types		
α	<i>x</i> , <i>y</i>	Subprogram
Short-precision real	Short-precision real	SYAX
Long-precision real	Long-precision real	DYAX
Short-precision complex	Short-precision complex	CYAX
Long-precision complex	Long-precision complex	ZYAX
Short-precision real	Short-precision complex	CSYAX
Long-precision real	Long-precision complex	ZDYAX

#### Syntax

Fortran	CALL SYAX   DYAX   CYAX   ZYAX   CSYAX   ZDYAX (n, alpha, x, incx, y, incy)
C and C++	syax   dyax   cyax   zyax   csyax   zdyax (n, alpha, x, incx, y, incy);
PL/I	CALL SYAX   DYAX   CYAX   ZYAX   CSYAX   ZDYAX (n, alpha, x, incx, y, incy);

#### On Entry

n

is the number of elements in vector  $\mathbf{x}$  and  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

alpha

is the scalar  $\alpha$ . Specified as: a number of the data type indicated in Table 55.

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 55. incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer. It can have any value.

See "On Return."

incy

is the stride for vector y. Specified as: a fullword integer. It can have any value.

#### On Return

y

is the vector  $\mathbf{y}$  of length n, containing the result of the computation  $\alpha \mathbf{x}$ . Returned as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 55.

#### **Notes**

1. If you specify the same vector for **x** and **y**, then *incx* and *incy* must be equal; otherwise, results are unpredictable.

2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{y}$ , they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$\begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_n \end{bmatrix} \leftarrow \alpha \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$

See reference [73]. If n is 0, no computation is performed. For CYAX, intermediate results are accumulated in long precision.

#### **Error Condition**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x** and **y** with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors **x** and **y** that have strides of opposite signs. For y, which has negative stride, results are stored beginning in element Y(5).

Call Statement and Input

**Example 3:** This example shows a vector, **x**, with 0 stride. **x** is treated like a vector of length n, all of whose elements are the same as the single element in x.

**Example 4:** This example shows how SYAX can be used to compute a scalar value. In this case both vectors  $\mathbf{x}$  and  $\mathbf{y}$  contain scalar values, and the strides for both vectors are 0. The number of elements to be processed, n, is 1.

#### Call Statement and Input

**Example 5:** This example shows a scalar,  $\alpha$ , and vectors  $\mathbf{x}$  and  $\mathbf{y}$ , containing complex numbers, where both vectors have a stride of 1.

#### Call Statement and Input

N ALPHA X INCX Y INCY

| | | | | | | |

CALL CYAX(3, ALPHA, X, 1, Y, 1)

ALPHA = 
$$(2.0, 3.0)$$

X =  $((1.0, 2.0), (2.0, 0.0), (3.0, 5.0))$ 

Output

Y =  $((-4.0, 7.0), (4.0, 6.0), (-9.0, 19.0))$ 

**Example 6:** This example shows a scalar,  $\alpha$ , containing a real number, and vectors  $\mathbf{x}$  and  $\mathbf{y}$ , containing complex numbers, where both vectors have a stride of 1

## SZAXPY, DZAXPY, CZAXPY, and ZZAXPY—Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in a Vector Z

These subprograms perform the following computation, using the scalar  $\alpha$  and vectors  $\mathbf{x}$ ,  $\mathbf{y}$ , and  $\mathbf{z}$ :

 $z \leftarrow y + \alpha x$ 

Table 56. Data Types	
α, <b>x</b> , <b>y</b> , <b>z</b>	Subprogram
Short-precision real	SZAXPY
Long-precision real	DZAXPY
Short-precision complex	CZAXPY
Long-precision complex	ZZAXPY

#### Syntax

Fortran	CALL SZAXPY   DZAXPY   CZAXPY   ZZAXPY (n, alpha, x, incx, y, incy, z, incz)
C and C++	szaxpy   dzaxpy   czaxpy   zzaxpy (n, alpha, x, incx, y, incy, z, incz);
PL/I	CALL SZAXPY   DZAXPY   CZAXPY   ZZAXPY (n, alpha, x, incx, y, incy, z, incz);

#### On Entry

n

is the number of elements in vectors x, y, and z. Specified as: a fullword integer;  $n \ge 0$ .

alpha

is the scalar  $\alpha$ . Specified as: a number of the data type indicated in Table 56.

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 56. incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer. It can have any value.

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 56. incy

is the stride for vector y. Specified as: a fullword integer. It can have any value.

See "On Return."

incz

is the stride for vector z. Specified as: a fullword integer. It can have any value.

#### On Return

z

is the vector  $\mathbf{z}$  of length n, containing the result of the computation  $\mathbf{y} + \alpha \mathbf{x}$ . Returned as: a one-dimensional array of (at least) length 1 + (n-1)|incz|, containing numbers of the data type indicated in Table 56.

#### **Notes**

- 1. If you specify the same vector for  $\mathbf{x}$  and  $\mathbf{z}$ , then incx and incz must be equal; otherwise, results are unpredictable. The same is true for  $\mathbf{y}$  and  $\mathbf{z}$ .
- 2. If you specify different vectors for  $\mathbf{x}$  and  $\mathbf{z}$ , they must have no common elements; otherwise, results are unpredictable. The same is true for  $\mathbf{y}$  and  $\mathbf{z}$ . See "Concepts" on page 55.

**Function:** The computation is expressed as follows:

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ z_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

See reference [73]. If n is 0, no computation is performed. For CZAXPY, intermediate results are accumulated in long precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows vectors **x** and **y** with positive strides.

Call Statement and Input

**Example 2:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite sign, and an output vector  $\mathbf{z}$  having a positive stride. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(5), which is 1.0.

**Example 3:** This example shows a vector, **x**, with 0 stride, and a vector, **z**, with negative stride. x is treated like a vector of length n, all of whose elements are the same as the single element in x. For vector z, results are stored beginning in element Z(5).

Call Statement and Input

N ALPHA X INCX Y INCY Z INCZ

| | | | | | | | | | | | |

CALL SZAXPY(5, 2.0, X, 0, Y, 1, Z, -1)

$$X = (1.0)$$
 $Y = (5.0, 4.0, 3.0, 2.0, 1.0)$ 

Output

 $Z = (3.0, 4.0, 5.0, 6.0, 7.0)$ 

**Example 4:** This example shows a vector, **y**, with 0 stride. **y** is treated like a vector of length n, all of whose elements are the same as the single element in y.

Call Statement and Input

**Example 5:** This example shows how SZAXPY can be used to compute a scalar value. In this case, vectors **x** and **y** contain scalar values. The strides of all vectors, x, y, and z, are 0. The number of elements to be processed, n, is 1.

Call Statement and Input

**Example 6:** This example shows vectors **x** and **y**, containing complex numbers and having positive strides.

### Sparse Vector-Scalar Subprograms

This section contains the sparse vector-scalar subprogram descriptions.

# SSCTR, DSCTR, CSCTR, ZSCTR—Scatter the Elements of a Sparse Vector X in Compressed-Vector Storage Mode into Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode

These subprograms scatter the elements of sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode, into specified elements of sparse vector  $\mathbf{y}$ , stored in full-vector storage mode.

Table 57. Data Types	
<i>x</i> , <i>y</i>	Subprogram
Short-precision real	SSCTR
Long-precision real	DSCTR
Short-precision complex	CSCTR
Long-precision complex	ZSCTR

#### Syntax

Fortran	CALL SSCTR   DSCTR   CSCTR   ZSCTR (nz, x, indx, y)
C and C++	ssctr   dsctr   csctr   zsctr (nz, x, indx, y);
PL/I	CALL SSCTR   DSCTR   CSCTR   ZSCTR (nz, x, indx, y);

#### On Entry

nz

is the number of elements in sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \ge 0$ .

is the sparse vector **x**, containing *nz* elements, stored in compressed-vector storage mode in an array, referred to as X. Specified as: a one-dimensional array of (at least) length *nz*, containing numbers of the data type indicated in Table 57.

#### indx

is the array, referred to as INDX, containing the nz indices that indicate the positions of the elements of the sparse vector  $\boldsymbol{x}$  when in full-vector storage mode. They also indicate the positions in vector  $\boldsymbol{y}$  into which the elements are copied.

Specified as: a one-dimensional array of (at least) length *nz*, containing fullword integers.

See "On Return."

#### On Return

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for i = 1, nz, into which nz elements of vector  $\mathbf{x}$  are copied at positions indicated by the indices array INDX.

Returned as: a one-dimensional array of (at least) length max(INDX(i)) for i = 1, nz, containing numbers of the data type indicated in Table 57.

#### **Notes**

- 1. Each value specified in array INDX must be unique; otherwise, results are unpredictable.
- 2. Vectors **x** and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. For a description of how sparse vectors are stored, see "Sparse Vector" on page 60.

Function: The copy is expressed as follows:

$$y_{\text{INDX}(i)} \leftarrow x_i \quad \text{for } i = 1, nz$$

where:

x is a sparse vector, stored in compressed-vector storage mode.
INDX is the indices array for sparse vector x.
y is a sparse vector, stored in full-vector storage mode.

See reference [29]. If nz is 0, no copy is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: nz < 0

**Example 1:** This example shows how to use SSCTR to copy a sparse vector **x** of length 5 into the following vector **y**, where the elements of array INDX are in ascending order:

$$Y = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)$$

Call Statement and Input

**Example 2:** This example shows how to use SSCTR to copy a sparse vector  $\mathbf{x}$  of length 5 into the following vector  $\mathbf{y}$ , where the elements of array INDX are in random order:

$$Y = (6.0, 2.0, 4.0, 7.0, 6.0, 10.0, -2.0, 8.0, 9.0, 0.0)$$

**Example 3:** This example shows how to use CSCTR to copy a sparse vector  $\mathbf{x}$  of length 3 into the following vector  $\mathbf{y}$ , where the elements of array INDX are in random order:

$$Y = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))$$

= ((3.0, 4.0), (-2.0, 3.0), (5.0, 6.0), (1.0, 2.0))

Call Statement and Input

Υ

## SGTHR, DGTHR, CGTHR, and ZGTHR—Gather Specified Elements of a Sparse Vector Y in Full-Vector Storage Mode into a Sparse Vector X in Compressed-Vector Storage Mode

These subprograms gather specified elements of vector y, stored in full-vector storage mode, into sparse vector x, stored in compressed-vector storage mode.

Table 58. Data Types	
<i>x</i> , <i>y</i>	Subprogram
Short-precision real	SGTHR
Long-precision real	DGTHR
Short-precision complex	CGTHR
Long-precision complex	ZGTHR

#### **Syntax**

Fortran	CALL SGTHR   DGTHR   CGTHR   ZGTHR (nz, y, x, indx)
C and C++	sgthr   dgthr   cgthr   zgthr (nz, y, x, indx);
PL/I	CALL SGTHR   DGTHR   CGTHR   ZGTHR (nz, y, x, indx);

#### On Entry

nz

is the number of elements in sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \ge 0$ .

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for i = 1, nz, from which nz elements are copied from positions indicated by the indices array INDX.

Specified as: a one-dimensional array of (at least) length  $\max(INDX(i))$  for i = 1, nz, containing numbers of the data type indicated in Table 58.

x See "On Return."

indx

is the array, referred to as INDX, containing the nz indices that indicate the positions of the elements of the sparse vector  $\mathbf{x}$  when in full-vector storage mode. They also indicate the positions in vector  $\mathbf{y}$  from which elements are copied.

Specified as: a one-dimensional array of (at least) length *nz*, containing fullword integers.

#### On Return

Х

is the sparse vector  $\mathbf{x}$ , containing  $n\mathbf{z}$  elements, stored in compressed-vector storage mode in an array, referred to as X, into which are copied the elements of vector  $\mathbf{y}$  from positions indicated by the indices array INDX.

Returned as: a one-dimensional array of (at least) length *nz*, containing numbers of the data type indicated in Table 58.

#### **Notes**

- 1. Vectors **x** and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. For a description of how sparse vectors are stored, see "Sparse Vector" on page 60.

Function: The copy is expressed as follows:

$$x_i \leftarrow y_{INDX(i)}$$
 for  $i = 1$ ,  $nz$ 

where:

x is a sparse vector, stored in compressed-vector storage mode.
INDX is the indices array for sparse vector x.
y is a sparse vector, stored in full-vector storage mode.

See reference [29]. If nz is 0, no copy is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: nz < 0

**Example 1:** This example shows how to use SGTHR to copy specified elements of a vector  $\mathbf{y}$  into a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in ascending order.

Call Statement and Input

**Example 2:** This example shows how to use SGTHR to copy specified elements of a vector  $\mathbf{y}$  into a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in random order. (Note that the element 0.0 occurs in output vector  $\mathbf{x}$ . This does not produce an error.)

Call Statement and Input

Output

$$X = (7.0, 4.0, 6.0, 0.0, -2.0)$$

Example 3: This example shows how to use CGTHR to copy specified elements of a vector, y, into a sparse vector, x, of length 3, where the elements of array INDX are in random order.

# SGTHRZ, DGTHRZ, CGTHRZ, and ZGTHRZ—Gather Specified Elements of a Sparse Vector Y in Full-Vector Mode into a Sparse Vector X in Compressed-Vector Mode, and Zero the Same Specified Elements of Y

These subprograms gather specified elements of sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, into sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode, and zero the same specified elements of vector  $\mathbf{y}$ .

Table 59. Data Types	
<i>x</i> , <i>y</i>	Subprogram
Short-precision real	SGTHRZ
Long-precision real	DGTHRZ
Short-precision complex	CGTHRZ
Long-precision complex	ZGTHRZ

#### Syntax

Fortran	CALL SGTHRZ   DGTHRZ   CGTHRZ   ZGTHRZ (nz, y, x, indx)
C and C++	sgthrz   dgthrz   cgthrz   zgthrz (nz, y, x, indx);
PL/I	CALL SGTHRZ   DGTHRZ   CGTHRZ   ZGTHRZ (nz, y, x, indx);

#### On Entry

nz

is the number of elements in sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \ge 0$ .

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for i = 1, nz, from which nz elements are copied from positions indicated by the indices array INDX.

Specified as: a one-dimensional array of (at least) length max(INDX(i)) for i = 1, nz, containing numbers of the data type indicated in Table 59.

x See "On Return."

indx

is the array, referred to as INDX, containing the nz indices that indicate the positions of the elements of the sparse vector  $\boldsymbol{x}$  when in full-vector storage mode. They also indicate the positions in vector  $\boldsymbol{y}$  from which elements are copied then set to zero.

Specified as: a one-dimensional array of (at least) length *nz*, containing fullword integers.

#### On Return

У

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for i=1,  $n\mathbf{z}$ , whose elements are set to zero at positions indicated by the indices array INDX.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 59.

Х

is the sparse vector  $\mathbf{x}$ , containing nz elements stored in compressed-vector storage mode in an array, referred to as X, into which are copied the elements of vector  $\mathbf{y}$  from positions indicated by the indices array INDX.

Returned as: a one-dimensional array of (at least) length *nz*, containing numbers of the data type indicated in Table 59 on page 285.

#### **Notes**

- 1. Each value specified in array INDX must be unique; otherwise, results are unpredictable.
- 2. Vectors **x** and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. For a description of how sparse vectors are stored, see "Sparse Vector" on page 60.

Function: The copy is expressed as follows:

```
x_i \leftarrow y_{\text{INDX}(i)}

y_{\text{INDX}(i)} \leftarrow 0.0 (for SGTHRZ and DGTHRZ)

y_{\text{INDX}(i)} \leftarrow (0.0,0.0) (for CGTHRZ and ZGTHRZ)

for i = 1,nz
```

#### where:

x is a sparse vector, stored in compressed-vector storage mode.
INDX is the indices array for sparse vector x.
y is a sparse vector, stored in full-vector storage mode.

See reference [29]. If nz is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: nz < 0

**Example 1:** This example shows how to use SGTHRZ to copy specified elements of a vector  $\mathbf{y}$  into a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in ascending order.

**Example 2:** This example shows how to use SGTHRZ to copy specified elements of a vector  $\mathbf{y}$  into a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in random order. (Note that the element 0.0 occurs in output vector  $\mathbf{x}$ . This does not produce an error.)

# Call Statement and Input

**Example 3:** This example shows how to use CGTHRZ to copy specified elements of a vector  $\mathbf{y}$  into a sparse vector  $\mathbf{x}$  of length 3, where the elements of array INDX are in random order.

# SAXPYI, DAXPYI, CAXPYI, and ZAXPYI—Multiply a Sparse Vector X in Compressed-Vector Storage Mode by a Scalar, Add to a Sparse Vector Y in Full-Vector Storage Mode, and Store in the Vector Y

These subprograms multiply sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode, by scalar  $\alpha$ , add it to sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, and store the result in vector  $\mathbf{y}$ .

Table 60. Data Types	
α, <b>x</b> , <b>y</b>	Subprogram
Short-precision real	SAXPYI
Long-precision real	DAXPYI
Short-precision complex	CAXPYI
Long-precision complex	ZAXPYI

# Syntax

Fortran	ortran CALL SAXPYI   DAXPYI   CAXPYI   ZAXPYI (nz, alpha, x, indx, y)	
C and C++ saxpyi   daxpyi   caxpyi   zaxpyi (nz, alpha, x, indx, y);		
PL/I	CALL SAXPYI   DAXPYI   CAXPYI   ZAXPYI (nz, alpha, x, indx, y);	

# On Entry

nz

is the number of elements in sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode. Specified as: a fullword integer;  $n\mathbf{z} \ge 0$ .

alpha

is the scalar  $\alpha$ . Specified as: a number of the data type indicated in Table 60.

Х

is the sparse vector  $\mathbf{x}$ , containing  $n\mathbf{z}$  elements, stored in compressed-vector storage mode in an array, referred to as X. Specified as: a one-dimensional array of (at least) length  $n\mathbf{z}$ , containing numbers of the data type indicated in Table 60.

indx

is the array, referred to as INDX, containing the nz indices that indicate the positions of the elements of the sparse vector  $\mathbf{x}$  when in full-vector storage mode. They also indicate the positions of the elements in vector  $\mathbf{y}$  that are used in the computation.

Specified as: a one-dimensional array of (at least) length *nz*, containing fullword integers.

У

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(\mathbf{i}))$  for i=1, nz. Specified as: a one-dimensional array of (at least) length  $\max(\text{INDX}(\mathbf{i}))$  for i=1, nz, containing numbers of the data type indicated in Table 60.

# On Return

V

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length  $\max(\text{INDX}(i))$  for i=1, nz containing the results of the computation, stored at positions indicated by the indices array INDX.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 60 on page 288.

# Notes

- 1. Each value specified in array INDX must be unique; otherwise, results are unpredictable.
- 2. Vectors **x** and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. For a description of how sparse vectors are stored, see "Sparse Vector" on page 60.

Function: The computation is expressed as follows:

$$y_{\text{INDX}(i)} \leftarrow y_{\text{INDX}(i)} + \alpha x_i$$
 for  $i = 1$ ,  $nz$ 

where:

x is a sparse vector, stored in compressed-vector storage mode.
INDX is the indices array for sparse vector x.
y is a sparse vector, stored in full-vector storage mode.

See reference [29]. If  $\alpha$  or nz is zero, no computation is performed. For SAXPYI and CAXPYI, intermediate results are accumulated in long-precision.

# **Error Conditions**

Computational Errors: None

Input-Argument Errors: nz < 0

**Example 1:** This example shows how to use SAXPYI to perform a computation using a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in ascending order.

Call Statement and Input

**Example 2:** This example shows how to use SAXPYI to perform a computation using a sparse vector **x** of length 5, where the elements of array INDX are in random order.

# Call Statement and Input

**Example 3:** This example shows how to use CAXPYI to perform a computation using a sparse vector **x** of length 3, where the elements of array INDX are in random order.

# SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI—Dot Product of a Sparse Vector X in Compressed-Vector Storage Mode and a Sparse Vector Y in Full-Vector Storage Mode

SDOTI, DDOTI, CDOTUI, and ZDOTUI compute the dot product of sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode, and full vector  $\mathbf{y}$ , stored in full-vector storage mode.

CDOTCI and ZDOTCI compute the dot product of the complex conjugate of sparse vector  $\mathbf{x}$ , stored in compressed-vector storage mode, and full vector  $\mathbf{y}$ , stored in full-vector storage mode.

Table 61. Data Types		
x, y, Result	Subprogram	
Short-precision real	SDOTI	
Long-precision real	DDOTI	
Short-precision complex	CDOTUI	
Long-precision complex	ZDOTUI	
Short-precision complex	CDOTCI	
Long-precision complex	ZDOTCI	

# Syntax

Fortran	SDOTI   DDOTI   CDOTUI   ZDOTUI   CDOTCI   ZDOTCI (nz, x, indx, y)
C and C++	sdoti   ddoti   cdotui   zdotui   cdotci   zdotci (nz, x, indx, y);
PL/I	SDOTI   DDOTI   CDOTUI   ZDOTUI   CDOTCI   ZDOTCI (nz, x, indx, y);

# On Entry

nz

is the number of elements in sparse vector x, stored in compressed-vector storage mode. Specified as: a fullword integer;  $nz \ge 0$ .

Χ

is the sparse vector  $\mathbf{x}$ , containing nz elements, stored in compressed-vector storage mode in an array, referred to as X. Specified as: a one-dimensional array of (at least) length nz, containing numbers of the data type indicated in Table 61.

indx

is the array, referred to as INDX, containing the nz indices that indicate the positions of the elements of the sparse vector  $\mathbf{x}$  when in full-vector storage mode. They also indicate the positions of elements in vector  $\mathbf{y}$  that are used in the computation.

Specified as: a one-dimensional array of (at least) length nz, containing fullword integers.

is the sparse vector  $\mathbf{y}$ , stored in full-vector storage mode, of (at least) length max(INDX(i)) for i = 1, nz. Specified as: a one-dimensional array of (at least) length max(INDX(i)) for i = 1, nz, containing numbers of the data type indicated in Table 61.

On Return

Function value

is the result of the dot product computation.

Returned as: a number of the data type indicated in Table 61 on page 291.

# Note

- 1. Declare this function in your program as returning a value of the data type indicated in Table 61 on page 291.
- 2. For a description of how sparse vectors are stored, see "Sparse Vector" on page 60.

**Function:** For SDOTI, DDOTI, CDOTUI, and ZDOTUI, the dot product computation is expressed as follows:

$$\sum_{i=1}^{nz} x_i y_{\text{INDX}(i)} = x_1 y_{\text{INDX}(1)} + x_2 y_{\text{INDX}(2)} + \dots + x_{nz} y_{\text{INDX}(nz)}$$

For CDOTCI and ZDOTCI, the dot product computation is expressed as follows:

$$\sum_{i=1}^{nz} \overline{x}_i y_{\text{INDX}(i)} = \overline{x}_1 y_{\text{INDX}(1)} + \overline{x}_2 y_{\text{INDX}(2)} + \dots + \overline{x}_{nz} y_{\text{INDX}(nz)}$$

where:

**x** is a sparse vector, stored in compressed-vector storage mode.

 $\bar{x}$  is the complex conjugate of a sparse vector, stored in compressed - vector storage mode.

INDX is the indices array for sparse vector  $\mathbf{x}$ .

y is a sparse vector, stored in full-vector storage mode.

See reference [29]. The result is returned as the function value. If *nz* is 0, then zero is returned as the value of the function.

For SDOTI, CDOTUI, and CDOTCI, intermediate results are accumulated in long-precision.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: nz < 0

**Example 1:** This example shows how to use SDOTI to compute a dot product using a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in ascending order.

Function Reference and Input

**Example 2:** This example shows how to use SDOTI to compute a dot product using a sparse vector  $\mathbf{x}$  of length 5, where the elements of array INDX are in random order.

Function Reference and Input

**Example 3:** This example shows how to use CDOTUI to compute a dot product using a sparse vector  $\mathbf{x}$  of length 3, where the elements of array INDX are in ascending order.

Function Reference and Input

**Example 4:** This example shows how to use CDOTCI to compute a dot product using the complex conjugate of a sparse vector  $\mathbf{x}$  of length 3, where the elements of array INDX are in random order.

Function Reference and Input

# SDOTI, DDOTI, CDOTUI, ZDOTUI, CDOTCI, and ZDOTCI

```
NZ X INDX Y
DOTT = CDOTCI(3, X, INDX, Y)
        = ((1.0, 2.0), (3.0, 4.0), (5.0, 6.0))
        = (4, 1, 3)
INDX
        = ((6.0, 5.0), (-2.0, 3.0), (15.0, 4.0), (9.0, 0.0))
Output
DOTT
       = (146.0, -97.0)
```

# **Matrix-Vector Subprograms**

This section contains the matrix-vector subprogram descriptions.

# SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX—Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose

SGEMV and DGEMV compute the matrix-vector product for either a real general matrix or its transpose, using the scalars  $\alpha$  and  $\beta$ , vectors  $\textbf{\textit{x}}$  and  $\textbf{\textit{y}}$ , and matrix  $\textbf{\textit{A}}$  or its transpose:

$$y \leftarrow \beta y + \alpha A x$$
$$y \leftarrow \beta y + \alpha A^{\mathsf{T}} x$$

CGEMV and ZGEMV compute the matrix-vector product for either a complex general matrix, its transpose, or its conjugate transpose, using the scalars  $\alpha$  and  $\beta$ , vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

$$y \leftarrow \beta y + \alpha Ax$$
  
 $y \leftarrow \beta y + \alpha A^{T}x$   
 $y \leftarrow \beta y + \alpha A^{H}x$ 

SGEMX and DGEMX compute the matrix-vector product for a real general matrix, using the scalar  $\alpha$ , vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and matrix  $\mathbf{A}$ :

$$y \leftarrow y + \alpha Ax$$

SGEMTX and DGEMTX compute the matrix-vector product for the transpose of a real general matrix, using the scalar  $\alpha$ , vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and the transpose of matrix  $\mathbf{A}$ :

$$y \leftarrow y + \alpha A^{T} x$$

Table 62. Data Types	
α, β, <b>x</b> , <b>y</b> , <b>A</b>	Subprogram
Short-precision real	SGEMV, SGEMX, and SGEMTX
Long-precision real	DGEMV, DGEMX, and DGEMTX
Short-precision complex	CGEMV
Long-precision complex	ZGEMV

**Note:** SGEMV and DGEMV are Level 2 BLAS subroutines. It is suggested that these subroutines be used instead of SGEMX, DGEMX, SGEMTX, and DGEMTX, which are provided only for compatibility with earlier releases of ESSL.

# Syntax

Fortran	CALL SGEMV   DGEMV   CGEMV   ZGEMV (transa, m, n, alpha, a, lda, x, incx, beta, y, incy)
	CALL SGEMX   DGEMX   SGEMTX   DGEMTX ( m, n, alpha, a, lda, x, incx, y, incy)
C and C++	sgemv   dgemv   cgemv   zgemv (transa, m, n, alpha, a, lda, x, incx, beta, y, incy);
	sgemx   dgemx   sgemtx   dgemtx ( m, n, alpha, a, lda, x, incx, y, incy);
PL/I	CALL SGEMV   DGEMV   CGEMV   ZGEMV (transa, m, n, alpha, a, lda, x, incx, beta, y, incy);
	CALL SGEMX   DGEMX   SGEMTX   DGEMTX ( m, n, alpha, a, lda, x, incx, y, incy);

```
On Entry
transa
    indicates the form of matrix A to use in the computation, where:
   If transa = 'N', A is used in the computation.
    If transa = 'T', A^T is used in the computation.
    If transa = 'C', A^H is used in the computation.
    Specified as: a single character. It must be 'N', 'T', or 'C'.
m
    is the number of rows in matrix A, and:
    For SGEMV, DGEMV, CGEMV, and ZGEMV:
        If transa = 'N', it is the length of vector \mathbf{y}.
        If transa = 'T' or 'C', it is the length of vector x.
    For SGEMX and DGEMX, it is the length of vector y.
    For SGEMTX and DGEMTX, it is the length of vector x.
    Specified as: a fullword integer; 0 \le m \le lda.
n
    is the number of columns in matrix A, and:
    For SGEMV, DGEMV, CGEMV, and ZGEMV:
        If transa = 'N', it is the length of vector x.
        If transa = 'T' or 'C', it is the length of vector y.
    For SGEMX and DGEMX, it is the length of vector x.
    For SGEMTX and DGEMTX, it is the length of vector y.
    Specified as: a fullword integer; n \ge 0.
alpha
    is the scaling constant \alpha. Specified as: a number of the data type indicated in
    Table 62 on page 296.
а
    is the m by n matrix \boldsymbol{A}, where:
    For SGEMV, DGEMV, CGEMV, and ZGEMV:
        If transa = 'N', A is used in the computation.
        If transa = {}^{\mathsf{T}}\mathsf{T}, A^{\mathsf{T}} is used in the computation.
        If transa = 'C', A^H is used in the computation.
    For SGEMX and DGEMX, A is used in the computation.
    For SGEMTX and DGEMTX, A^{T} is used in the computation.
    Note: No data should be moved to form A^T or A^H; that is, the matrix A should
            always be stored in its untransposed form.
```

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 62 on page 296.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

```
X
   is the vector x, where:
   For SGEMV, DGEMV, CGEMV, and ZGEMV:
       If transa = 'N', it has length n.
       If transa = 'T' or 'C', it has length m.
   For SGEMX and DGEMX, it has length n.
   For SGEMTX and DGEMTX, it has length m.
   Specified as: a one-dimensional array, containing numbers of the data type
   indicated in Table 62 on page 296, where:
   For SGEMV, DGEMV, CGEMV, and ZGEMV:
       If transa = 'N', it must have at least 1+(n-1)|incx| elements.
       If transa = 'T' or 'C', it must have at least 1+(m-1)|incx| elements.
   For SGEMX and DGEMX, it must have at least 1+(n-1)|incx| elements.
   For SGEMTX and DGEMTX, it must have at least 1+(m-1)|incx| elements.
incx
   is the stride for vector \mathbf{x}. Specified as: a fullword integer; It can have any value.
beta
   is the scaling constant β. Specified as: a number of the data type indicated in
   Table 62 on page 296.
   is the vector \mathbf{y}, where:
   For SGEMV, DGEMV, CGEMV, and ZGEMV:
       If transa = 'N', it has length m.
       If transa = 'T' or 'C', it has length n.
   For SGEMX and DGEMX, it has length m.
   For SGEMTX and DGEMTX, it has length n.
   Specified as: a one-dimensional array, containing numbers of the data type
   indicated in Table 62 on page 296, where:
   For SGEMV, DGEMV, CGEMV, and ZGEMV:
       If transa = 'N', it must have at least 1+(m-1)|incy| elements.
       If transa = 'T' or 'C', it must have at least 1+(n-1)|incy| elements.
   For SGEMX and DGEMX, it must have at least 1+(m-1)|incy| elements.
   For SGEMTX and DGEMTX, it must have at least 1+(n-1)|incy| elements.
incy
   is the stride for vector \mathbf{y}. Specified as: a fullword integer; incy > 0 or incy < 0.
On Return
   is the vector \mathbf{y}, containing the result of the computation, where:
   For SGEMV, DGEMV, CGEMV, and ZGEMV:
       If transa = 'N', it has length m.
       If transa = 'T' or 'C', it has length n.
```

For SGEMX and DGEMX, it has length m.

For SGEMTX and DGEMTX, it has length *n*.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 62 on page 296.

# Notes

- 1. For SGEMV and DGEMV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 2. The SGEMV, DGEMV, CGEMV, and ZGEMV subroutines accept lowercase letters for the *transa* argument.
- 3. In the SGEMV, DGEMV, CGEMV, and ZGEMV subroutines, *incx* = 0 is valid; however, the Level 2 BLAS standard considers *incx* = 0 to be invalid. See references [34] and [35].
- 4. Vector **y** must have no common elements with matrix **A** or vector **x**; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The possible computations that can be performed by these subroutines are described in the following sections. Varying implementation techniques are used for this computation to improve performance. As a result, accuracy of the computational result may vary for different computations.

For SGEMV, CGEMV, SGEMX, and SGEMTX, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are stored.

See references [34], [35], [38], [46], and [73]. No computation is performed if m or n is 0 or if  $\alpha$  is zero and  $\beta$  is one.

*General Matrix:* For SGEMV, DGEMV, CGEMV, and ZGEMV, the matrix-vector product for a general matrix:

$$y \leftarrow \beta y + \alpha Ax$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

For SGEMX and DGEMX, the matrix-vector product for a real general matrix:

$$y \leftarrow y + \alpha Ax$$

is expressed as follows:

# SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

$$\begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \ddots \\ \vdots & & \ddots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

In these expressions:

y is a vector of length m.

 $\alpha$  is a scalar.

 $\beta$  is a scalar.

A is an m by n matrix.

x is a vector of length n.

*Transpose of a General Matrix:* For SGEMV, DGEMV, CGEMV and ZGEMV, the matrix-vector product for the transpose of a general matrix:

$$y \leftarrow \beta y + \alpha A^T x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \vdots & & \ddots \\ a_{1n} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$$

For SGEMTX and DGEMTX, the matrix-vector product for the transpose of a real general matrix:

$$y \leftarrow y + \alpha A^T x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ a_{1n} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_m \end{bmatrix}$$

In these expressions:

y is a vector of length n.

 $\alpha$  is a scalar.

 $\beta$  is a scalar.

 $A^{T}$  is the transpose of matrix A, where A is an m by n matrix.

x is a vector of length m.

Conjugate Transpose of a General Matrix: For CGEMV and ZGEMV, the matrix-vector product for the conjugate transpose of a general matrix:

$$y \leftarrow \beta y + \alpha A^{H} x$$

is expressed as follows:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} \overline{a}_{11} & \dots & \overline{a}_{m1} \\ \vdots & \ddots & \vdots \\ \overline{a}_{1n} & \dots & \overline{a}_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$$

# where:

y is a vector of length n.

 $\alpha$  is a scalar.

 $\beta$  is a scalar.

 $A^{H}$  is the conjugate transpose of matrix A, where A is an m by n matrix. x is a vector of length m.

# **Error Conditions**

Resource Errors: Unable to allocate internal work area (for SGEMV, DGEMV, CGEMV, and ZGEMV).

Computational Errors: None

Input-Argument Errors

- 1. transa ≠ 'N', 'T', or 'C'
- 2. m < 0
- 3. m > Ida
- 4. n < 0
- 5.  $Ida \leq 0$
- 6. incy = 0

**Example 1:** This example shows the computation for TRANSA equal to 'N', where the real general matrix A is used in the computation. Because Ida is 10 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=10 and  $F2-F1+1 \ge 3$ . In this example, array A is declared as A(1:10,0:2).

$$X = (3.0, 2.0, 1.0)$$
 $Y = (4.0, ..., 5.0, ..., 2.0, ..., 3.0)$ 

Output
 $Y = (14.0, ..., 19.0, ..., 17.0, ..., 20.0)$ 

Example 2: This example shows the computation for TRANSA equal to 'T', where the transpose of the real general matrix A is used in the computation. Array A must follow the same rules as given in Example 1. In this example, array A is declared as A(-1:8,1:3).

Call Statement and Input

**Example 3:** This example shows the computation for TRANSA equal to 'N', where the complex general matrix **A** is used in the computation.

**Example 4:** This example shows the computation for TRANSA equal to 'T', where the transpose of complex general matrix  $\bf A$  is used in the computation. Because  $\beta$  is zero, the result of the computation is  $\alpha {\bf A}^{T}{\bf x}$ 

# Call Statement and Input

**Example 5:** This example shows the computation for TRANSA equal to 'C', where the conjugate transpose of the complex general matrix  $\boldsymbol{A}$  is used in the computation.

Call Statement and Input

**Example 6:** This example shows a matrix, A, contained in a larger array, A. The strides of vectors x and y are positive. Because Ida is 10 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=10 and F2-F1+1  $\geq$  3. For this example, array A is declared as A(1:10,0:2).

**Example 7:** This example shows a matrix,  $\mathbf{A}$ , contained in a larger array, A. The strides of vectors  $\mathbf{x}$  and  $\mathbf{y}$  are of opposite sign. For  $\mathbf{y}$ , which has negative stride, processing begins at element Y(7), which is 4.0. Array A must follow the same rules as given in Example 6. For this example, array A is declared as A(-1:8,1:3).

Call Statement and Input

**Example 8:** This example shows a matrix, A, contained in a larger array, A, and the first element of the matrix is not the first element of the array. Array A must follow the same rules as given in Example 6. For this example, array A is declared as A(1:10,1:3).

**Example 9:** This example shows a matrix, A, and an array, A, having the same number of rows. For this case, m and lda are equal. Because lda is 4 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=4 and  $F2-F1+1 \ge 3$ . For this example, array A is declared as A(1:4,0:2).

Call Statement and Input

$$X = (3.0, 2.0, 1.0)$$
  
 $Y = (4.0, 5.0, 2.0, 3.0)$ 

Output

$$Y = (14.0, 19.0, 17.0, 20.0)$$

**Example 10:** This example shows a matrix, A, and an array, A, having the same number of rows. For this case, m and lda are equal. Because lda is 4 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=4 and  $F2-F1+1 \ge 3$ . For this example, array A is declared as A(1:4,0:2).

# SGEMV, DGEMV, CGEMV, ZGEMV, SGEMX, DGEMX, SGEMTX, and DGEMTX

Example 11: This example shows a computation in which alpha is greater than 1. Array A must follow the same rules as given in Example 10. For this example, array A is declared as A(-1:2,1:3).

# SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC—Rank-One Update of a General Matrix

SGER, DGER, CGERU, and ZGERU compute the rank-one update of a general matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vector  $\boldsymbol{x}$ , and the transpose of vector  $\boldsymbol{y}$ :

$$A \leftarrow A + \alpha x y^T$$

CGERC and ZGERC compute the rank-one update of a general matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vector  $\boldsymbol{x}$ , and the conjugate transpose of vector  $\boldsymbol{y}$ :

$$A \leftarrow A + \alpha xy^{H}$$

Table 63. Data Types	
α, <b>A</b> , <b>x</b> , <b>y</b>	Subprogram
Short-precision real	SGER
Long-precision real	DGER
Short-precision complex	CGERU and CGERC
Long-precision complex	ZGERU and ZGERC

**Note:** For compatibility with earlier releases of ESSL, you can use the names SGER1 and DGER1 for SGER and DGER, respectively.

# Syntax

Fortran	CALL SGER   DGER   CGERU   ZGERU   CGERC   ZGERC (m, n, alpha, x, incx, y, incy, a, lda)
C and C++	sger   dger   cgeru   zgeru   cgerc   zgerc (m, n, alpha, x, incx, y, incy, a, lda);
PL/I	CALL SGER   DGER   CGERU   ZGERU   CGERC   ZGERC (m, n, alpha, x, incx, y, incy, a, lda);

On Entry

m

is the number of rows in matrix A and the number of elements in vector x. Specified as: a fullword integer;  $0 \le m \le lda$ .

n

is the number of columns in matrix A and the number of elements in vector y. Specified as: a fullword integer;  $n \ge 0$ .

alpha

is the scaling constant  $\alpha$ . Specified as: a number of the data type indicated in Table 63.

х

is the vector  $\mathbf{x}$  of length m. Specified as: a one-dimensional array of (at least) length 1+(m-1)|incx|, containing numbers of the data type indicated in Table 63.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

is the vector  $\mathbf{y}$  of length n, whose transpose or conjugate transpose is used in the computation.

**Note:** No data should be moved to form  $y^T$  or  $y^H$ ; that is, the vector y should always be stored in its untransposed form.

Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 63.

incv

is the stride for vector **y**. Specified as: a fullword integer. It can have any value.

а

is the m by n matrix A. Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 63 on page 307.

lda

is the size of the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

# On Return

а

is the m by n matrix  $\boldsymbol{A}$ , containing the result of the computation.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 63 on page 307.

#### **Notes**

- 1. In these subroutines, incx = 0 and incy = 0 are valid; however, the Level 2 BLAS standard considers incx = 0 and incy = 0 to be invalid. See references [34] and [35].
- 2. Matrix **A** can have no common elements with vectors **x** and **y**; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** SGER, DGER, CGERU, and ZGERU compute the rank-one update of a general matrix:

$$A \leftarrow A + \alpha x v^{T}$$

where:

**A** is an *m* by *n* matrix.

 $\alpha$  is a scalar.

x is a vector of length m.

 $y^{\mathsf{T}}$  is the transpose of vector y of length n.

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} [y_1 \dots y_n]$$

It can also be expressed as:

# SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} + \alpha x_1 y_1 & \dots & a_{1n} + \alpha x_1 y_n \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} + \alpha x_m y_1 & \dots & a_{mn} + \alpha x_m y_n \end{bmatrix}$$

CGERC and ZGERC compute a slightly different rank-one update of a general matrix:

$$A \leftarrow A + \alpha xy^{H}$$

where:

A is an m by n matrix.

 $\alpha$  is a scalar.

**x** is a vector of length *m*.

 $y^{H}$  is the conjugate transpose of vector y of length n.

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} [\bar{y}_1 \dots \bar{y}_n]$$

It can also be expressed as:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} + \alpha x_1 \overline{y}_1 & \dots & a_{1n} + \alpha x_1 \overline{y}_n \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} + \alpha x_m \overline{y}_1 & \dots & a_{mn} + \alpha x_m \overline{y}_n \end{bmatrix}$$

See references [34], [35], and [73]. No computation is performed if m, n, or  $\alpha$  is zero. For CGERU and CGERC, intermediate results are accumulated in long precision. For SGER, intermediate results are accumulated in long precision on some platforms.

# **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors

1. m < 0

2. n < 0

 $3. Ida \leq 0$ 

4. m > Ida

**Example 1:** This example shows a matrix, **A**, contained in a larger array, A. The strides of vectors  $\mathbf{x}$  and  $\mathbf{y}$  are positive. Because *lda* is 10 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=10 and  $F2-F1+1 \ge 3$ . For this example, array A is declared as A(1:10,0:2).

# Call Statement and Input

# Output

$$A = \begin{bmatrix} 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \\ & & & & \\ & & & \\ &$$

Example 2: This example shows a matrix, A, contained in a larger array, A. The strides of vectors **x** and **y** are of opposite sign. For **y**, which has negative stride, processing begins at element Y(5), which is 1.0. Array A must follow the same rules as given in Example 1. For this example, array A is declared as A(-1:8,1:3).

Output

A =(same as input A in Example 1)

**Example 3:** This example shows a matrix, A, contained in a larger array, A, and the first element of the matrix is not the first element of the array. Array A must follow the same rules as given in Example 1. For this example, array A is declared as A(1:10,1:3).

Call Statement and Input

Output

$$A = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 4:** This example shows a matrix, A, and array, A, having the same number of rows. For this case, m and lda are equal. Because lda is 4 and n is 3, array A must be declared as A(E1:E2,F1:F2), where E2-E1+1=4 and F2-F1+1  $\geq$  3. For this example, array A is declared as A(1:4,0:2).

# SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 2.0 & 2.0 & 4.0 \\ 3.0 & 2.0 & 2.0 \\ 4.0 & 2.0 & 1.0 \end{bmatrix}$$

Output

$$A = \begin{bmatrix} 4.0 & 8.0 & 12.0 \\ 4.0 & 6.0 & 10.0 \\ 4.0 & 4.0 & 5.0 \\ 8.0 & 10.0 & 13.0 \end{bmatrix}$$

**Example 5:** This example shows a computation in which scalar value for alpha is greater than 1. Array A must follow the same rules as given in Example 4. For this example, array A is declared as A(-1:2,1:3).

Call Statement and Input

Output

$$A = \begin{bmatrix} 7.0 & 14.0 & 21.0 \\ 6.0 & 10.0 & 16.0 \\ 5.0 & 6.0 & 8.0 \\ 12.0 & 18.0 & 25.0 \end{bmatrix}$$

**Example 6:** This example shows a rank-one update in which all data items contain complex numbers, and the transpose  $\mathbf{y}^{\mathsf{T}}$  is used in the computation. Matrix **A** is contained in a larger array, A. The strides of vectors **x** and **y** are positive. The Fortran DIMENSION statement for array A must follow the same rules as given in Example 1. For this example, array A is declared as A(1:10,0:2).

Output

$$A = \begin{bmatrix} (-2.0, & 6.0) & (7.0, & 13.0) & (5.0, & 1.0) \\ (6.0, & 11.0) & (23.0, & 9.0) & (8.0, & 4.0) \\ (6.0, & 7.0) & (5.0, & 8.0) & (8.0, & 0.0) \\ (3.0, & 12.0) & (14.0, & 21.0) & (15.0, & 1.0) \\ (11.0, & 5.0) & (11.0, & 6.0) & (3.0, & -2.0) \\ & & & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ &$$

**Example 7:** This example shows a rank-one update in which all data items contain complex numbers, and the conjugate transpose  $y^H$  is used in the computation. Matrix A is contained in a larger array, A. The strides of vectors x and y are positive. The Fortran DIMENSION statement for array A must follow the same rules as given in Example 1. For this example, array A is declared as A(1:10,0:2).

# Call Statement and Input

Output

# SGER, DGER, CGERU, ZGERU, CGERC, and ZGERC

A =	(6.0, (10.0,	-5.0) 3.0) 0.0)	(7.0, (23.0, (5.0, (14.0, (11.0,	9.0) 8.0) 21.0)	(8.0, (6.0, (7.0,	2.0)
			•		•	ļ
	•		•		•	
			•			İ
					•	į

# SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, ZHEMV, SSLMX, and DSLMX—Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix

SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV compute the matrix-vector product for either a real symmetric matrix or a complex Hermitian matrix, using the scalars  $\alpha$  and  $\beta$ , matrix A, and vectors x and y:

$$y \leftarrow \beta y + \alpha Ax$$

SSLMX and DSLMX compute the matrix-vector product for a real symmetric matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , and vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ :

$$y \leftarrow y + \alpha Ax$$

The following storage modes are used:

- For SSPMV, DSPMV, CHPMV, and ZHPMV, matrix **A** is stored in upper- or lower-packed storage mode.
- For SSYMV, DSYMV, CHEMV, and ZHEMV, matrix A is stored in upper or lower storage mode.
- For SSLMX and DSLMX, matrix **A** is stored in lower-packed storage mode.

Table 64. Data Types	
α, β, <b>Α</b> , <b>x</b> , <b>y</b>	Subprogram
Short-precision real	SSPMV, SSYMV, and SSLMX
Long-precision real	DSPMV, DSYMV, and DSLMX
Short-precision complex	CHPMV and CHEMV
Long-precision complex	ZHPMV and ZHEMV

**Note:** SSPMV and DSPMV are Level 2 BLAS subroutines. You should use these subroutines instead of SSLMX and DSLMX, which are provided only for compatibility with earlier releases of ESSL.

# Syntax

Fortran	CALL SSPMV   DSPMV   CHPMV   ZHPMV (uplo, n, alpha, ap, x, incx, beta, y, incy)	
	CALL SSYMV   DSYMV   CHEMV   ZHEMV (uplo, n, alpha, a, lda, x, incx, beta, y, incy)	
	CALL SSLMX   DSLMX (n, alpha, ap, x, incx, y, incy)	
C and C++	sspmv   dspmv   chpmv   zhpmv (uplo, n, alpha, ap, x, incx, beta, y, incy);	
	ssymv   dsymv   chemv   zhemv (uplo, n, alpha, a, lda, x, incx, beta, y, incy);	
	sslmx   dslmx (n, alpha, ap, x, incx, y, incy);	
PL/I	CALL SSPMV   DSPMV   CHPMV   ZHPMV (uplo, n, alpha, ap, x, incx, beta, y, incy);	
	CALL SSYMV   DSYMV   CHEMV   ZHEMV (uplo, n, alpha, a, lda, x, incx, beta, y, incy);	
	CALL SSLMX   DSLMX (n, alpha, ap, x, incx, y, incy);	

On Entry

uplo

indicates the storage mode used for matrix **A**, where:

If *uplo* = 'U', **A** is stored in upper-packed or upper storage mode.

If *uplo* = 'L', **A** is stored in lower-packed or lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

n

is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$  and the order of matrix  $\mathbf{A}$ . Specified as: a fullword integer;  $n \ge 0$ .

alpha

is the scaling constant  $\alpha$ . Specified as: a number of the data type indicated in Table 64 on page 315.

ap

has the following meaning:

For SSPMV and DSPMV, ap is the real symmetric matrix  $\boldsymbol{A}$  of order n, stored in upper- or lower-packed storage mode.

For CHPMV and ZHPMV, ap is the complex Hermitian matrix A of order n, stored in upper- or lower-packed storage mode.

For SSLMX and DSLMX, ap is the real symmetric matrix  $\boldsymbol{A}$  of order n, stored in lower-packed storage mode.

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 64 on page 315.

а

has the following meaning:

For SSYMV and DSYMV, a is the real symmetric matrix A of order n, stored in upper or lower storage mode.

For CHEMV and ZHEMV, a is the complex Hermitian matrix  $\boldsymbol{A}$  of order n, stored in upper or lower storage mode.

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 64 on page 315.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 64 on page 315.

incx

is the stride for vector **x**. Specified as: a fullword integer, where:

For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV, incx < 0 or incx > 0.

For SSLMX and DSLMX, incx can have any value.

beta

is the scaling constant  $\beta$ . Specified as: a number of the data type indicated in Table 64 on page 315.

У

is the vector  $\mathbf{y}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 64 on page 315.

incy

is the stride for vector  $\mathbf{y}$ . Specified as: a fullword integer; incy > 0 or incy < 0.

# On Return

V

is the vector  $\mathbf{y}$  of length n, containing the result of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 64 on page 315.

# Notes

- 1. All subroutines accept lowercase letters for the uplo argument.
- 2. The vector **y** must have no common elements with vector **x** or matrix **A**; otherwise, results are unpredictable. See "Concepts" on page 55.
- On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix *A* are assumed to be zero, so you do not have to set these values.
- 4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines perform the computations described in the two sections below. See references [34], [35], and [73]. For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV, if n is zero or if  $\alpha$  is zero and  $\beta$  is one, no computation is performed. For SSLMX and DSLMX, if n or  $\alpha$  is zero, no computation is performed.

For SSLMX, SSPMV, SSYMV, CHPMV, and CHEMV, intermediate results are accumulated in long precision. However, several intermediate stores may occur for each element of the vector  $\mathbf{v}$ .

For SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, and ZHEMV: These subroutines compute the matrix-vector product for either a real symmetric matrix or a complex Hermitian matrix:

$$y \leftarrow \beta y + \alpha Ax$$

#### where:

**y** is a vector of length *n*.

 $\boldsymbol{\alpha}$  is a scalar.

 $\beta$  is a scalar.

**A** is a real symmetric or complex Hermitian matrix of order *n*.

**x** is a vector of length *n*.

It is expressed as follows:

# SSPMV, DSPMV, CHPMV, ZHPMV, SSYMV, DSYMV, CHEMV, ZHEMV, SSLMX, and DSLMX

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \beta \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & \cdot \\$$

For SSLMX and DSLMX: These subroutines compute the matrix-vector product for a real symmetric matrix stored in lower-packed storage mode:

$$y \leftarrow y + \alpha Ax$$

where:

y is a vector of length n.

 $\alpha$  is a scalar.

A is a real symmetric matrix of order n.

x is a vector of length n.

It is expressed as follows:

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix} + \alpha \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

# **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. *uplo* ≠ 'L' or 'U'
- 2. n < 0
- 3. Ida < n
- $4. Ida \leq 0$
- 5. incx = 0
- 6. incy = 0

**Example 1:** This example shows vectors **x** and **y** with positive strides and a real symmetric matrix **A** of order 3, stored in lower-packed storage mode. Matrix **A** is:

**Example 2:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is 1.0. The real symmetric matrix  $\mathbf{A}$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

Call Statement and Input

**Example 3:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  with positive stride and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. Matrix  $\mathbf{A}$  is:

$$\begin{bmatrix} (1.0, 0.0) & (3.0, 5.0) & (2.0, -3.0) \\ (3.0, -5.0) & (7.0, 0.0) & (4.0, -8.0) \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, 0.0) \end{bmatrix}$$

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.

**Example 4:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is (1.0, 2.0). The complex Hermitian matrix  $\mathbf{A}$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.

Call Statement and Input

**Example 5:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  with positive strides and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

Call Statement and Input

= (39.0, . , 34.0, . , 25.0)

**Example 6:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is 1.0. The real symmetric matrix  $\mathbf{A}$  of order 3 is stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

$$X = (4.0, ., 2.0, ., 1.0)$$
  
 $Y = (6.0, 5.0, 4.0)$ 

Output

$$A = (36.0, 54.0, 36.0)$$

**Example 7:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  with positive stride and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in lower storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.

Call Statement and Input

UPLO N ALPHA A LDA X INCX BETA Y INCY

| | | | | | | | | | | | | | | |

CALL CHEMV('L', 3, ALPHA, A, 3, X, 1, BETA, Y, 2)

ALPHA = 
$$(1.0, 0.0)$$

$$A = \begin{bmatrix} (1.0, .) & . & . & . \\ (3.0, -5.0) & (7.0, .) & . & . \\ (2.0, 3.0) & (4.0, 8.0) & (6.0, .) \end{bmatrix}$$

$$X = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))$$

BETA =  $(1.0, 0.0)$ 

Y =  $((1.0, 0.0), ..., (2.0, -1.0), ..., (2.0, 1.0))$ 

Output

**Example 8:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is (1.0, 2.0). The complex Hermitian matrix  $\mathbf{A}$  of order 3 is stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

= ((32.0, 21.0), . , (87.0, -8.0), . , (32.0, 64.0))

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.

Call Statement and Input

Υ

**Example 9:** This example shows vectors x and y with positive strides and a real symmetric matrix A of order 3. Matrix A is:

# SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1 —Rank-One Update of a Real Symmetric or Complex Hermitian Matrix

SSPR, DSPR, SSYR, DSYR, SSLR1, and DSLR1 compute the rank-one update of a real symmetric matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vector  $\boldsymbol{x}$ , and its transpose  $\boldsymbol{x}^T$ :

# $\mathbf{A} \leftarrow \mathbf{A} + \alpha \mathbf{x} \mathbf{x}^{\mathsf{T}}$

CHPR, ZHPR, CHER, and ZHER compute the rank-one update of a complex Hermitian matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vector  $\boldsymbol{x}$ , and its conjugate transpose  $\boldsymbol{x}^H$ :

### $A \leftarrow A + \alpha x x^H$

The following storage modes are used:

- For SSPR, DSPR, CHPR, and ZHPR, matrix **A** is stored in upper- or lower-packed storage mode.
- For SSYR, DSYR, CHER, and ZHER, matrix A is stored in upper or lower storage mode.
- For SSLR1 and DSLR1, matrix **A** is stored in lower-packed storage mode.

Table 65. Data Types		
A, x	α	Subprogram
Short-precision real	Short-precision real	SSPR, SSYR, and SSLR1
Long-precision real	Long-precision real	DSPR, DSYR, and DSLR1
Short-precision complex	Short-precision real	CHPR and CHER
Long-precision complex	Long-precision real	ZHPR and ZHER

**Note:** SSPR and DSPR are Level 2 BLAS subroutines. You should use these subroutines instead of SSLR1 and DSLR1, which are only provided for compatibility with earlier releases of ESSL.

# Syntax

Fortran	CALL SSPR   DSPR   CHPR   ZHPR (uplo, n, alpha, x, incx, ap)
	CALL SSYR   DSYR   CHER   ZHER (uplo, n, alpha, x, incx, a, lda)
	CALL SSLR1   DSLR1 (n, alpha, x, incx, ap)
C and C++	sspr   dspr   chpr   zhpr (uplo, n, alpha, x, incx, ap);
	ssyr   dsyr   cher   zher (uplo, n, alpha, x, incx, a, lda);
	sslr1   dslr1 (n, alpha, x, incx, ap);
PL/I	CALL SSPR   DSPR   CHPR   ZHPR (uplo, n, alpha, x, incx, ap);
	CALL SSYR   DSYR   CHER   ZHER (uplo, n, alpha, x, incx, a, lda);
	CALL SSLR1   DSLR1 (n, alpha, x, incx, ap);

On Entry

# SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

uplo

indicates the storage mode used for matrix A, where:

If *uplo* = 'U', **A** is stored in upper-packed or upper storage mode.

If *uplo* = 'L', **A** is stored in lower-packed or lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

n

is the number of elements in vector  $\mathbf{x}$  and the order of matrix  $\mathbf{A}$ . Specified as: a fullword integer;  $n \ge 0$ .

alpha

is the scaling constant  $\alpha$ . Specified as: a number of the data type indicated in Table 65 on page 323.

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 65 on page 323.

incx

is the stride for vector **x**. Specified as: a fullword integer, where:

For SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, and ZHER, *incx* < 0 or *incx* > 0.

For SSLR1 and DSLR1, incx can have any value.

ар

has the following meaning:

For SSPR and DSPR, ap is the real symmetric matrix A of order n, stored in upper- or lower-packed storage mode.

For CHPR and ZHPR, ap is the complex Hermitian matrix  $\boldsymbol{A}$  of order n, stored in upper- or lower-packed storage mode.

For SSLR1 and DSLR1, ap is the real symmetric matrix  $\boldsymbol{A}$  of order n, stored in lower-packed storage mode.

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 65 on page 323.

а

has the following meaning:

For SSYR and DSYR, *a* is the real symmetric matrix *A* of order *n*, stored in upper or lower storage mode.

For CHER and ZHER, *a* is the complex Hermitian matrix *A* of order *n*, stored in upper or lower storage mode.

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 65 on page 323.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

#### On Return

ар

is the matrix A of order n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 65 on page 323.

а

is the matrix  $\mathbf{A}$  of order n, containing the results of the computation. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 65 on page 323.

#### **Notes**

- 1. All subroutines accept lowercase letters for the *uplo* argument.
- 2. The vector **x** must have no common elements with matrix **A**; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\mathbf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.
- 4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines perform the computations described in the two sections below. See references [34], [35], and [73]. If n or  $\alpha$  is 0, no computation is performed.

For CHPR and CHER, intermediate results are accumulated in long precision. For SSPR, SSYR, and SSLR1, intermediate results are accumulated in long precision on some platforms.

For SSPR, DSPR, SSYR, DSYR, SSLR1, and DSLR1: These subroutines compute the rank-one update of a real symmetric matrix:

$$A \leftarrow A + \alpha x x^T$$

where:

**A** is a real symmetric matrix of order *n*.

 $\alpha$  is a scalar.

**x** is a vector of length *n*.

 $\mathbf{x}^{\mathsf{T}}$  is the transpose of vector  $\mathbf{x}$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} [x_1 \dots x_n]$$

For CHPR, ZHPR, CHER, and ZHER: These subroutines compute the rank-one update of a complex Hermitian matrix:

$$A \leftarrow A + \alpha x x^H$$

where:

# SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

**A** is a complex Hermitian matrix of order *n*.

 $\alpha$  is a scalar.

**x** is a vector of length *n*.

 $\mathbf{x}^{H}$  is the conjugate transpose of vector  $\mathbf{x}$ .

It is expressed as follows:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} [\bar{x}_1 & \dots & \bar{x}_n]$$

#### **Error Condition**

Computational Errors: None

Input-Argument Errors

- 1. *uplo* ≠ 'L' or 'U'
- 2. n < 0
- 3. incx = 0
- $4. Ida \leq 0$
- 5. Ida < n

**Example 1:** This example shows a vector  $\mathbf{x}$  with a positive stride, and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. Matrix  $\mathbf{A}$  is:

Call Statement and Input

**Example 2:** This example shows a vector **x** with a negative stride, and a real symmetric matrix **A** of order 3, stored in upper-packed storage mode. It uses the same input matrix **A** as in Example 1.

**Example 3:** This example shows a vector **x** with a positive stride, and a complex Hermitian matrix **A** of order 3, stored in lower-packed storage mode. Matrix **A** is:

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\bf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

Call Statement and Input

**Example 4:** This example shows a vector  $\mathbf{x}$  with a negative stride, and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in upper-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\mathbf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

**Example 5:** This example shows a vector  $\mathbf{x}$  with a positive stride, and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

# Call Statement and Input

#### Output

$$A = \begin{bmatrix} 17.0 & . & . \\ 10.0 & 10.0 & . \\ 5.0 & 9.0 & 4.0 \end{bmatrix}$$

**Example 6:** This example shows a vector  $\mathbf{x}$  with a negative stride, and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

#### Call Statement and Input

# Output

$$A = \begin{bmatrix} 17.0 & 10.0 & 5.0 \\ . & 10.0 & 9.0 \\ . & . & 4.0 \\ . & . & . \end{bmatrix}$$

**Example 7:** This example shows a vector  $\mathbf{x}$  with a positive stride, and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in lower storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\bf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

Call Statement and Input

UPLO N ALPHA X INCX A LDA

| | | | | | | | | | |

CALL CHER('L', 3, 1.0, X, 1, A, 3)

X = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))

A = 
$$\begin{bmatrix} (1.0, ...) & ... & .$$

Output

$$A = \begin{bmatrix} (6.0, 0.0) & . & . \\ (7.0, -13.0) & (23.0, 0.0) & . \\ (13.0, 1.0) & (16.0, 24.0) & (31.0, 0.0) \end{bmatrix}$$

**Example 8:** This example shows a vector  $\mathbf{x}$  with a negative stride, and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\bf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq 0.0$ , they are set to zero.

Call Statement and Input

Output

$$A = \begin{bmatrix} (6.0, 0.0) & (7.0, 13.0) & (13.0, -1.0) \\ . & (23.0, 0.0) & (16.0, -24.0) \\ . & . & (31.0, 0.0) \end{bmatrix}$$

**Example 9:** This example shows a vector  $\mathbf{x}$  with a positive stride, and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

# SSPR, DSPR, CHPR, ZHPR, SSYR, DSYR, CHER, ZHER, SSLR1, and DSLR1

# SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2—Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix

SSPR2, DSPR2, SSYR2, DSYR2, SSLR2, and DSLR2 compute the rank-two update of a real symmetric matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ , and their transposes  $\boldsymbol{x}^{\mathsf{T}}$  and  $\boldsymbol{y}^{\mathsf{T}}$ :

$$\mathbf{A} \leftarrow \mathbf{A} + \alpha \mathbf{x} \mathbf{y}^\mathsf{T} + \alpha \mathbf{y} \mathbf{x}^\mathsf{T}$$

CHPR2, ZHPR2, CHER2, and ZHER2, compute the rank-two update of a complex Hermitian matrix, using the scalar  $\alpha$ , matrix  $\boldsymbol{A}$ , vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ , and their conjugate transposes  $\boldsymbol{x}^H$  and  $\boldsymbol{y}^H$ :

$$A \leftarrow A + \alpha x y^{\mathrm{H}} + \overline{\alpha} y x^{\mathrm{H}}$$

The following storage modes are used:

- For SSPR2, DSPR2, CHPR2, and ZHPR2, matrix **A** is stored in upper- or lower-packed storage mode.
- For SSYR2, DSYR2, CHER2, and ZHER2, matrix A is stored in upper or lower storage mode.
- For SSLR2 and DSLR2, matrix **A** is stored in lower-packed storage mode.

Table 66. Data Types	
α, <b>A</b> , <b>x</b> , <b>y</b>	Subprogram
Short-precision real	SSPR2, SSYR2, and SSLR2
Long-precision real	DSPR2, DSYR2, and DSLR2
Short-precision complex	CHPR2 and CHER2
Long-precision complex	ZHPR2 and ZHER2

**Note:** SSPR2 and DSPR2 are Level 2 BLAS subroutines. You should use these subroutines instead of SSLR2 and DSLR2, which are only provided for compatibility with earlier releases of ESSL.

# Syntax

Fortran	CALL SSPR2   DSPR2   CHPR2   ZHPR2 (uplo, n, alpha, x, incx, y, incy, ap)
	CALL SSYR2   DSYR2   CHER2   ZHER2 (uplo, n, alpha, x, incx, y, incy, a, lda)
	CALL SSLR2   DSLR2 (n, alpha, x, incx, y, incy, ap)
C and C++	sspr2   dspr2   chpr2   zhpr2 (uplo, n, alpha, x, incx, y, incy, ap);
	ssyr2   dsyr2   cher2   zher2 (uplo, n, alpha, x, incx, y, incy, a, lda);
	sslr2   dslr2 (n, alpha, x, incx, y, incy, ap);
PL/I	CALL SSPR2   DSPR2   CHPR2   ZHPR2 (uplo, n, alpha, x, incx, y, incy, ap);
	CALL SSYR2   DSYR2   CHER2   ZHER2 (uplo, n, alpha, x, incx, y, incy, a lda);
	CALL SSLR2   DSLR2 (n, alpha, x, incx, y, incy, ap);

```
On Entry
olau
   indicates the storage mode used for matrix A, where:
   If uplo = 'U', A is stored in upper-packed or upper storage mode.
   If uplo = 'L', A is stored in lower-packed or lower storage mode.
   Specified as: a single character. It must be 'U&csq or 'L'.
    is the number of elements in vectors x and y and the order of matrix A.
    Specified as: a fullword integer; n \ge 0.
alpha
   is the scaling constant \alpha. Specified as: a number of the data type indicated in
   Table 66 on page 331.
   is the vector x of length n. Specified as: a one-dimensional array of (at least)
   length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 66
    on page 331.
incx
   is the stride for vector x.
   Specified as: a fullword integer, where:
   For SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, and ZHER2,
   incx < 0 \text{ or } incx > 0.
   For SSLR2 and DSLR2, incx can have any value.
   is the vector y of length n. Specified as: a one-dimensional array of (at least)
   length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 66
   on page 331.
incy
   is the stride for vector y. Specified as: a fullword integer, where:
   For SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, and ZHER2,
    incy < 0 \text{ or } incy > 0.
    For SSLR2 and DSLR2, incy can have any value.
ap
   has the following meaning:
   For SSPR2 and DSPR2, ap is the real symmetric matrix \boldsymbol{A} of order n, stored in
   upper- or lower-packed storage mode.
   For CHPR2 and ZHPR2, ap is the complex Hermitian matrix A of order n,
    stored in upper- or lower-packed storage mode.
   For SSLR2 and DSLR2, ap is the real symmetric matrix A of order n, stored in
   lower-packed storage mode.
```

has the following meaning:

For SSYR2 and DSYR2, a is the real symmetric matrix A of order n, stored in upper or lower storage mode.

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing

numbers of the data type indicated in Table 66 on page 331.

For CHER2 and ZHER2, a is the complex Hermitian matrix A of order n, stored in upper or lower storage mode.

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 66 on page 331.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

#### On Return

ap

is the matrix  $\mathbf{A}$  of order n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 66 on page 331.

а

is the matrix  $\boldsymbol{A}$  of order n, containing the results of the computation. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 66 on page 331.

#### Notes

- 1. All subroutines accept lowercase letters for the uplo argument.
- 2. The vectors **x** and **y** must have no common elements with matrix **A**; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\bf A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq z$  zero, the imaginary parts of the diagonal elements are set to zero.
- 4. For a description of how symmetric matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper- or lower-packed storage mode and upper or lower storage mode, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines perform the computation described in the two sections below. See references [34], [35], and [73]. If n or  $\alpha$  is zero, no computation is performed.

For SSPR2, SSYR2, SSLR2, CHPR2, and CHER2, intermediate results are accumulated in long precision.

SSPR2, DSPR2, SSYR2, DSYR2, SSLR2, and DSLR2: These subroutines compute the rank-two update of a real symmetric matrix:

$$\mathbf{A} \leftarrow \mathbf{A} + \alpha \mathbf{x} \mathbf{y}^\mathsf{T} + \alpha \mathbf{y} \mathbf{x}^\mathsf{T}$$

# where:

 $\boldsymbol{A}$  is a real symmetric matrix of order  $\boldsymbol{n}$ .  $\boldsymbol{\alpha}$  is a scalar.  $\boldsymbol{x}$  is a vector of length  $\boldsymbol{n}$ .  $\boldsymbol{x}^{\mathsf{T}}$  is the transpose of vector  $\boldsymbol{x}$ .  $\boldsymbol{y}$  is a vector of length  $\boldsymbol{n}$ .  $\boldsymbol{y}^{\mathsf{T}}$  is the transpose of vector  $\boldsymbol{y}$ .

It is expressed as follows:

# SSPR2, DSPR2, CHPR2, ZHPR2, SSYR2, DSYR2, CHER2, ZHER2, SSLR2, and DSLR2

$$\begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} y_1 \dots y_n \end{bmatrix}$$

$$+ \alpha \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} [x_1 \dots x_n]$$

CHPR2, ZHPR2, CHER2, and ZHER2: These subroutines compute the rank-two update of a complex Hermitian matrix:

$$A \leftarrow A + \alpha x y^{\mathrm{H}} + \overline{\alpha} y x^{\mathrm{H}}$$

where:

**A** is a complex Hermitian matrix of order *n*.

 $\alpha$  is a scalar.

x is a vector of length n.

 $x^{H}$  is the conjugate transpose of vector x.

y is a vector of length n.

 $y^{H}$  is the conjugate transpose of vector y.

It is expressed as follows:

$$\begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots & \vdots \\ \vdots & \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} + \alpha \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} \bar{y}_1 \dots \bar{y}_n \end{bmatrix}$$

$$+ \overline{\alpha} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} [\overline{x}_1 \dots \overline{x}_n]$$

#### **Error Condition**

Computational Errors: None

Input-Argument Errors

1. *uplo* ≠ 'L' or 'U'

2. n < 0

3. incx = 0

$$4. incy = 0$$

5.  $Ida \leq 0$ 

6. Ida < n

**Example 1:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  with positive strides and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. Matrix  $\mathbf{A}$  is:

Call Statement and Input

**Example 2:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is 3.0. The real symmetric matrix  $\mathbf{A}$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

Call Statement and Input

**Example 3:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  with positive stride and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. Matrix  $\mathbf{A}$  is:

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\bf A$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq z$  zero, the imaginary parts of the diagonal elements are set to zero.

Call Statement and Input

```
UPLO N
                     ALPHA
                             X INCX Y INCY AP
CALL CHPR2( 'L' , 3 , ALPHA , X , 1 , Y , 2 , AP )
ALPHA
        = (1.0, 0.0)
        = ((1.0, 2.0), (4.0, 0.0), (3.0, 4.0))
Χ
Υ
        = ((1.0, 0.0), ., (2.0, -1.0), ., (2.0, 1.0))
AΡ
        = ((1.0, .), (3.0, -5.0), (2.0, 3.0), (7.0, .),
            (4.0, 8.0), (6.0, .)
Output
AΡ
        = ((3.0, 0.0), (7.0, -10.0), (9.0, 4.0), (23.0, 0.0),
            (14.0, 23.0), (26.0, 0.0))
```

**Example 4:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is (1.0,2.0). The complex Hermitian matrix  $\mathbf{A}$  of order 3 is stored in upper-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\mathbf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq \text{zero}$ , the imaginary parts of the diagonal elements are set to zero.

Call Statement and Input

**Example 5:** This example shows vectors **x** and **y** with positive strides, and a real symmetric matrix **A** of order 3, stored in lower storage mode. It uses the same input matrix **A** as in Example 1.

Output

$$A = \begin{bmatrix} 38.0 & . & . \\ 23.0 & 18.0 & . \\ 13.0 & 14.0 & 7.0 \end{bmatrix}$$

**Example 6:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is 3.0. The real symmetric matrix  $\mathbf{A}$  of order 3 is stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

Call Statement and Input

Output

$$A = \begin{bmatrix} 38.0 & 23.0 & 13.0 \\ . & 18.0 & 14.0 \\ . & . & 7.0 \\ . & . & . \end{bmatrix}$$

**Example 7:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  with positive stride, and a complex Hermitian matrix  $\mathbf{A}$  of order 3, stored in lower storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\mathbf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq \text{zero}$ , the imaginary parts of the diagonal elements are set to zero.

# Call Statement and Input

# Output

$$A = \begin{bmatrix} (3.0, 0.0) & . & . \\ (7.0, -10.0) & (23.0, 0.0) & . \\ (9.0, 4.0) & (14.0, 23.0) & (26.0, 0.0) \end{bmatrix}$$

**Example 8:** This example shows vector  $\mathbf{x}$  and  $\mathbf{y}$  having strides of opposite signs. For  $\mathbf{x}$ , which has negative stride, processing begins at element X(5), which is (1.0, 2.0). The complex Hermitian matrix  $\mathbf{A}$  of order 3 is stored in upper storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 3.

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix  $\mathbf{A}$  are assumed to be zero, so you do not have to set these values. On output, if  $\alpha \neq \text{zero}$ , the imaginary parts of the diagonal elements are set to zero.

#### Call Statement and Input

$$ALPHA = \begin{bmatrix} (1.0, 0.0) \\ (1.0,$$

Output

$$A = \begin{bmatrix} (3.0, 0.0) & (7.0, 10.0) & (9.0, -4.0) \\ . & (23.0, 0.0) & (14.0, -23.0) \\ . & . & (26.0, 0.0) \end{bmatrix}$$

**Example 9:** This example shows vectors  $\mathbf{x}$  and  $\mathbf{y}$  with positive strides and a real symmetric matrix  $\mathbf{A}$  of order 3, stored in lower-packed storage mode. It uses the same input matrix  $\mathbf{A}$  as in Example 1.

```
Call Statement and Input
```

# SGBMV, DGBMV, CGBMV, and ZGBMV—Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose

SGBMV and DGBMV compute the matrix-vector product for either a real general band matrix or its transpose, where the general band matrix is stored in BLAS-general-band storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and general band matrix  $\mathbf{A}$  or its transpose:

$$y \leftarrow \beta y + \alpha A x$$
$$y \leftarrow \beta y + \alpha A^{\mathsf{T}} x$$

CGBMV and ZGBMV compute the matrix-vector product for either a complex general band matrix, its transpose, or its conjugate transpose, where the general band matrix is stored in BLAS-general-band storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $\mathbf{x}$  and  $\mathbf{y}$ , and general band matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

$$y \leftarrow \beta y + \alpha Ax$$
  
 $y \leftarrow \beta y + \alpha A^{T}x$   
 $y \leftarrow \beta y + \alpha A^{H}x$ 

Table 67. Data Types	
α, β, <b>x</b> , <b>y</b> , <b>A</b>	Subprogram
Short-precision real	SGBMV
Long-precision real	DGBMV
Short-precision complex	CGBMV
Long-precision complex	ZGBMV

# Syntax

Fortran	CALL SGBMV   DGBMV   CGBMV   ZGBMV (transa, m, n, ml, mu, alpha, a, lda, x, incx, beta, y, incy)
C and C++	sgbmv   dgbmv   cgbmv   zgbmv (transa, m, n, ml, mu, alpha, a, lda, x, incx, beta, y, incy);
PL/I	CALL SGBMV   DGBMV   CGBMV   ZGBMV (transa, m, n, ml, mu, alpha, a, lda, x, incx, beta, y, incy);

# On Entry

#### transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If transa = 'T',  $A^T$  is used in the computation.

If  $transa = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}$ ,  $A^{\mathsf{H}}$  is used in the computation.

Specified as: a single character. It must be 'N', 'T', or 'C'.

m

is the number of rows in matrix A, and:

If transa = 'N', it is the length of vector y.

If transa = 'T' or 'C', it is the length of vector x.

```
Specified as: a fullword integer; m \ge 0.
n
    is the number of columns in matrix A, and:
    If transa = 'N', it is the length of vector x.
    If transa = 'T' or 'C', it is the length of vector y.
    Specified as: a fullword integer; n \ge 0.
ml
    is the lower band width ml of the matrix A. Specified as: a fullword integer;
    ml \geq 0.
mu
    is the upper band width mu of the matrix A. Specified as: a fullword integer;
alpha
    is the scaling constant \alpha. Specified as: a number of the data type indicated in
    Table 67 on page 340.
    is the m by n general band matrix A, stored in BLAS-general-band storage
    mode. It has an upper band width mu and a lower band width ml. Also:
    If transa = 'N', A is used in the computation.
    If transa = 'T', A^T is used in the computation.
    If transa = {}^{t}C^{t}, A^{H} is used in the computation.
    Note: No data should be moved to form A^T or A^H; that is, the matrix A should
            always be stored in its untransposed form in BLAS-general-band
            storage mode.
    Specified as: an Ida by (at least) n array, containing numbers of the data type
    indicated in Table 67 on page 340, where lda \ge ml+mu+1.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
   integer; Ida > 0 and Ida \ge mI + mu + 1.
Χ
    is the vector x, where:
    If transa = 'N', it has length n.
    If transa = 'T' or 'C', it has length m.
    Specified as: a one-dimensional array, containing numbers of the data type
    indicated in Table 67 on page 340, where:
    If transa = 'N', it must have at least 1+(n-1)|incx| elements.
    If transa = 'T' or 'C', it must have at least 1+(m-1)|incx| elements.
incx
    is the stride for vector \mathbf{x}. Specified as: a fullword integer; incx > 0 or incx < 0.
beta
    is the scaling constant \beta. Specified as: a number of the data type indicated in
    Table 67 on page 340.
V
    is the vector y, where:
    If transa = 'N', it has length m.
    If transa = 'T' or 'C', it has length n.
```

Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 67 on page 340, where:

```
If transa = 'N', it must have at least 1+(m-1)|incy| elements.
```

If transa = 'T' or 'C', it must have at least 1+(n-1)|incy| elements. incv

is the stride for vector  $\mathbf{y}$ . Specified as: a fullword integer; incy > 0 or incy < 0.

#### On Return

У

is the vector  $\mathbf{y}$ , containing the result of the computation, where:

```
If transa = 'N', it has length m.
```

If transa = 'T' or 'C', it has length n.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 67 on page 340.

#### **Notes**

- 1. For SGBMV and DGBMV, if you specify 'C' for the transa argument, it is interpreted as though you specified 'T'.
- 2. All subroutines accept lowercase letters for the transa argument.
- 3. Vector **y** must have no common elements with matrix **A** or vector **x**; otherwise, results are unpredictable. See "Concepts" on page 55.
- 4. To achieve optimal performance, use lda = mu+ml+1.
- 5. For general band matrices, if you specify  $ml \ge m$  or  $mu \ge n$ , ESSL assumes, only for purposes of the computation, that the lower band width is m-1 or the upper band width is n-1, respectively. However, ESSL uses the original values for ml and mu for the purposes of finding the locations of element  $a_{11}$  and all other elements in the array specified for **A**, as described in "General Band Matrix" on page 76. For an illustration of this technique, see "Example 4" on page 345.
- 6. For a description of how a general band matrix is stored in BLAS-general-band storage mode in an array, see "General Band Matrix" on page 76.

Function: The possible computations that can be performed by these subroutines are described in the following sections. Varying implementation techniques are used for this computation to improve performance. As a result, accuracy of the computational result may vary for different computations.

In all the computations, general band matrix **A** is stored in its untransposed form in an array, using BLAS-general-band storage mode.

For SGBMV and CGBMV, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are truncated to short precision and stored.

See references [34], [35], [38], [46], and [73]. No computation is performed if m or n is 0 or if  $\alpha$  is zero and  $\beta$  is one.

General Band Matrix: For SGBMV, DGBMV, CGBMV, and ZGBMV, the matrix-vector product for a general band matrix is expressed as follows:

$$y \leftarrow \beta y + \alpha Ax$$

#### where:

**x** is a vector of length *n*.

y is a vector of length m.

 $\alpha$  is a scalar.

 $\beta$  is a scalar.

 $\boldsymbol{A}$  is an m by n general band matrix, having a lower band width of ml and an upper band width of mu.

*Transpose of a General Band Matrix:* For SGBMV, DGBMV, CGBMV, and ZGBMV, the matrix-vector product for the transpose of a general band matrix is expressed as:

$$y \leftarrow \beta y + \alpha A^T x$$

#### where:

 $\boldsymbol{x}$  is a vector of length m.

y is a vector of length n.

 $\alpha$  is a scalar.

 $\beta$  is a scalar.

 $A^T$  is the transpose of an m by n general band matrix A, having a lower band width of ml and an upper band width of mu.

Conjugate Transpose of a General Band Matrix: For CGBMV and ZGBMV, the matrix-vector product for the conjugate transpose of a general band matrix is expressed as follows:

$$y \leftarrow \beta y + \alpha A^{H} x$$

#### where:

x is a vector of length m.

**y** is a vector of length *n*.

 $\alpha$  is a scalar.

β is a scalar.

 $A^{H}$  is the conjugate transpose of an m by n general band matrix A of order n, having a lower band width of ml and an upper band width of mu.

# **Error Conditions**

Computational Errors: None

#### Input-Argument Errors

```
1. transa ≠ 'N', 'T', or 'C'
```

2. m < 0

3. n < 0

4. ml < 0

5. mu < 0

6.  $Ida \leq 0$ 

7. Ida < ml+mu+1

8. incx = 0

9. 
$$incy = 0$$

**Example 1:** This example shows how to use SGBMV to perform the computation  $\mathbf{y} \leftarrow \beta \mathbf{y} + \alpha \mathbf{A} \mathbf{x}$ , where TRANSA is equal to 'N', and the following real general band matrix  $\mathbf{A}$  is used in the computation. Matrix  $\mathbf{A}$  is:

Call Statement and Input

$$Y = (1.0, 2.0, 3.0, 4.0)$$

$$Y = (1.0, ., 2.0, ., 3.0, ., 4.0, ., 5.0, .)$$

Output

$$Y = (22.0, ., 60.0, ., 90.0, ., 120.0, ., 140.0, .)$$

**Example 2:** This example shows how to use SGBMV to perform the computation  $\mathbf{y} \leftarrow \beta \mathbf{y} + \alpha \mathbf{A}^\mathsf{T} \mathbf{x}$ , where TRANSA is equal to 'T', and the transpose of a real general band matrix  $\mathbf{A}$  is used in the computation. It uses the same input as Example 1.

Call Statement and Input

**Example 3:** This example shows how to use CGBMV to perform the computation  $\mathbf{y} \leftarrow \beta \mathbf{y} + \alpha \mathbf{A}^H \mathbf{x}$ , where TRANSA is equal to 'C', and the complex conjugate of the following general band matrix  $\mathbf{A}$  is used in the computation. Matrix  $\mathbf{A}$  is:

### Call Statement and Input

# Output

**Example 4:** This example shows how to use SGBMV to perform the computation  $y \leftarrow \beta y + \alpha Ax$ , where  $ml \ge m$  and  $mu \ge n$ , TRANSA is equal to 'N', and the following real general band matrix A is used in the computation. Matrix A is:

# SGBMV, DGBMV, CGBMV, and ZGBMV

```
X = (1.0, 2.0, 3.0, 4.0, 5.0)

Y = (40.0, ., 80.0, ., 120.0, ., 160.0, .)
```

# SSBMV, DSBMV, CHBMV, and ZHBMV—Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix

SSBMV and DSBMV compute the matrix-vector product for a real symmetric band matrix. CHBMV and ZHBMV compute the matrix-vector product for a complex Hermitian band matrix. The band matrix  $\boldsymbol{A}$  is stored in either upper- or lower-band-packed storage mode. It uses the scalars  $\alpha$  and  $\beta$ , vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ , and band matrix  $\boldsymbol{A}$ :

$$y \leftarrow \beta y + \alpha A x$$
$$y \leftarrow \beta y + \alpha A x$$

Table 68. Data Types	
α, β, <b>x</b> , <b>y</b> , <b>A</b>	Subprogram
Short-precision real	SSBMV
Long-precision real	DSBMV
Short-precision complex	CHBMV
Long-precision complex	ZHBMV

### Syntax

Fortran	CALL SSBMV   DSBMV   CHBMV   ZHBMV (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy)
C and C++	ssbmv   dsbmv   chbmv   zhbmv (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy);
PL/I	CALL SSBMV   DSBMV   CHBMV   ZHBMV (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy);

# On Entry

uplo

indicates the storage mode used for matrix  $\boldsymbol{A}$ , where either the upper or lower triangle can be stored:

If uplo = 'U', **A** is stored in upper-band-packed storage mode.

If uplo = 'L', **A** is stored in lower-band-packed storage mode.

Specified as: a single character. It must be 'U' or 'L'.

n

is the order of matrix A and the number of elements in vectors x and y. Specified as: a fullword integer;  $n \ge 0$ .

k

is the half band width k of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer;  $k \ge 0$ . alpha

is the scaling constant  $\alpha$ . Specified as: a number of the data type indicated in Table 68.

а

is the real symmetric or complex Hermitian band matrix  $\boldsymbol{A}$  of order n, having a half band width of k, where:

If *uplo* = 'U', **A** is stored in upper-band-packed storage mode.

If *uplo* = 'L', **A** is stored in lower-band-packed storage mode.

Specified as: an *Ida* by (at least) n array, containing numbers of the data type indicated in Table 68, where  $Ida \ge k+1$ .

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge k+1$ .

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 68 on page 347.

incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0 or incx < 0. beta

is the scaling constant  $\beta$ . Specified as: a number of the data type indicated in Table 68 on page 347.

is the vector **y** of length *n*. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 68 on page 347.

incy

is the stride for vector  $\mathbf{y}$ . Specified as: a fullword integer; incy > 0 or incy < 0.

#### On Return

У

is the vector  $\mathbf{y}$  of length n, containing the result of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 68 on page 347.

#### **Notes**

- 1. All subroutines accept lowercase letters for the uplo argument.
- 2. Vector **y** must have no common elements with matrix **A** or vector **x**; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. To achieve optimal performance in these subroutines, use Ida = k+1.
- 4. The imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.
- 5. For real symmetric and complex Hermitian band matrices, if you specify k ≥ n, ESSL assumes, only for purposes of the computation, that the half band width of matrix A is n-1; that is, it processes matrix A, of order n, as though it is a (nonbanded) real symmetric or complex Hermitian matrix. However, ESSL uses the original value for k for the purposes of finding the locations of element a<sub>11</sub> and all other elements in the array specified for A, as described in the storage modes referenced in the next note. For an illustration of this technique, see "Example 3" on page 350.
- 6. For a description of how a real symmetric band matrix is stored, see "Upper-Band-Packed Storage Mode" on page 83 or "Lower-Band-Packed Storage Mode" on page 84. For a description of how a complex Hermitian band matrix is stored, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines perform the following matrix-vector product, using a real symmetric or complex Hermitian band matrix **A**, stored in either upper- or lower-band-packed storage mode:

$$y \leftarrow \beta y + \alpha Ax$$

where:

 $\boldsymbol{x}$  and  $\boldsymbol{y}$  are vectors of length  $\boldsymbol{n}$ .  $\alpha$  and  $\beta$  are scalars.

 $\boldsymbol{A}$  is an real symmetric or complex Hermitian band matrix of order n, having a half band width of k.

For SSBMV and CHBMV, intermediate results are accumulated in long precision. Occasionally, for performance reasons, these intermediate results are truncated to short precision and stored.

See references [34], [38], [46], and [73]. No computation is performed if n is 0 or if  $\alpha$  is zero and  $\beta$  is one.

# **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. *uplo* ≠ 'U' or 'L'
- 2. n < 0
- 3. k < 0
- $4. Ida \leq 0$
- 5. Ida < k+1
- 6. incx = 0
- 7. incy = 0

**Example 1:** This example shows how to use SSBMV to perform the matrix-vector product, where the real symmetric band matrix **A** of order 7 and half band width of 3 is stored in upper-band-packed storage mode. Matrix **A** is:

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)$$
  
 $Y = (1.0, ., 2.0, ., 3.0, ., 4.0, ., 5.0, ., 6.0, ., 7.0)$ 

Output

```
Y = (30.0, ., 78.0, ., 148.0, ., 244.0, ., 288.0, ., 316.0, ., 322.0)
```

**Example 2:** This example shows how to use CHBMV to perform the matrix-vector product, where the complex Hermitian band matrix **A** of order 7 and half band width of 3 is stored in lower-band-packed storage mode. Matrix **A** is:

```
(0.0, 0.0)
             (1.0, 1.0)
                        (1.0, 1.0) (1.0, 1.0)
                                                 (0.0, 0.0)
                                                             (0.0, 0.0)
(1.0, -1.0)
           (2.0, 0.0)
                        (2.0, 2.0)
                                    (2.0, 2.0)
                                                 (2.0, 2.0)
                                                             (0.0, 0.0)
                                                                          (0.0, 0.0)
(1.0, -1.0) (2.0, -2.0) (3.0, 0.0)
                                    (3.0, 3.0)
                                                 (3.0, 3.0)
                                                             (3.0, 3.0)
                                                                          (0.0, 0.0)
(1.0, -1.0) (2.0, -2.0) (3.0, -3.0) (4.0, 0.0)
                                                 (4.0, 4.0)
                                                             (4.0, 4.0)
                                                                          (4.0, 4.0)
 (0.0, 0.0) (2.0, -2.0) (3.0, -3.0) (4.0, -4.0)
                                                             (5.0, 5.0)
                                                                          (5.0, 5.0)
                                                (5.0, 0.0)
 (0.0, 0.0) (0.0, 0.0) (3.0, -3.0) (4.0, -4.0) (5.0, -5.0)
                                                            (6.0, 0.0)
                                                                          (6.0, 6.0)
 (0.0, 0.0) (0.0, 0.0) (0.0, 0.0) (4.0, -4.0) (5.0, -5.0) (6.0, -6.0)
                                                                         (7.0, 0.0)
```

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not need to set these values.

Call Statement and Input

Output

```
Y = ((48.0, 12.0), ., (124.0, 32.0), ., (228.0, 68.0), ., (360.0, 128.0), ., (360.0, 216.0), ., (300.0, 332.0), ., (168.0, 476.0))
```

**Example 3:** This example shows how to use SSBMV to perform the matrix-vector product, where  $n \ge k$ . Matrix **A** is a real 5 by 5 symmetric band matrix with a half band width of 5, stored in upper-band-packed storage mode. Matrix **A** is:

```
      1.0
      1.0
      1.0
      1.0
      1.0

      1.0
      2.0
      2.0
      2.0
      2.0

      1.0
      2.0
      3.0
      3.0
      3.0

      1.0
      2.0
      3.0
      4.0
      4.0

      1.0
      2.0
      3.0
      4.0
      5.0
```

### Call Statement and Input

```
X = (1.0, 2.0, 3.0, 4.0, 5.0)

Y = (1.0, ., 2.0, ., 3.0, ., 4.0, ., 5.0, .)
```

# Output

```
Y = (40.0, ., 78.0, ., 112.0, ., 140.0, ., 160.0, .)
```

# STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV—Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose

STRMV, DTRMV, STPMV, and DTPMV compute one of the following matrix-vector products, using the vector  $\mathbf{x}$  and triangular matrix  $\mathbf{A}$  or its transpose:

$$x \leftarrow Ax$$
$$x \leftarrow A^{T}x$$

CTRMV, ZTRMV, CTPMV, and ZTPMV compute one of the following matrix-vector products, using the vector  $\mathbf{x}$  and triangular matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

$$x \leftarrow Ax$$
 $x \leftarrow A^{T}x$ 
 $x \leftarrow A^{H}x$ 

Matrix **A** can be either upper or lower triangular, where:

- For the \_TRMV subroutines, it is stored in upper- or lower-triangular storage mode, respectively.
- For the \_TPMV subroutines, it is stored in upper- or lower-triangular-packed storage mode, respectively.

Table 69. Data Types	
A, x	Subprogram
Short-precision real	STRMV and STPMV
Long-precision real	DTRMV and DTPMV
Short-precision complex	CTRMV and CTPMV
Long-precision complex	ZTRMV and ZTPMV

#### Syntax

Fortran	CALL STRMV   DTRMV   CTRMV   ZTRMV (uplo, transa, diag, n, a, lda, x, incx)
	CALL STPMV   DTPMV   CTPMV   ZTPMV (uplo, transa, diag, n, ap, x, incx)
C and C++	strmv   dtrmv   ctrmv   ztrmv (uplo, transa, diag, n, a, lda, x, incx);
	stpmv   dtpmv   ctpmv   ztpmv (uplo, transa, diag, n, ap, x, incx);
PL/I	CALL STRMV   DTRMV   CTRMV   ZTRMV (uplo, transa, diag, n, a, lda, x, incx);
	CALL STPMV   DTPMV   CTPMV   ZTPMV (uplo, transa, diag, n, ap, x, incx);

On Entry

uplo

indicates whether matrix **A** is an upper or lower triangular matrix, where:

If uplo = 'U', **A** is an upper triangular matrix.

If uplo = 'L', **A** is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

# STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

#### transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If transa = 'T',  $A^T$  is used in the computation.

If  $transa = {}^{\mathsf{L}}C^{\mathsf{L}}$ ,  $A^{\mathsf{H}}$  is used in the computation.

Specified as: a single character. It must be 'N', 'T', or 'C'. diag

indicates the characteristics of the diagonal of matrix **A**, where:

If diag = 'U', **A** is a unit triangular matrix.

If diag = 'N', **A** is not a unit triangular matrix.

Specified as: a single character. It must be 'U' or 'N'.

is the order of triangular matrix **A**. Specified as: a fullword integer;  $0 \le n \le Ida$ .

is the upper or lower triangular matrix  $\boldsymbol{A}$  of order n, stored in upper- or lower-triangular storage mode, respectively.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 69 on page 352.

lda

n

а

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

ap

is the upper or lower triangular matrix  $\mathbf{A}$  of order n, stored in upper- or lower-triangular-packed storage mode, respectively. Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 69 on page 352.

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 69 on page 352.

incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0 or incx < 0.

#### On Return

Χ

is the vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 69 on page 352.

#### Notes

- 1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.
- 2. For STRMV, DTRMV, STPMV, and DTPMV if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 3. Matrix **A** and vector **x** must have no common elements; otherwise, results are unpredictable.

# STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

- 4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.
- 5. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see "Triangular Matrix" on page 73.

**Function:** These subroutines can perform the following matrix-vector product computations, using the triangular matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose, where  $\mathbf{A}$  can be either upper or lower triangular:

```
x \leftarrow Ax

x \leftarrow A^Tx

x \leftarrow A^Hx (for CTRMV, ZTRMV, CTPMV, and ZTPMV only)
```

#### where:

**x** is a vector of length *n*.

**A** is an upper or lower triangular matrix of order *n*. For \_TRMV, it is stored in upper- or lower-triangular storage mode, respectively. For \_TPMV, it is stored in upper- or lower-triangular-packed storage mode, respectively.

See references [32] and [38]. If *n* is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

uplo ≠ 'L' or 'U'
 transa ≠ 'T', 'N', or 'C'
 diag ≠ 'N' or 'U'
 n < 0</li>
 lda ≤ 0
 lda < n</li>
 incx = 0

**Example 1:** This example shows the computation  $x \leftarrow Ax$ . Matrix A is a real 4 by 4 lower triangular matrix that is unit triangular, stored in lower-triangular storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

$$X = (1.0, 2.0, 3.0, 4.0)$$

Output

$$X = (1.0, 3.0, 11.0, 24.0)$$

**Example 2:** This example shows the computation  $x \leftarrow A^T x$ . Matrix A is a real 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

$$X = (5.0, 4.0, 3.0, 2.0)$$

Output

$$X = (5.0, 14.0, 26.0, 41.0)$$

**Example 3:** This example shows the computation  $x \leftarrow A^H x$ . Matrix A is a complex 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular storage mode. Vector x is a vector of length 4. Matrix A is:

$$\begin{bmatrix} (1.0, 0.0) & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & (1.0, 0.0) & (2.0, 2.0) & (5.0, 5.0) \\ . & . & (1.0, 0.0) & (3.0, 3.0) \\ . & . & . & (1.0, 0.0) & (3.0, 0.0) \end{bmatrix}$$

# STRMV, DTRMV, CTRMV, ZTRMV, STPMV, DTPMV, CTPMV, and ZTPMV

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

Call Statement and Input

X = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))

Output

$$X = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))$$

**Example 4:** This example shows the computation  $x \leftarrow Ax$ . Matrix A is a real 4 by 4 lower triangular matrix that is unit triangular, stored in lower-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

**Example 5:** This example shows the computation  $x \leftarrow A^T x$ . Matrix A is a real 4 by 4 upper triangular matrix that is not unit triangular, stored in upper-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

Call Statement and Input

**Example 6:** This example shows the computation  $x \leftarrow A^H x$ . Matrix A is a complex 4 by 4 upper triangular matrix that is unit triangular, stored in upper-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

# STBMV, DTBMV, CTBMV, and ZTBMV—Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose

STBMV and DTBMV compute one of the following matrix-vector products, using the vector  $\mathbf{x}$  and triangular band matrix  $\mathbf{A}$  or its transpose:

$$x \leftarrow Ax$$
$$x \leftarrow A^{T}x$$

CTBMV and ZTBMV compute one of the following matrix-vector products, using the vector  $\mathbf{x}$  and triangular band matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

$$\begin{array}{l}
x \leftarrow Ax \\
x \leftarrow A^{\mathsf{T}}x \\
x \leftarrow A^{\mathsf{H}}x
\end{array}$$

Matrix **A** can be either upper or lower triangular and is stored in upper- or lower-triangular-band-packed storage mode, respectively.

Table 70. Data Types	
A, x	Subprogram
Short-precision real	STBMV
Long-precision real	DTBMV
Short-precision complex	CTBMV
Long-precision complex	ZTBMV

# Syntax

Fortran	CALL STBMV   DTBMV   CTBMV   ZTBMV (uplo, transa, diag, n, k, a, lda, x, incx)
C and C++	stbmv   dtbmv   ctbmv   ztbmv (uplo, transa, diag, n, k, a, lda, x, incx);
PL/I	CALL STBMV   DTBMV   CTBMV   ZTBMV (uplo, transa, diag, n, k, a, lda, x, incx);

#### On Entry

uplo

indicates whether matrix **A** is an upper or lower triangular band matrix, where:

If uplo = 'U', **A** is an upper triangular matrix.

If uplo = 'L', **A** is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If transa = 'T',  $A^T$  is used in the computation.

If transa = 'C',  $A^H$  is used in the computation.

Specified as: a single character. It must be 'N', 'T', or 'C'.

### diag

indicates the characteristics of the diagonal of matrix **A**, where:

If diag = 'U', **A** is a unit triangular matrix.

If diag = 'N', **A** is not a unit triangular matrix.

Specified as: a single character. It must be 'U' or 'N'.

is the order of triangular band matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

k

n

is the upper or lower band width k of the matrix A. Specified as: a fullword integer;  $k \ge 0$ .

а

is the upper or lower triangular band matrix  $\boldsymbol{A}$  of order  $\boldsymbol{n}$ , stored in upper- or lower-triangular-band-packed storage mode, respectively.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 70 on page 358.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge k+1$ .

χ

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 70 on page 358.

incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0 or incx < 0.

### On Return

Χ

is the vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 70 on page 358.

### Notes

- 1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.
- 2. For STBMV and DTBMV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 3. Matrix **A** and vector **x** must have no common elements; otherwise, results are unpredictable.
- 4. To achieve optimal performance in these subroutines, use lda = k+1.
- 5. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. As a result, you do not have to set these values.
- 6. For both upper and lower triangular band matrices, if you specify  $k \ge n$ , ESSL assumes, **only for purposes of the computation**, that the upper or lower band width of matrix A is n-1; that is, it processes matrix A, of order n, as though it is a (nonbanded) triangular matrix. However, ESSL uses the original

value for k for the purposes of finding the locations of element  $a_{11}$  and all other elements in the array specified for A, as described in "Triangular Band Matrix" on page 86. For an illustration of this technique, see "Example 4" on page 363.

- For a description of triangular band matrices and how they are stored in upperand lower-triangular-band-packed storage mode, see "Triangular Band Matrix" on page 86.
- 8. If you are using a lower triangular band matrix, you may want to use this alternate approach instead of using lower-triangular-band-packed storage mode. Leave matrix *A* in full-matrix storage mode when you pass it to ESSL and specify the *Ida* argument to be *Ida*+1, which is the leading dimension of matrix *A* plus 1. ESSL then processes the matrix elements in the same way as though you had set them up in lower-triangular-band-packed storage mode.

**Function:** These subroutines can perform the following matrix-vector product computations, using the triangular band matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose, where  $\mathbf{A}$  can be either upper or lower triangular:

```
x \leftarrow Ax

x \leftarrow A^{T}x

x \leftarrow A^{H}x (for CTBMV and ZTBMV only)
```

#### where:

x is a vector of length n.

**A** is an upper or lower triangular band matrix of order *n*, stored in upper- or lower-triangular-band-packed storage mode, respectively.

See references [34], [46], and [38]. If *n* is 0, no computation is performed.

### **Error Conditions**

Computational Errors: None

### Input-Argument Errors

```
    uplo ≠ 'L' or 'U'
    transa ≠ 'T', 'N', or 'C'
    diag ≠ 'N' or 'U'
    n < 0</li>
    k < 0</li>
    lda ≤ 0
    lda < k+1</li>
    incx = 0
```

**Example 1:** This example shows the computation  $x \leftarrow Ax$ . Matrix A is a real 7 by 7 upper triangular band matrix with a half band width of 3 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector x is a vector of length 7. Matrix A is:

Call Statement and Input

$$A = \begin{bmatrix} . & . & . & 1.0 & 2.0 & 3.0 & 4.0 \\ . & . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 \\ . & . & . & . & . & . & . \end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)$$

Output

$$X = (10.0, 28.0, 54.0, 88.0, 90.0, 78.0, 49.0)$$

**Example 2:** This example shows the computation  $x \leftarrow A^Tx$ . Matrix A is a real 7 by 7 lower triangular band matrix with a half band width of 3 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector x is a vector of length 7. Matrix A is:

Call Statement and Input

CALL STBMV('L', 'T', 'N', 7, 3, A, 5, X, 1)

$$A = \begin{bmatrix}
1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & 7.0 \\
1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & . \\
1.0 & 2.0 & 3.0 & 4.0 & 5.0 & 6.0 & . \\
1.0 & 2.0 & 3.0 & 4.0 & 5.0 & . & . \\
1.0 & 2.0 & 3.0 & 4.0 & 5.0 & . & . \\
1.0 & 2.0 & 3.0 & 4.0 & . & . & . \\
1.0 & 2.0 & 3.0 & 4.0 & . & . & .
\end{bmatrix}$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)$$

Output

$$X = (10.0, 28.0, 54.0, 88.0, 90.0, 78.0, 49.0)$$

**Example 3:** This example shows the computation  $x \leftarrow A^{H}x$ . Matrix **A** is a complex 7 by 7 upper triangular band matrix with a half band width of 3 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector x is a vector of length 7. Matrix A is:

### Call Statement and Input

$$X = ((1.0, 2.0), (2.0, 4.0), (3.0, 6.0), (4.0, 8.0), (5.0, 10.0), (6.0, 12.0), (7.0, 14.0))$$

### Output

$$X = ((1.0, 2.0), (7.0, 9.0), (24.0, 23.0), (58.0, 46.0), (112.0, 79.0), (186.0, 122.0), (280.0, 175.0))$$

**Example 4:** This example shows the computation  $\mathbf{x} \leftarrow \mathbf{A}^{\mathsf{T}}\mathbf{x}$ , where k > n. Matrix  $\mathbf{A}$  is a real 4 by 4 upper triangular band matrix with a half band width of 5 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector  $\mathbf{x}$  is a vector of length 4. Matrix  $\mathbf{A}$  is:

$$\left[\begin{array}{ccccc} 1.0 & 1.0 & 1.0 & 1.0 \\ . & 2.0 & 2.0 & 2.0 \\ . & . & 3.0 & 3.0 \\ . & . & 4.0 \end{array}\right]$$

Call Statement and Input

$$X = (1.0, 2.0, 3.0, 4.0)$$

Output

$$X = (1.0, 5.0, 14.0, 30.0)$$

# Sparse Matrix-Vector Subprograms

This section contains the sparse matrix-vector subprogram descriptions.

# DSMMX—Matrix-Vector Product for a Sparse Matrix in Compressed-Matrix Storage Mode

This subprogram computes the matrix-vector product for sparse matrix  $\mathbf{A}$ , stored in compressed-matrix storage mode, using the matrix and vectors  $\mathbf{x}$  and  $\mathbf{y}$ :

$$y \leftarrow Ax$$

where A, x, and y contain long-precision real numbers. You can use DSMTM to transpose matrix A before calling this subroutine. The resulting computation performed by this subroutine is then  $y \leftarrow A^T x$ .

### Syntax

Fortran	CALL DSMMX (m, nz, ac, ka, lda, x, y)
C and C++	dsmmx (m, nz, ac, ka, lda, x, y);
PL/I	CALL DSMMX (m, nz, ac, ka, lda, x, y);

### On Entry

m

is the number of rows in sparse matrix A and the number of elements in vector y. Specified as: a fullword integer;  $m \ge 0$ .

nz

is the maximum number of nonzero elements in each row of sparse matrix A. Specified as: a fullword integer;  $nz \ge 0$ .

ac

is the m by n sparse matrix A, stored in compressed-matrix storage mode in an array, referred to as AC. Specified as: an Ida by (at least) nz array, containing long-precision real numbers.

ka

is the array, referred to as KA, containing the column numbers of the matrix A elements stored in the corresponding positions in array AC. Specified as: an *Ida* by (at least) nz array, containing fullword integers, where  $1 \le$  (elements of KA)  $\le n$ .

lda

is the size of the leading dimension of the arrays specified for ac and ka. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

Χ

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length n, containing long-precision real numbers.

See "On Return."

### On Return

У

is the vector  $\mathbf{y}$  of length m, containing the result of the computation. Returned as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

### Notes

1. Matrix **A** must have no common elements with vectors **x** and **y**; otherwise, results are unpredictable.

- 2. For the KA array, where there are no corresponding nonzero elements in AC, you must still fill in a number between 1 and *n*. See the "Example" on page 366.
- 3. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 93.
- 4. If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 99, you should first use the DSRSM utility subroutine, described in "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979, to convert your sparse matrix to compressed-matrix storage mode.

**Function:** The matrix-vector product is computed for a sparse matrix, stored in compressed matrix mode:

$$y \leftarrow Ax$$

where:

 ${\bf A}$  is an m by n sparse matrix, stored in compressed-matrix storage mode in arrays AC and KA.

**x** is a vector of length *n*.

y is a vector of length m.

It is expressed as follows:

See reference [67]. If m is 0, no computation is performed; if nz is 0, output vector y is set to zero, because matrix A contains all zeros.

If your program uses a sparse matrix stored by rows and you want to use this subroutine, you should first convert your sparse matrix to compressed-matrix storage mode by using the DSRSM utility subroutine described in "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. m < 0
- 2. Ida < 0
- 3. m > Ida
- 4. nz < 0

**Example:** This example shows the matrix-vector product computed for the following sparse matrix  $\mathbf{A}$ , which is stored in compressed-matrix storage mode in arrays AC and KA. Matrix  $\mathbf{A}$  is:

### Call Statement and Input

$$AC = \begin{bmatrix} 4.0 & 7.0 & 0.0 & 0.0 \\ 4.0 & 3.0 & 2.0 & 0.0 \\ 4.0 & 2.0 & 4.0 & 0.0 \\ 4.0 & 7.0 & 1.0 & 0.0 \\ 4.0 & 1.0 & 3.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 3.0 \end{bmatrix}$$

$$\mathsf{KA} \quad = \quad \left[ \begin{array}{cccc} 1 & 3 & 1 & 1 \\ 2 & 1 & 4 & 1 \\ 3 & 2 & 5 & 1 \\ 4 & 3 & 6 & 1 \\ 5 & 1 & 4 & 1 \\ 6 & 1 & 2 & 5 \end{array} \right]$$

$$X = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$$

### Output

$$Y = (25.0, 19.0, 36.0, 43.0, 33.0, 42.0)$$

# **DSMTM—Transpose a Sparse Matrix in Compressed-Matrix Storage Mode**

This subprogram transposes sparse matrix A, stored in compressed-matrix storage mode, where A contains long-precision real numbers.

### Syntax

Fortran	CALL DSMTM (m, nz, ac, ka, lda, n, nt, at, kt, ldt, aux, naux)
C and C++	dsmtm (m, nz, ac, ka, lda, n, nt, at, kt, ldt, aux, naux);
PL/I	CALL DSMTM (m, nz, ac, ka, lda, n, nt, at, kt, ldt, aux, naux);

### On Entry

m

is the number of rows in sparse matrix **A**. Specified as: a fullword integer;  $m \ge 0$ .

nz

is the maximum number of nonzero elements in each row of sparse matrix A. Specified as: a fullword integer;  $nz \ge 0$ .

ac

is the m by n sparse matrix A, stored in compressed-matrix storage mode in an array, referred to as AC. Specified as: an Ida by (at least) nz array, containing long-precision real numbers.

ka

is the array, referred to as KA, containing the column numbers of the matrix A elements stored in the corresponding positions in array AC. Specified as: an *Ida* by (at least) nz array, containing fullword integers, where  $1 \le$  (elements of KA)  $\le n$ .

lda

is the size of the leading dimension of the arrays specified for ac and ka. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

n

is the number of columns in sparse matrix A. Specified as: a fullword integer;  $0 \le n \le ldt$  and  $n \ge (maximum column index in KA).$ 

nt

is the number of columns in output arrays AT and KT that are available for use. Specified as: a fullword integer; nt > 0.

at

See "On Return" on page 369.

kt

See "On Return" on page 369.

ldt

is the size of the leading dimension of the arrays specified for at and kt. Specified as: a fullword integer; ldt > 0 and  $ldt \ge n$ .

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing long-precision real numbers. They can have any value.

#### naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DSMTM dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n$ .

### On Return

n

is the number of rows in the transposed matrix  $A^{T}$ . Returned as: a fullword integer; n = (maximum column index in KA).

nt

is the maximum number of nonzero elements, nt, in each row of the transposed matrix  $A^T$ . Returned as: a fullword integer;  $nt \le m$ .

at

is the n by (at least) m sparse matrix transpose  $A^T$ , stored in compressed-matrix storage mode in an array, referred to as AT. Returned as: an Idt by (at least) nt array, containing long-precision real numbers.

kt

is the array, referred to as KT, containing the column numbers of the transposed matrix  $\mathbf{A}^{\mathsf{T}}$  elements, stored in the corresponding positions in array AT. Returned as: an ldt by (at least) nt array, containing fullword integers, where  $1 \leq (\text{elements of KT}) \leq m$ .

### Notes

- 1. In your C program, arguments *n* and *nt* must be passed by reference.
- The value specified for input argument nt should be greater than or equal to the number of nonzero elements you estimate to be in each row of the transposed sparse matrix A<sup>T</sup>. The output value is less than or equal to the input value you specify.
- 3. For the KA array, where there are no corresponding nonzero elements in AC, you must still fill in a number between 1 and *n*. See the "Example" on page 370.
- 4. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 93.
- 5. If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 99, you should first use the DSRSM utility subroutine, described in "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979, to convert your sparse matrix to compressed-matrix storage mode.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** A sparse matrix A, stored in arrays AC and KA in compressed-matrix storage mode, is transposed, forming  $A^T$ , and is stored in arrays AT and KT in compressed-matrix storage mode. See reference [67]. This subroutine is provided for when you want to do a matrix-vector product using a transposed matrix,  $A^T$ . First, you transpose a matrix, A, using this subroutine, then you call DSMMX with

the transposed matrix  $A^{T}$ . This results in the following computation being performed:  $y \leftarrow A^T x$ .

If your program uses a sparse matrix stored by rows and you want to use this subroutine, you should first convert your sparse matrix to compressed-matrix storage mode by using the DSRSM utility subroutine described in "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. m, n < 0
- 2. Ida, Idt < 1
- 3. Ida < m
- 4. Idt < n
- 5. nz < 0
- 6. *n* is less than the maximum column index in KA.
- 7. nt or ldt are too small.
- 8. When the following two errors occur, arrays AT, KT, and AUX are overwritten:

$$naux < n$$
  
 $nt \le 0$ 

9. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example shows how to transpose the following 5 by 4 sparse matrix A, which is stored in compressed-matrix storage mode in arrays AC and KA. Matrix A is:

The resulting 4 by 5 matrix transpose  $A^{T}$ , stored in compressed-matrix storage mode in arrays AT and KT, is as follows. Matrix  $A^{T}$  is:

As shown here, the value of N is larger than the actual number of columns in the matrix A. On output, the exact number of rows in the transposed matrix is returned in the output argument N.

On output, row 6 of AT and KT is is not accessed or modified by the subroutine. Column 4 and row 5 are accessed and modified. They are of no use in further computations and will not be used, because NT = 3 and M = 4.

### Call Statement and Input

$$KA = \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ 3 & 4 \\ 2 & 4 \\ 1 & 3 \end{bmatrix}$$

### Output

$$AT = \begin{bmatrix} 11.0 & 21.0 & 51.0 & 0.0 \\ 42.0 & 0.0 & 0.0 & 0.0 \\ 33.0 & 23.0 & 53.0 & 0.0 \\ 34.0 & 44.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \\ & & & & & & & \end{bmatrix}$$

$$KT = \begin{bmatrix} 1 & 2 & 5 & 1 \\ 4 & 1 & 1 & 1 \\ 3 & 2 & 5 & 1 \\ 3 & 4 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

## DSDMX—Matrix-Vector Product for a Sparse Matrix or Its Transpose in Compressed-Diagonal Storage Mode

This subprogram computes the matrix-vector product for square sparse matrix A, stored in compressed-diagonal storage mode, using either the matrix or its transpose, and vectors x and y:

$$y \leftarrow Ax$$
$$y \leftarrow A^{\mathsf{T}}x$$

where **A**, **x**, and **y** contain long-precision real numbers.

### Syntax

Fortran	CALL DSDMX (iopt, n, nd, ad, lda, trans, la, x, y)
C and C++	dsdmx (iopt, n, nd, ad, lda, trans, la, x, y);
PL/I	CALL DSDMX (iopt, n, nd, ad, lda, trans, la, x, y);

On Entry

iopt

indicates the storage variation used for sparse matrix A, stored in compressed-diagonal storage mode, where:

If iopt = 0, matrix **A** is a general sparse matrix, where all the nonzero diagonals in matrix **A** are used to set up the storage arrays.

If iopt = 1, matrix **A** is a symmetric sparse matrix, where only the nonzero main diagonal and one of each of the unique nonzero diagonals are used to set up the storage arrays.

Specified as: a fullword integer; iopt = 0 or 1.

n

is the order of sparse matrix  $\boldsymbol{A}$  and the number of elements in vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

nd

is the number of diagonals stored in the columns of array AD, as well as the number of columns in AD and the number of elements in array LA. Specified as: a fullword integer;  $nd \ge 0$ .

ad

is the sparse matrix  $\boldsymbol{A}$  of order n, stored in compressed diagonal storage in an array, referred to as AD. The *iopt* argument indicates the storage variation used for storing matrix **A**. The *trans* argument indicates the following:

If trans = 'N', **A** is used in the computation.

If  $trans = {}^{\mathsf{T}}\mathsf{T}$ ,  $A^{\mathsf{T}}$  is used in the computation.

**Note:** No data should be moved to form  $A^{T}$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: an *Ida* by (at least) *nd* array, containing long-precision real numbers:  $Ida \ge n$ .

lda

is the size of the leading dimension of the array specified for ad. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

#### trans

indicates the form of matrix **A** to use in the computation, where:

If trans = 'N', **A** is used in the computation.

If trans = 'T',  $A^T$  is used in the computation.

Specified as: a single character; trans = 'N' or 'T'.

la

is the array, referred to as LA, containing the diagonal numbers k for the diagonals stored in each corresponding column in array AD. (For an explanation of how diagonal numbers are assigned, see "Compressed-Diagonal Storage Mode" on page 94.)

Specified as: a one-dimensional array of (at least) length nd, containing fullword integers;  $1-n \le LA(i) \le n-1$ .

Х

is the vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array, containing long-precision real numbers.

У

See "On Return."

### On Return

У

is the vector  $\mathbf{y}$  of length n, containing the result of the computation. Returned as: a one-dimensional array, containing long-precision real numbers.

### Notes

- 1. All subroutines accept lowercase letters for the trans argument.
- 2. Matrix **A** must have no common elements with vectors **x** and **y**; otherwise, results are unpredictable.
- 3. For a description of how sparse matrices are stored in compressed-diagonal storage mode, see "Compressed-Diagonal Storage Mode" on page 94.

**Function:** The matrix-vector product of a square sparse matrix or its transpose, is computed for a matrix stored in compressed-diagonal storage mode:

$$y \leftarrow Ax$$
  
 $y \leftarrow A^{T}x$ 

### where:

 ${\bf A}$  is a sparse matrix of order n, stored in compressed-diagonal storage mode in AD and LA, using the storage variation for either general or symmetric sparse matrices, as indicated by the *iopt* argument.

**x** and **y** are vectors of length *n*.

It is expressed as follows for  $y \leftarrow Ax$ :

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} \dots a_{1n} \\ \vdots \\ a_{n1} \dots a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

It is expressed as follows for  $\mathbf{y} \leftarrow \mathbf{A}^{\mathsf{T}}\mathbf{x}$ :

If n is 0, no computation is performed; if nd is 0, output vector y is set to zero, because matrix A contains all zeros.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $iopt \neq 0$  or 1
- 2. n < 0
- $3. Ida \leq 0$
- 4. n > Ida
- 5. *trans* ≠ 'N' or 'T'
- 6. nd < 0
- 7.  $LA(j) \le -n$  or  $LA(j) \ge n$ , for any j = 1, n

**Example 1:** This example shows the matrix-vector product using *trans* = 'N', which is computed for the following sparse matrix A of order 6. The matrix is stored in compressed-matrix storage mode in arrays AD and LA using the storage variation for general sparse matrices, storing all nonzero diagonals. Matrix A is:

Call Statement and Input

= (1.0, 2.0, 3.0, 4.0, 5.0, 6.0)

= (0, -5, -4, -1, 2)

LA

Χ

Output

$$Y = (25.0, 19.0, 36.0, 43.0, 33.0, 42.0)$$

**Example 2:** This example shows the matrix-vector product using trans = 'N', which is computed for the following sparse matrix  $\boldsymbol{A}$  of order 6. The matrix is stored in compressed-matrix storage mode in arrays AD and LA using the storage variation for symmetric sparse matrices, storing the nonzero main diagonal and one of each of the unique nonzero diagonals. Matrix  $\boldsymbol{A}$  is:

Call Statement and Input

LA = 
$$(0, 2, -4)$$
  
X =  $(1.0, 2.0, 3.0, 4.0, 5.0, 6.0)$ 

Output

$$Y = (125.0, 296.0, 287.0, 500.0, 395.0, 632.0)$$

**Example 3:** This example is the same as Example 1 except that it shows the matrix-vector product for the transpose of a matrix, using trans = 'T'. It is computed using the transpose of the following sparse matrix A of order 6, which is stored in compressed-matrix storage mode in arrays AD and LA, using the storage variation for general sparse matrices, storing all nonzero diagonals. It uses the same matrix A as in Example 1.

Call Statement and Input

### **DSDMX**

## **Chapter 9. Matrix Operations**

The matrix operation subroutines are described in this chapter.

### **Overview of the Matrix Operation Subroutines**

Some of the matrix operation subroutines were designed in accordance with the Level 3 BLAS de facto standard. If these subroutines do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subroutines, the updates could require modifications of the calling application program. For details on the Level 3 BLAS, see reference [32]. The matrix operation subroutines also include the commonly used matrix operations: addition, subtraction, multiplication, and transposition (Table 71).

Table 71. List of Matrix Operation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Matrix Addition for General Matrices or Their Transposes	SGEADD CGEADD	DGEADD ZGEADD	381
Matrix Subtraction for General Matrices or Their Transposes	SGESUB CGESUB	DGESUB ZGESUB	388
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes	SGEMUL CGEMUL	DGEMUL ZGEMUL DGEMLP§	395
Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm	SGEMMS CGEMMS	DGEMMS ZGEMMS	405
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM◆ CGEMM◆	DGEMM◆ ZGEMM◆	411
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM◆ CSYMM◆ CHEMM◆	DSYMM◆ ZSYMM◆ ZHEMM◆	420
Triangular Matrix-Matrix Product	STRMM◆ CTRMM◆	DTRMM◆ ZTRMM◆	428
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK+ CSYRK+ CHERK+	DSYRK◆ ZSYRK◆ ZHERK◆	435
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K◆ CSYR2K◆ CHER2K◆	DSYR2K◆ ZSYR2K◆ ZHER2K◆	442
General Matrix Transpose (In-Place)	SGETMI CGETMI	DGETMI ZGETMI	450
General Matrix Transpose (Out-of-Place)	SGETMO CGETMO	DGETMO ZGETMO	453

Level 3 BLAS

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<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

### **Use Considerations**

This section describes some key points about using the matrix operations subroutines.

# Specifying Normal, Transposed, or Conjugate Transposed Input Matrices

On each invocation, the matrix operation subroutines can perform one of several possible computations, using different forms of the input matrices **A** and **B**. For the real and complex versions of the subroutines, there are four and nine combinations, respectively, depending on the characters specified for the *transa* and *transb* arguments:

'N' Normal form

'T' Transposed form subroutines)

'C' Conjugate transposed form

The four and nine possible combinations are defined as follows:

Real Combinations	Complex Combinations
AB	AB
<b>A</b> <sup>⊤</sup> <b>B</b>	$A^{T}B$
	AHB
<i>AB</i> <sup>⊤</sup>	<i>AB</i> <sup>⊤</sup>
$A^{T}B^{T}$	<b>A</b> ⊺ <b>B</b> ⊺
	<b>A</b> H <b>B</b> T
	<i>AB</i> H
	<b>A</b> ⊺ <b>B</b> H
	<b>A</b> H <b>B</b> H

## **Transposing or Conjugate Transposing:**

This section describes some key points about using transposed and conjugate transposed matrices.

### On Input

In every case, the input arrays for the matrix, its transpose, or its conjugate transpose should be stored in the original untransposed form. You then specify the desired form of the matrix to be used in the computation in the *transa* or *transb* arguments. For a description of matrix transpose and matrix conjugate transpose, see "Matrices" on page 62.

### On Output

If you want to compute the transpose or the conjugate transpose of a matrix operation—that is, the output stored in matrix *C*—you should use the matrix identities described in Special Usage for each subroutine description. Examples are provided in the subroutine descriptions to show the use of these matrix identities. This accomplishes the transpose or conjugate transpose as part of the multiply operation.

## **Performance and Accuracy Considerations**

This section describes some key points about performance and accuracy in the matrix operations subroutines.

### In General

- The matrix operation subroutines use algorithms that are tuned specifically to the workstation processors they run on. The techniques involve using any one of several computational methods, based on certain operation counts and sizes of data.
- 2. The short-precision multiplication subroutines provide increased accuracy by partially accumulating results in long precision.
- 3. Strassen's method is not stable for certain row or column scalings of the input matrices A and B. Therefore, for matrices A and B with divergent exponent values, Strassen's method may give inaccurate results. For these cases, you should use the \_GEMUL or \_GEMM subroutines.
- 4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

### For Large Matrices

If you are using large square matrices in your matrix multiplication operations, you get better performance by using SGEMMS, DGEMMS, CGEMMS, and ZGEMMS. These subroutines use Winograd's variation of Strassen's algorithm for both real and complex matrices.

## **For Combined Operations**

If you want to perform a combined matrix multiplication and addition with scaling, SGEMM, DGEMM, CGEMM, and ZGEMM provide better performance than if you perform the parts of the computation separately in your program. See references [32] and [35].

# **Matrix Operation Subroutines**

This section contains the matrix operation subroutine descriptions.

# SGEADD, DGEADD, CGEADD, and ZGEADD—Matrix Addition for General Matrices or Their Transposes

These subroutines can perform any one of the following matrix additions, using matrices  $\boldsymbol{A}$  and  $\boldsymbol{B}$  or their transposes, and matrix  $\boldsymbol{C}$ :

 $C \leftarrow A + B$ 

 $C \leftarrow A^{T} + B$ 

 $C \leftarrow A + B^T$ 

 $C \leftarrow A^{T} + B^{T}$ 

Table 72. Data Types	
A, B, C	Subroutine
Short-precision real	SGEADD
Long-precision real	DGEADD
Short-precision complex	CGEADD
Long-precision complex	ZGEADD

### Syntax

Fortran	CALL SGEADD   DGEADD   CGEADD   ZGEADD (a, Ida, transa, b, Idb, transb, c, Idc, m, n)
C and C++	sgeadd   dgeadd   cgeadd   zgeadd (a, lda, transa, b, ldb, transb, c, ldc, m, n);
PL/I	CALL SGEADD   DGEADD   CGEADD   ZGEADD (a, Ida, transa, b, Idb, transb, c, Idc, m, n);

### On Entry

а

is the matrix **A**, where:

If transa = 'N', **A** is used in the computation, and **A** has m rows and n columns.

If  $transa = {}^{t}T^{t}$ ,  $\mathbf{A}^{T}$  is used in the computation, and  $\mathbf{A}$  has n rows and m columns.

**Note:** No data should be moved to form  $A^T$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 72, where:

If transa = 'N', its size must be lda by (at least) n.

If transa = 'T', its size must be lda by (at least) m.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and:

If transa = 'N',  $Ida \ge m$ .

If transa = 'T',  $lda \ge n$ .

transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If  $transa = {}^{\mathsf{T}}\mathsf{T}^{\mathsf{T}}$ ,  $A^{\mathsf{T}}$  is used in the computation.

```
Specified as: a single character; transa = 'N' or 'T'.
b
    is the matrix B, where:
    If transb = 'N', B is used in the computation, and B has m rows and n
    columns.
    If transb = {}^{\mathsf{T}}\mathsf{T}, \mathbf{B}^{\mathsf{T}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    Note: No data should be moved to form B^T; that is, the matrix B should
           always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 72 on page 381, where:
    If transb = 'N', its size must be ldb by (at least) n.
    If transb = 'T', its size must be ldb by (at least) m.
ldb
    is the leading dimension of the array specified for b. Specified as: a fullword
   integer; Idb > 0 and:
    If transb = 'N', ldb \ge m.
    If transb = 'T', ldb \ge n.
transb
    indicates the form of matrix B to use in the computation, where:
    If transb = 'N', B is used in the computation.
   If transb = 'T', B^T is used in the computation.
    Specified as: a single character; transb = 'N' or 'T'.
С
    See "On Return."
ldc
   is the leading dimension of the array specified for c. Specified as: a fullword
   integer; ldc > 0 and ldc \ge m.
m
    is the number of rows in matrix C. Specified as: a fullword integer;
    0 \le m \le ldc.
   is the number of columns in matrix C. Specified as: a fullword integer; 0 \le n.
On Return
    is the m by n matrix C, containing the results of the computation. Returned as:
    an ldc by (at least) n array, containing numbers of the data type indicated in
   Table 72 on page 381.
Notes
 1. All subroutines accept lowercase letters for the transa and transb arguments.
```

2. Matrix C must have no common elements with matrices A or B. However, C may (exactly) coincide with  $\mathbf{A}$  if transa = 'N', and  $\mathbf{C}$  may (exactly) coincide with **B** if transb = 'N'. Otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The matrix sum is expressed as follows, where  $a_{ij}$ ,  $b_{ij}$ , and  $c_{ij}$  are elements of matrices **A**, **B**, and **C**, respectively:

$$c_{ij} = a_{ij} + b_{ij}$$
 for  $C \leftarrow A + B$   
 $c_{ij} = a_{ij} + b_{ji}$  for  $C \leftarrow A + B^T$   
 $c_{ij} = a_{ji} + b_{ij}$  for  $C \leftarrow A^T + B$   
 $c_{ij} = a_{ji} + b_{ji}$  for  $C \leftarrow A^T + B^T$   
for  $i = 1$ ,  $m$  and  $j = 1$ ,  $n$ 

If m or n is 0, no computation is performed.

**Special Usage:** You can compute the transpose  $C^T$  of each of the four computations listed under "Function" by using the following matrix identities:

$$(A+B)^{\mathsf{T}} = A^{\mathsf{T}}+B^{\mathsf{T}}$$
  
 $(A+B^{\mathsf{T}})^{\mathsf{T}} = A^{\mathsf{T}}+B$   
 $(A^{\mathsf{T}}+B)^{\mathsf{T}} = A+B^{\mathsf{T}}$   
 $(A^{\mathsf{T}}+B^{\mathsf{T}})^{\mathsf{T}} = A+B$ 

Be careful that your output array receiving  $C^T$  has dimensions large enough to hold the transposed matrix. See "Example 4" on page 385.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. Ida, Idb,  $Idc \le 0$
- 2. m, n < 0
- 3. m > ldc
- 4. transa, transb ≠ 'N' or 'T'
- 5. transa = 'N' and m > Ida
- 6. transa = 'T' and n > Ida
- 7. transb = 'N' and m > ldb
- 8. transb = 'T' and n > ldb

**Example 1:** This example shows the computation  $C \leftarrow A+B$ , where A and C are contained in larger arrays A and C, respectively, and B is the same size as array B, in which it is contained.

Call Statement and Input

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 \\ 21.0 & 22.0 & 23.0 \\ 31.0 & 32.0 & 33.0 \\ 41.0 & 42.0 & 43.0 \end{bmatrix}$$

Output

**Example 2:** This example shows the computation  $C \leftarrow A^T + B$ , where A, B, and Care the same size as arrays A, B, and C, in which they are contained.

### Call Statement and Input

Output

**Example 3:** This example shows computation  $C \leftarrow A + B^T$ , where A is contained in a larger array A, and **B** and **C** are the same size as arrays B and C, in which they are contained.

Call Statement and Input

Output

**Example 4:** This example shows how to produce the transpose of the result of the computation performed in "Example 3" on page 384,  $C \leftarrow A + B^{T}$ , which uses the calling sequence:

You instead code a calling sequence for  $C^T \leftarrow A^T + B$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 3. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see "Special Usage" on page 383.

Call Statement and Input

$$B = \begin{bmatrix} 11.0 & 12.0 & 13.0 & 14.0 \\ 21.0 & 22.0 & 23.0 & 24.0 \\ 31.0 & 32.0 & 33.0 & 34.0 \end{bmatrix}$$

Output

**Example 5:** This example shows the computation  $C \leftarrow A^T + B^T$ , where A, B, and C are the same size as the arrays A, B, and C, in which they are contained.

### Call Statement and Input

### Output

**Example 6:** This example shows the computation  $C \leftarrow A+B$ , where A, B, and C are contained in larger arrays A, B, and C, respectively, and the arrays contain complex data.

### Call Statement and Input

Output

$$C = \begin{bmatrix} (2.0, 13.0) & (11.0, 9.0) & (4.0, 11.0) \\ (6.0, 8.0) & (14.0, 11.0) & (7.0, 11.0) \\ (9.0, 5.0) & (11.0, 10.0) & (5.0, 12.0) \\ (13.0, 8.0) & (9.0, 10.0) & (2.0, 10.0) \\ & & & & & & \\ \end{bmatrix}$$

# SGESUB, DGESUB, CGESUB, and ZGESUB—Matrix Subtraction for General Matrices or Their Transposes

These subroutines can perform any one of the following matrix subtractions, using matrices  $\boldsymbol{A}$  and  $\boldsymbol{B}$  or their transposes, and matrix  $\boldsymbol{C}$ :

 $C \leftarrow A - B$ 

 $C \leftarrow A^{T} - B$ 

 $C \leftarrow A - B^{T}$ 

 $C \leftarrow A^{T} - B^{T}$ 

Table 73. Data Types	
A, B, C	Subroutine
Short-precision real	SGESUB
Long-precision real	DGESUB
Short-precision complex	CGESUB
Long-precision complex	ZGESUB

### Syntax

Fortran	CALL SGESUB   DGESUB   CGESUB   ZGESUB (a, Ida, transa, b, Idb, transb, c, Idc, m, n)
C and C++	sgesub   dgesub   cgesub   zgesub (a, lda, transa, b, ldb, transb, c, ldc, m, n);
PL/I	CALL SGESUB   DGESUB   CGESUB   ZGESUB (a, Ida, transa, b, Idb, transb, c, Idc, m, n);

### On Entry

а

is the matrix **A**, where:

If  $transa = {}^{t}N{}^{t}$ , **A** is used in the computation, and **A** has m rows and n columns.

If  $transa = {}^{\mathsf{T}}\mathsf{T}$ ,  $\mathbf{A}^{\mathsf{T}}$  is used in the computation, and  $\mathbf{A}$  has n rows and m columns.

**Note:** No data should be moved to form  $A^T$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 73, where:

If transa = 'N', its size must be lda by (at least) n.

If transa = 'T', its size must be lda by (at least) m.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and:

If transa = 'N',  $Ida \ge m$ .

If transa = 'T',  $lda \ge n$ .

### transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If transa = 'T',  $A^T$  is used in the computation.

```
Specified as: a single character; transa = 'N' or 'T'.
b
    is the matrix B, where:
    If transb = 'N', B is used in the computation, and B has m rows and n
    columns.
    If transb = {}^{\mathsf{T}}\mathsf{T}, \mathbf{B}^{\mathsf{T}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    Note: No data should be moved to form B^{T}; that is, the matrix B should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 72 on page 381, where:
    If transb = 'N', its size must be ldb by (at least) n.
    If transb = 'T', its size must be ldb by (at least) m.
ldb
    is the leading dimension of the array specified for b. Specified as: a fullword
    integer; ldb > 0 and:
    If transb = 'N', ldb \ge m.
    If transb = 'T', ldb \ge n.
transb
    indicates the form of matrix B to use in the computation, where:
    If transb = 'N', B is used in the computation.
    If transb = {}^{\mathsf{T}}\mathsf{T}, \mathbf{B}^{\mathsf{T}} is used in the computation.
    Specified as: a single character; transb = 'N' or 'T'.
С
    See "On Return."
ldc
    is the leading dimension of the array specified for c. Specified as: a fullword
    integer; ldc > 0 and ldc \ge m.
m
    is the number of rows in matrix C. Specified as: a fullword integer;
    0 \le m \le ldc.
n
    is the number of columns in matrix C. Specified as: a fullword integer; 0 \le n.
On Return
    is the m by n matrix C, containing the results of the computation. Returned as:
    an ldc by (at least) n array, containing numbers of the data type indicated in
    Table 73 on page 388.
Notes
 1. All subroutines accept lowercase letters for the transa and transb arguments.
```

Matrix C must have no common elements with matrices A or B. However, C may (exactly) coincide with A if transa = 'N', and C may (exactly) coincide with B if transb = 'N'. Otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The matrix subtraction is expressed as follows, where  $a_{ij}$ ,  $b_{ij}$ , and  $c_{ij}$  are elements of matrices **A**, **B**, and **C**, respectively:

$$c_{ij} = a_{ij} - b_{ij}$$
 for  $C \leftarrow A - B$   
 $c_{ij} = a_{ij} - b_{ji}$  for  $C \leftarrow A - B^T$   
 $c_{ij} = a_{ji} - b_{ij}$  for  $C \leftarrow A^T - B$   
 $c_{ij} = a_{ji} - b_{ji}$  for  $C \leftarrow A^T - B^T$   
for  $i = 1$ ,  $m$  and  $j = 1$ ,  $n$ 

If m or n is 0, no computation is performed.

**Special Usage:** You can compute the transpose  $C^{T}$  of each of the four computations listed under "Function" by using the following matrix identities:

$$(A-B)^{\mathsf{T}} = A^{\mathsf{T}}-B^{\mathsf{T}}$$
  
 $(A-B^{\mathsf{T}})^{\mathsf{T}} = A^{\mathsf{T}}-B$   
 $(A^{\mathsf{T}}-B)^{\mathsf{T}} = A-B^{\mathsf{T}}$   
 $(A^{\mathsf{T}}-B^{\mathsf{T}})^{\mathsf{T}} = A-B$ 

Be careful that your output array receiving  $C^T$  has dimensions large enough to hold the transposed matrix. See "Example 5" on page 392.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. Ida, Idb,  $Idc \le 0$
- 2. m, n < 0
- 3. m > ldc
- 4. transa, transb ≠ 'N' or 'T'
- 5. transa = 'N' and m > Ida
- 6. transa = 'T' and n > Ida
- 7. transb = 'N' and m > ldb
- 8. transb = 'T' and n > ldb

**Example 1:** This example shows the computation  $C \leftarrow A - B$ , where A and C are contained in larger arrays A and C, respectively, and B is the same size as array B, in which it is contained.

Call Statement and Input

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 \\ -21.0 & -22.0 & -23.0 \\ -31.0 & -32.0 & -33.0 \\ -41.0 & -42.0 & -43.0 \end{bmatrix}$$

Output

**Example 2:** This example shows the computation  $C \leftarrow A^T - B$ , where A, B, and C are the same size as arrays A, B, and C, in which they are contained.

Call Statement and Input

Output

$$C = \begin{bmatrix} 110011.0 & 210012.0 & 310013.0 \\ 120021.0 & 220022.0 & 320023.0 \\ 130031.0 & 230032.0 & 330033.0 \\ 140041.0 & 240042.0 & 340043.0 \end{bmatrix}$$

**Example 3:** This example shows computation  $C \leftarrow A - B^T$ , where A is contained in a larger array A, and B and C are the same size as arrays B and C, in which they are contained.

Call Statement and Input

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{bmatrix}$$

Output

**Example 4:** This example shows the computation  $C \leftarrow A^T - B^T$ , where A, B, and C are the same size as the arrays A, B, and C, in which they are contained.

Call Statement and Input

$$B = \begin{vmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{vmatrix}$$

Output

**Example 5:** This example shows how to produce the transpose of the result of the computation performed in "Example 4,"  $C \leftarrow A^T - B^T$ , which uses the calling sequence:

You instead code a calling sequence for  $C^T \leftarrow A - B$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 4. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see "Special Usage" on page 390.

### Call Statement and Input

$$B = \begin{bmatrix} -11.0 & -12.0 & -13.0 & -14.0 \\ -21.0 & -22.0 & -23.0 & -24.0 \\ -31.0 & -32.0 & -33.0 & -34.0 \end{bmatrix}$$

### Output

**Example 6:** This example shows the computation  $C \leftarrow A - B$ , where A, B, and C are contained in larger arrays A, B, and C, respectively, and the arrays contain complex data.

### Call Statement and Input

Output

### SGESUB, DGESUB, CGESUB, and ZGESUB

$$C = \begin{bmatrix} (0.0, -3.0) & (7.0, -5.0) & (-2.0, 7.0) \\ (-2.0, 0.0) & (2.0, -5.0) & (-5.0, 5.0) \\ (-3.0, 1.0) & (3.0, 0.0) & (-3.0, 2.0) \\ (-1.0, 4.0) & (-3.0, 2.0) & (0.0, -2.0) \\ & & & & & & \end{bmatrix}$$

# SGEMUL, DGEMUL, CGEMUL, and ZGEMUL—Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes

SGEMUL and DGEMUL can perform any one of the following matrix multiplications, using matrices **A** and **B** or their transposes, and matrix **C**:

$$C \leftarrow AB$$
  $C \leftarrow AB^{T}$   $C \leftarrow A^{T}B^{T}$ 

CGEMUL and ZGEMUL can perform any one of the following matrix multiplications, using matrices  $\boldsymbol{A}$  and  $\boldsymbol{B}$ , their transposes or their conjugate transposes, and matrix  $\boldsymbol{C}$ :

Table 74. Data Types	
A, B, C	Subroutine
Short-precision real	SGEMUL
Long-precision real	DGEMUL
Short-precision complex	CGEMUL
Long-precision complex	ZGEMUL

#### Syntax

Fortran	CALL SGEMUL   DGEMUL   CGEMUL   ZGEMUL (a, Ida, transa, b, Idb, transb, c, Idc, I, m, n)
C and C++	sgemul   dgemul   cgemul   zgemul (a, Ida, transa, b, Idb, transb, c, Idc, I, m, n);
PL/I	CALL SGEMUL   DGEMUL   CGEMUL   ZGEMUL (a, Ida, transa, b, Idb, transb, c, Idc, I, m, n);
APL2	SGEMUL   DGEMUL   CGEMUL   ZGEMUL a Ida transa b Idb transb ' c' Idc I m n

On Entry

а

is the matrix **A**, where:

If transa = 'N', **A** is used in the computation, and **A** has *I* rows and *m* columns.

If  $transa = {}^{t}T^{t}$ ,  $\mathbf{A}^{T}$  is used in the computation, and  $\mathbf{A}$  has m rows and I columns.

If  $transa = {}^{t}C^{t}$ ,  $A^{H}$  is used in the computation, and A has m rows and I columns.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 74, where:

If transa = 'N', its size must be lda by (at least) m.

If transa = 'T' or 'C', its size must be Ida by (at least) I.

```
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer: Ida > 0 and:
    If transa = 'N', Ida \ge I.
    If transa = 'T' \text{ or } 'C', Ida \ge m.
transa
    indicates the form of matrix A to use in the computation, where:
    If transa = 'N', A is used in the computation.
    If transa = 'T', A^T is used in the computation.
    If transa = 'C', A^H is used in the computation.
    Specified as: a single character; transa = 'N' or 'T' for SGEMUL and
    DGEMUL; transa = 'N', 'T', or 'C' for CGEMUL and ZGEMUL.
    is the matrix B, where:
    If transb = 'N', B is used in the computation, and B has m rows and n
    columns.
    If transb = {}^{\mathsf{T}}\mathsf{T}, \mathbf{B}^{\mathsf{T}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    If transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, B^{\mathsf{H}} is used in the computation, and B has n rows and m
    columns.
    Note: No data should be moved to form B^{T} or B^{H}; that is, the matrix B should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 74 on page 395, where:
    If transb = 'N', its size must be ldb by (at least) n.
    If transb = 'T' or 'C', its size must be ldb by (at least) m.
ldb
    is the leading dimension of the array specified for b. Specified as: a fullword
    integer; Idb > 0 and:
    If transb = 'N', ldb \ge m.
    If transb = 'T' \text{ or } 'C', Idb \ge n.
    indicates the form of matrix B to use in the computation, where:
    If transb = 'N', B is used in the computation.
    If transb = 'T', B^T is used in the computation.
    If transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, B^{\mathsf{H}} is used in the computation.
    Specified as: a single character; transb = 'N' or 'T' for SGEMUL and
    DGEMUL; transb = 'N', 'T', or 'C' for CGEMUL and ZGEMUL.
С
    See "On Return" on page 397.
ldc
    is the leading dimension of the array specified for c. Specified as: a fullword
    integer; ldc > 0 and ldc \ge l.
1
    is the number of rows in matrix C. Specified as: a fullword integer; 0 \le l \le ldc.
```

m

has the following meaning, where:

If transa = 'N', it is the number of columns in matrix **A**.

If transa = 'T' or 'C', it is the number of rows in matrix **A**.

In addition:

If transb = 'N', it is the number of rows in matrix **B**.

If transb = 'T' or 'C', it is the number of columns in matrix **B**.

Specified as: a fullword integer;  $m \ge 0$ .

n

is the number of columns in matrix C. Specified as: a fullword integer;  $n \ge 0$ .

#### On Return

С

is the *I* by n matrix C, containing the results of the computation. Returned as: an *Idc* by (at least) n numbers of the data type indicated in Table 74 on page 395.

#### **Notes**

- 1. All subroutines accept lowercase letters for the *transa* and *transb* arguments.
- 2. Matrix *C* must have no common elements with matrices *A* or *B*; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The matrix multiplication is expressed as follows, where  $a_{ik}$ ,  $b_{kj}$ , and  $c_{ij}$  are elements of matrices **A**, **B**, and **C**, respectively:

$$c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj} \quad \text{for } C \leftarrow A B$$

$$c_{ij} = \sum_{k=1}^{m} a_{ki} b_{kj} \quad \text{for } C \leftarrow A^{T} B$$

$$c_{ij} = \sum_{k=1}^{m} \overline{a}_{ki} b_{kj} \quad \text{for } C \leftarrow A^{H} B$$

$$c_{ij} = \sum_{k=1}^{m} a_{ik} b_{jk} \quad \text{for } C \leftarrow A B^{T}$$

$$c_{ij} = \sum_{k=1}^{m} a_{ki} b_{jk} \quad \text{for } C \leftarrow A^{T} B^{T}$$

$$c_{ij} = \sum_{k=1}^{m} \overline{a}_{ki} b_{jk} \quad \text{for } C \leftarrow A^{H} B^{T}$$

$$c_{ij} = \sum_{k=1}^{m} a_{ik} \overline{b}_{jk} \quad \text{for } C \leftarrow A B^{H}$$

$$c_{ij} = \sum_{k=1}^{m} a_{ki} \overline{b}_{jk} \quad \text{for } C \leftarrow A^{T} B^{H}$$

$$c_{ij} = \sum_{k=1}^{m} \overline{a}_{ki} \overline{b}_{jk} \quad \text{for } C \leftarrow A^{H} B^{H}$$

$$for \quad i = 1, l \text{ and } j = 1, n$$

See reference [38]. If l or n is 0, no computation is performed. If l and n are greater than 0, and m is 0, an l by n matrix of zeros is returned.

#### Special Usage

Equivalence Rules: By using the following equivalence rules, you can compute the transpose  $C^{T}$  or the conjugate transpose  $C^{H}$  of some of the computations performed by these subroutines:

Transpose	Conjugate Transpose
$(\mathbf{A}\mathbf{B})^{\top} = \mathbf{B}^{\top}\mathbf{A}^{\top}$	$(\mathbf{A}\mathbf{B})H = \mathbf{B}H\mathbf{A}H$
$(\mathbf{A}^{T}\mathbf{B})^{T} = \mathbf{B}^{T}\mathbf{A}$	$(A \vdash B) \vdash = B \vdash A$
$(\mathbf{A}\mathbf{B}^{T})^{T} = \mathbf{B}\mathbf{A}^{T}$	$(\mathbf{A}\mathbf{B}^{H})^{H} = \mathbf{B}\mathbf{A}^{H}$
$(\mathbf{A}^{T}\mathbf{B}^{T})^{T} = \mathbf{B}\mathbf{A}$	$(A^{H}B^{H})^{H} = BA$

When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your output array, receiving  $\mathbf{C}^{\mathsf{T}}$  or  $\mathbf{C}^{\mathsf{H}}$ , has dimensions large enough to hold the resulting transposed or conjugate transposed matrix. See "Example 2" on page 400 and "Example 4" on page 401.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area (CGEMUL and ZGEMUL only).

Computational Errors: None

#### Input-Argument Errors

- 1. Ida, Idb,  $Idc \le 0$
- 2. l, m, n < 0
- 3. I > Idc
- 4. transa, transb ≠ 'N' or 'T' for SGEMUL and DGEMUL
- 5. transa, transb ≠ 'N', 'T', or 'C' for CGEMUL and ZGEMUL
- 6. transa = 'N' and I > Ida
- 7. transa = 'T' or 'C' and m > Ida
- 8. transb = 'N' and m > ldb
- 9. transb = 'T' or 'C' and n > ldb

**Example 1:** This example shows the computation  $C \leftarrow AB$ , where A, B, and C are contained in larger arrays A, B, and C, respectively.

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ . & . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ & & & & & & \\ \end{bmatrix}$$

#### Output

**Example 2:** This example shows how to produce the transpose of the result of the computation performed in "Example 1,"  $C \leftarrow AB$ , which uses the calling sequence:

You instead code a calling sequence for  $C^T \leftarrow B^T A^T$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 1. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see "Special Usage" on page 398.

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \end{bmatrix}$$

#### Output

**Example 3:** This example shows the computation  $C \leftarrow A^TB$ , where A and C are contained in larger arrays A and C, respectively, and B is the same size as the

$$A = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \\ & & & & & & \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 6.0 & 4.0 & 1.0 & 1.0 & 0.0 & -1.0 \\ 4.0 & 26.0 & -5.0 & -5.0 & 8.0 & -15.0 \\ 1.0 & -5.0 & 5.0 & 5.0 & -1.0 & 3.0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \end{bmatrix}$$

**Example 4:** This example shows how to produce the transpose of the result of the computation performed in "Example 3" on page 400,  $C \leftarrow A^TB$ , which uses the calling sequence:

You instead code the calling sequence for  $C^T \leftarrow B^T A$ , as shown below, where the resulting matrix  $C^T$  in the output array CT is the transpose of the matrix in the output array C in Example 3. Note that the array CT has dimensions large enough to receive the transposed matrix. For a description of all the matrix identities, see "Special Usage" on page 398.

Call Statement and Input

B = 
$$\begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

$$A = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \\ & & & & & \end{bmatrix}$$

Output

$$CT = \begin{bmatrix} 6.0 & 4.0 & 1.0 \\ 4.0 & 26.0 & -5.0 \\ 1.0 & -5.0 & 5.0 \\ 1.0 & -5.0 & 5.0 \\ 0.0 & 8.0 & -1.0 \\ -1.0 & -15.0 & 3.0 \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix}$$

**Example 5:** This example shows the computation  $C \leftarrow AB^T$ , where **A** and **C** are contained in larger arrays A and C, respectively, and B is the same size as the array B in which it is contained.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \\ & & & \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 10.0 & -10.0 & 4.0 \\ -10.0 & 20.0 & -2.0 \\ 4.0 & -2.0 & 2.0 \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix}$$

**Example 6:** This example shows the computation  $C \leftarrow A^T B^T$ , where A, B, and C are the same size as the arrays A, B, and C in which they are contained. (Based on the dimensions of the matrices, **A** is actually a column vector, and **C** is actually a row vector.)

$$A = \begin{bmatrix} 1.0 \\ 2.0 \\ 1.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \end{bmatrix}$$

Output

$$B = \begin{bmatrix} -3.0 & 10.0 & -2.0 \end{bmatrix}$$

**Example 7:** This example shows the computation  $C \leftarrow A^TB$  using complex data, where A, B, and C are contained in larger arrays A, B, and C, respectively.

Call Statement and Input

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 4.0) \\ (4.0, 6.0) & (7.0, 1.0) \\ (6.0, 3.0) & (2.0, 5.0) \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ \end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 9.0) & (2.0, 6.0) & (5.0, 6.0) \\ (2.0, 5.0) & (6.0, 2.0) & (6.0, 4.0) \\ (2.0, 6.0) & (5.0, 4.0) & (2.0, 6.0) \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & &$$

Output

$$C = \begin{bmatrix} (-45.0, 85.0) & (20.0, 93.0) & (-13.0, 110.0) \\ (-50.0, 90.0) & (12.0, 79.0) & (3.0, 94.0) \\ & & & & & & & & \end{bmatrix}$$

**Example 8:** This example shows the computation  $C \leftarrow AB^H$  using complex data, where A and C are contained in larger arrays A and C, respectively, and C is the same size as the array C in which it is contained.

#### SGEMUL, DGEMUL, CGEMUL, and ZGEMUL

$$A = \begin{bmatrix} (1.0, 2.0) & (-3.0, 2.0) \\ (2.0, 6.0) & (4.0, 5.0) \\ (1.0, 2.0) & (-1.0, 8.0) \\ & & & \end{bmatrix}$$

B = 
$$\begin{bmatrix} (1.0, 3.0) & (-3.0, 2.0) \\ (2.0, 5.0) & (4.0, 6.0) \\ (1.0, 1.0) & (-1.0, 9.0) \end{bmatrix}$$

#### Output

# SGEMMS, DGEMMS, CGEMMS, and ZGEMMS—Matrix Multiplication for General Matrices, Their Transposes, or Conjugate Transposes Using Winograd's Variation of Strassen's Algorithm

These subroutines use Winograd's variation of the Strassen's algorithm to perform the matrix multiplication for both real and complex matrices. SGEMMS and DGEMMS can perform any one of the following matrix multiplications, using matrices **A** and **B** or their transposes, and matrix **C**:

$$\begin{array}{cccc} C \leftarrow AB & & C \leftarrow AB^{T} \\ C \leftarrow A^{T}B & & C \leftarrow A^{T}B^{T} \end{array}$$

CGEMMS and ZGEMMS can perform any one of the following matrix multiplications, using matrices  $\boldsymbol{A}$  and  $\boldsymbol{B}$ , their transposes or their conjugate transposes, and matrix  $\boldsymbol{C}$ :

$C \leftarrow AB$	$C \leftarrow AB^{T}$	<i>C</i> ← <i>AB</i> H
$C \leftarrow A^{T}B$	$C \leftarrow A^{T}B^{T}$	$C \leftarrow A^{T}B^{H}$
$C \leftarrow A^{H}B$	$C \leftarrow A^{H}B^{T}$	$C \leftarrow A H B H$

Table 75. Data Types		
A, B, C	aux	Subroutine
Short-precision real	Short-precision real	SGEMMS
Long-precision real	Long-precision real	DGEMMS
Short-precision complex	Short-precision real	CGEMMS
Long-precision complex	Long-precision real	ZGEMMS

#### Syntax

Fortran	CALL SGEMMS   DGEMMS   CGEMMS   ZGEMMS (a, Ida, transa, b, Idb, transb, c, Idc, I, m, n, aux, naux)
C and C++	sgemms   dgemms   cgemms   zgemms (a, lda, transa, b, ldb, transb, c, ldc, l, m, n, aux, naux);
PL/I	CALL SGEMMS   DGEMMS   CGEMMS   ZGEMMS (a, Ida, transa, b, Idb, transb, c, Idc, I, m, n, aux, naux);

On Entry

а

is the matrix **A**, where:

If transa = 'N', **A** is used in the computation, and **A** has *I* rows and *m* columns.

If  $transa = {}^{\mathsf{T}}\mathsf{T}^{\mathsf{T}}$ ,  $\mathbf{A}^{\mathsf{T}}$  is used in the computation, and  $\mathbf{A}$  has m rows and I columns

If  $transa = {}^{t}C^{t}$ ,  $A^{H}$  is used in the computation, and A has m rows and I columns.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix A should always be stored in its untransposed form.

```
Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 75, where:
    If transa = 'N', its size must be lda by (at least) m.
    If transa = 'T' or 'C', its size must be Ida by (at least) I.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0 and:
    If transa = 'N', Ida \ge I.
    If transa = 'T' \text{ or } 'C', Ida \ge m.
transa
    indicates the form of matrix A to use in the computation, where:
    If transa = 'N', A is used in the computation.
    If transa = 'T', A^T is used in the computation.
    If transa = 'C', A^H is used in the computation.
    Specified as: a single character; transa = 'N' or 'T' for SGEMMS and
    DGEMMS; transa = 'N', 'T', or 'C' for CGEMMS and ZGEMMS.
    is the matrix B, where:
    If transb = 'N', B is used in the computation, and B has m rows and n
    columns.
    If transb = {}^{\mathsf{T}}\mathsf{T}^{\mathsf{T}}, \mathbf{B}^{\mathsf{T}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    If transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, B^{\mathsf{H}} is used in the computation, and B has n rows and m
    columns.
    Note: No data should be moved to form B^{T} or B^{H}; that is, the matrix B should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 75 on page 405, where:
    If transb = 'N', its size must be ldb by (at least) n.
    If transb = 'T' or 'C', its size must be ldb by (at least) m.
ldb
    is the leading dimension of the array specified for b. Specified as: a fullword
    integer; Idb > 0 and:
    If transb = 'N', ldb \ge m.
    If transb = 'T' \text{ or 'C'}, Idb \ge n.
    indicates the form of matrix B to use in the computation, where:
    If transb = 'N', B is used in the computation.
    If transb = 'T', B^T is used in the computation.
    If transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, B^{\mathsf{H}} is used in the computation.
    Specified as: a single character; transb = 'N' or 'T' for SGEMMS and
    DGEMMS; transb = 'N', 'T', or 'C' for CGEMMS and ZGEMMS.
С
    See "On Return" on page 408.
```

#### SGEMMS, DGEMMS, CGEMMS, and ZGEMMS

is the leading dimension of the array specified for c. Specified as: a fullword integer; Idc > 0 and Idc ≥ I.

is the number of rows in matrix C. Specified as: a fullword integer; 0 ≤ I ≤ Idc.

m has the following meaning, where:

If transa = 'N', it is the number of columns in matrix A.

If transa = 'T' or 'C', it is the number of rows in matrix A.

In addition:

If transb = 'N', it is the number of rows in matrix B.

If transb = 'T' or 'C', it is the number of columns in matrix B.

Specified as: a fullword integer; m ≥ 0.

n is the number of columns in matrix C. Specified as: a fullword integer; n ≥ 0.

is the number of columns in matrix c. Specified as: a fullword integer;  $n \ge 0$  aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage containing numbers of the data type indicated in Table 75 on page 405.

#### naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*.

Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SGEMMS, DGEMMS, CGEMMS, and ZGEMMS dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,

When this subroutine uses Strassen's algorithm:

For SGEMMS and DGEMMS:

```
Use naux = max[(n)(l), 0.7m(l+n)].
```

For CGEMMS and ZGEMMS:

```
Use naux = \max[(n)(1), 0.7m(1+n)] + nb1 + nb2, where:

If l \ge n, then nb1 \ge (1)(n+20) and nb2 \ge \max[(n)(1), (m)(n+20)].

If l < n, then nb1 \ge (m)(n+20) and nb2 \ge \max[(n)(1), (1)(m+20)].
```

When this subroutine uses the direct method ( $\_GEMUL$ ), use  $naux \ge 0$ .

#### Notes:

- 1. In most cases, these formulas provide an overestimate.
- 2. For an explanation of when this subroutine uses the direct method versus Strassen's algorithm, see "Notes" on page 408.

#### On Return

C

is the *l* by n matrix C, containing the results of the computation. Returned as: an *ldc* by (at least) n array, containing numbers of the data type indicated in Table 75 on page 405.

#### **Notes**

- 1. There are two instances when these subroutines use the direct method (GEMUL), rather than using Strassen's algorithm:
  - When either or both of the input matrices are small
  - For CGEMMS and ZGEMMS, when input matrices **A** and **B** overlap

In these instances when the direct method is used, the subroutine does not use auxiliary storage, and you can specify naux = 0.

- 2. For CGEMMS and ZGEMMS, one of the input matrices, **A** or **B**, is rearranged during the computation and restored to its original form on return. Keep this in mind when diagnosing an abnormal termination.
- 3. All subroutines accept lowercase letters for the *transa* and *transb* arguments.
- Matrix C must have no common elements with matrices A or B; otherwise, results are unpredictable. See "Concepts" on page 55.
- 5. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The matrix multiplications performed by these subroutines are functionally equivalent to those performed by SGEMUL, DGEMUL, CGEMUL, and ZGEMUL. For details on the computations performed, see "Function" on page 397.

SGEMMS, DGEMMS, CGEMMS, and ZGEMMS use Winograd's variation of the Strassen's algorithm with minor changes for tuning purposes. (See pages 45 and 46 in reference [11].) The subroutines compute matrix multiplication for both real and complex matrices of large sizes. Complex matrix multiplication uses a special technique, using three real matrix multiplications and five real matrix additions. Each of these three resulting matrix multiplications then uses Strassen's algorithm.

Strassen's Algorithm: The steps of Strassen's algorithm can be repeated up to four times by these subroutines, with each step reducing the dimensions of the matrix by a factor of two. The number of steps used by this subroutine depends on the size of the input matrices. Each step reduces the number of operations by about 10% from the normal matrix multiplication. On the other hand, if the matrix is small, a normal matrix multiplication is performed without using the Strassen's algorithm, and no improvement is gained. For details about small matrices, see "Notes."

Complex Matrix Multiplication: The complex multiplication is performed by forming the real and imaginary parts of the input matrices. These subroutines uses three real matrix multiplications and five real matrix additions, instead of the normal four real matrix multiplications and two real matrix additions. Using only three real matrix multiplications allows the subroutine to achieve up to a 25% reduction in matrix operations, which can result in a significant savings in computing time for large matrices.

Accuracy Considerations: Strassen's method is not stable for certain row or column scalings of the input matrices **A** and **B**. Therefore, for matrices **A** and **B** with divergent exponent values Strassen's method may give inaccurate results. For these cases, you should use the \_GEMUL or \_GEMM subroutines.

**Special Usage:** The equivalence rules, defined for matrix multiplication of  $\boldsymbol{A}$  and  $\boldsymbol{B}$  in "Special Usage" on page 398, also apply to these subroutines. You should use the equivalence rules when you want to transpose or conjugate transpose the result of the multiplication computation. When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your output array, receiving  $\boldsymbol{C}^T$  or  $\boldsymbol{C}^H$ , has dimensions large enough to hold the resulting transposed or conjugate transposed matrix. See "Example 2" on page 400 and "Example 4" on page 401.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. Ida, Idb,  $Idc \le 0$
- 2. l, m, n < 0
- 3. I > Idc
- 4. transa, transb ≠ 'N' or 'T' for SGEMMS and DGEMMS
- 5. transa, transb ≠ 'N', 'T', or 'C' for CGEMMS and ZGEMMS
- 6. transa = 'N'and l > Ida
- 7. transa = 'T' or 'C' and m > lda
- 8. transb = 'N' and m > ldb
- 9. transb = 'T' or 'C' and n > ldb
- 10. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows the computation  $C \leftarrow AB$ , where A, B, and C are contained in larger arrays A, B, and C, respectively. It shows how to code the calling sequence for SGEMMS, but does not use the Strassen algorithm for doing the computation. The calling sequence is shown below. The input and output, other than auxiliary storage, is the same as in "Example 1" on page 399 for SGEMUL.

Call Statement and Input

**Example 2:** This example shows the computation  $C \leftarrow AB^H$ , where A and C are contained in larger arrays A and C, respectively, and B is the same size as the array B in which it is contained. The arrays contain complex data. This example shows how to code the calling sequence for CGEMMS, but does not use the Strassen algorithm for doing the computation. The calling sequence is shown below. The input and output, other than auxiliary storage, is the same as in "Example 8" on page 403 for CGEMUL.

## SGEMMS, DGEMMS, CGEMMS, and ZGEMMS

Call Statement and Input

A LDA TRANSA B LDB TRANSB C LDC L M CALL CGEMMS( A , 4 , 'N' , B , 3 , 'C' , C , 4 , 3 , 2 , 3 , AUX , 0 )

# SGEMM, DGEMM, CGEMM, and ZGEMM—Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes

SGEMM and DGEMM can perform any one of the following combined matrix computations, using scalars  $\alpha$  and  $\beta$ , matrices  $\textbf{\textit{A}}$  and  $\textbf{\textit{B}}$  or their transposes, and matrix  $\textbf{\textit{C}}$ :

$$C \leftarrow \alpha AB + \beta C$$
 $C \leftarrow \alpha AB^{T} + \beta C$  $C \leftarrow \alpha A^{T}B + \beta C$  $C \leftarrow \alpha A^{T}B^{T} + \beta C$ 

CGEMM and ZGEMM can perform any one of the following combined matrix computations, using scalars  $\alpha$  and  $\beta$ , matrices A and B, their transposes or their conjugate transposes, and matrix C:

$\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{T} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{H} + \beta \mathbf{C}$
$\mathbf{C} \leftarrow \alpha \mathbf{A}^{T} \mathbf{B} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A}^{T} \mathbf{B}^{T} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A}^{T} \mathbf{B}^{H} + \beta \mathbf{C}$
$\mathbf{C} \leftarrow \alpha \mathbf{A}^{H} \mathbf{B} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A}^{H} \mathbf{B}^{T} + \beta \mathbf{C}$	$\mathbf{C} \leftarrow \alpha \mathbf{A}^{H} \mathbf{B}^{H} + \beta \mathbf{C}$

Table 76. Data Types	
<b>Α</b> , <b>Β</b> , <b>C</b> , α, β	Subroutine
Short-precision real	SGEMM
Long-precision real	DGEMM
Short-precision complex	CGEMM
Long-precision complex	ZGEMM

#### Syntax

Fortran	CALL SGEMM   DGEMM   CGEMM   ZGEMM (transa, transb, I, n, m, alpha, a, Ida, b, Idb, beta, c, Idc)
C and C++	sgemm   dgemm   cgemm   zgemm (transa, transb, I, n, m, alpha, a, Ida, b, Idb, beta, c, Idc);
PL/I	CALL SGEMM   DGEMM   CGEMM   ZGEMM (transa, transb, I, n, m, alpha, a, Ida, b, Idb, beta, c, Idc);

#### On Entry

#### transa

indicates the form of matrix  $\boldsymbol{A}$  to use in the computation, where:

If transa = 'N', **A** is used in the computation.

If transa = 'T',  $A^T$  is used in the computation.

If transa = 'C',  $A^H$  is used in the computation.

Specified as: a single character; *transa* = 'N', 'T', or 'C'. *transb* 

indicates the form of matrix **B** to use in the computation, where:

If transb = 'N', **B** is used in the computation.

If transb = 'T',  $B^T$  is used in the computation.

If  $transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}$ ,  $B^{\mathsf{H}}$  is used in the computation.

Specified as: a single character; *transb* = 'N', 'T', or 'C'.

```
I
    is the number of rows in matrix C. Specified as: a fullword integer; 0 \le l \le ldc.
    is the number of columns in matrix C. Specified as: a fullword integer; n \ge 0.
m
    has the following meaning, where:
    If transa = 'N', it is the number of columns in matrix A.
    If transa = 'T' or 'C', it is the number of rows in matrix A.
    In addition:
    If transb = 'N', it is the number of rows in matrix B.
    If transb = 'T' or 'C', it is the number of columns in matrix B.
    Specified as: a fullword integer; m \ge 0.
alpha
    is the scalar \alpha. Specified as: a number of the data type indicated in Table 76
    on page 411.
    is the matrix A, where:
    If transa = 'N', A is used in the computation, and A has I rows and m
    columns.
    If transa = 'T', A^T is used in the computation, and A has m rows and I
    columns.
    If transa = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, \mathbf{A}^{\mathsf{H}} is used in the computation, and \mathbf{A} has m rows and I
    columns.
    Note: No data should be moved to form A^T or A^H; that is, the matrix A should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 76 on page 411, where:
    If transa = 'N', its size must be lda by (at least) m.
    If transa = 'T' or 'C', its size must be Ida by (at least) I.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0 and:
    If transa = 'N', Ida \ge I.
    If transa = 'T' \text{ or } 'C', Ida \ge m.
    is the matrix B, where:
    If transb = 'N', B is used in the computation, and B has m rows and n
    columns.
    If transb = {}^{\mathsf{T}}\mathsf{T}, \mathbf{B}^{\mathsf{T}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    If transb = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}, \mathbf{B}^{\mathsf{H}} is used in the computation, and \mathbf{B} has n rows and m
    columns.
    Note: No data should be moved to form B^T or B^H; that is, the matrix B should
```

always be stored in its untransposed form.

Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 76 on page 411, where:

If transb = 'N', its size must be ldb by (at least) n.

If transb = 'T' or 'C', its size must be ldb by (at least) m.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and:

If transb = 'N',  $ldb \ge m$ .

If  $transb = 'T' \text{ or } 'C', Idb \ge n.$ 

beta

is the scalar  $\beta$ . Specified as: a number of the data type indicated in Table 76 on page 411.

С

is the *I* by n matrix C. Specified as: a two-dimensional array, containing numbers of the data type indicated in Table 76 on page 411.

ldc

is the leading dimension of the array specified for c. Specified as: a fullword integer; ldc > 0 and  $ldc \ge l$ .

#### On Return

С

is the *l* by n matrix C, containing the results of the computation. Returned as: an *ldc* by (at least) n array, containing numbers of the data type indicated in Table 76 on page 411.

#### Notes

- 1. All subroutines accept lowercase letters for the transa and transb arguments.
- 2. For SGEMM and DGEMM, if you specify 'C' for the *transa* or *transb* argument, it is interpreted as though you specified 'T'.
- 3. Matrix *C* must have no common elements with matrices *A* or *B*; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The combined matrix addition and multiplication is expressed as follows, where  $a_{ik}$ ,  $b_{ki}$ , and  $c_{ii}$  are elements of matrices **A**, **B**, and **C**, respectively:

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ik} b_{kj}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} b_{kj}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} \overline{a}_{ki} b_{kj}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ik} b_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathsf{T}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} b_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{T}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

$$c_{ij} = \left(\alpha \sum_{k=1}^{m} a_{ki} \overline{b}_{jk}\right) + \beta c_{ij} \quad \text{for } \mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$$

See references [32] and [38]. In the following three cases, no computation is performed:

- / is 0.
- n is 0.
- $\beta$  is 1 and  $\alpha$  is 0.

Assuming the above conditions do not exist, if  $\beta \neq 1$  and m is 0, then  $\beta C$  is returned.

#### Special Usage

Equivalence Rules: The equivalence rules, defined for matrix multiplication of **A** and **B** in "Special Usage" on page 398, also apply to the matrix multiplication part of the computation performed by this subroutine. You should use the equivalent rules when you want to transpose or conjugate transpose the multiplication part of the computation. When coding the calling sequences for these cases, be careful to code your matrix arguments and dimension arguments in the order indicated by the rule. Also, be careful that your input and output array C has dimensions large enough to hold the resulting matrix. See "Example 4" on page 417.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area (CGEMM and ZGEMM only).

Computational Errors: None

Input-Argument Errors

- 1. Ida, Idb,  $Idc \le 0$
- 2. l, m, n < 0
- 3. I > Idc
- 4. transa, transb ≠ 'N', 'T', or 'C'
- 5. transa = 'N' and l > Ida
- 6. transa = 'T' or 'C' and m > Ida
- 7. transb = 'N' and m > ldb
- 8. transb = 'T' or 'C' and n > ldb

**Example 1:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$ , where  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  are contained in larger arrays A, B, and C, respectively.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & -1.0 & -1.0 & 4.0 \\ 2.0 & 0.0 & 1.0 & 1.0 & -1.0 \\ 1.0 & -1.0 & -1.0 & 1.0 & 2.0 \\ -3.0 & 2.0 & 2.0 & 2.0 & 0.0 \\ 4.0 & 0.0 & -2.0 & 1.0 & -1.0 \\ -1.0 & -1.0 & 1.0 & -3.0 & 2.0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ & \ddots & \ddots & \ddots & \vdots \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 24.0 & 13.0 & -5.0 & 3.0 \\ -3.0 & -4.0 & 2.0 & 4.0 \\ 4.0 & 1.0 & 2.0 & 5.0 \\ -2.0 & 6.0 & -1.0 & -9.0 \\ -4.0 & -6.0 & 5.0 & 5.0 \\ 16.0 & 7.0 & -4.0 & 7.0 \\ & & & & & & & \end{bmatrix}$$

**Example 2:** This example shows the computation  $C \leftarrow \alpha AB^{T} + \beta C$ , where A and C are contained in larger arrays A and C, respectively, and B is the same size as array B in which it is contained.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \\ & & & \end{bmatrix}$$

$$B = \begin{vmatrix} 1.0 & -3.0 \\ 2.0 & 4.0 \\ 1.0 & -1.0 \end{vmatrix}$$

$$C = \begin{bmatrix} 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ 0.5 & 0.5 & 0.5 \\ \vdots & \vdots & \ddots & \vdots \\ . & . & . & . \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 11.0 & -9.0 & 5.0 \\ -9.0 & 21.0 & -1.0 \\ 5.0 & -1.0 & 3.0 \\ & & & & \\ & & & & \\ \end{bmatrix}$$

**Example 3:** This example shows the computation  $C \leftarrow \alpha AB + \beta C$  using complex data, where **A**, **B**, and **C** are contained in larger arrays, A, B, and C, respectively.

ALPHA = 
$$(1.0, 0.0)$$
  
BETA =  $(2.0, 0.0)$ 

$$A = \begin{pmatrix} (1.0, 5.0) & (9.0, 2.0) & (1.0, 9.0) \\ (2.0, 4.0) & (8.0, 3.0) & (1.0, 8.0) \\ (3.0, 3.0) & (7.0, 5.0) & (1.0, 7.0) \\ (4.0, 2.0) & (4.0, 7.0) & (1.0, 5.0) \\ (5.0, 1.0) & (5.0, 1.0) & (1.0, 6.0) \\ (6.0, 6.0) & (3.0, 6.0) & (1.0, 4.0) \\ & & & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & &$$

B = 
$$\begin{vmatrix} (1.0, 8.0) & (2.0, 7.0) \\ (4.0, 4.0) & (6.0, 8.0) \\ (6.0, 2.0) & (4.0, 5.0) \\ & & & & & & \\ \end{vmatrix}$$

$$C = \begin{pmatrix} (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ (0.5, 0.0) & (0.5, 0.0) \\ & & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & & \\ & &$$

Output

**Example 4:** This example shows how to obtain the conjugate transpose of **AB**<sup>H</sup>.

$$\left(\boldsymbol{A}\boldsymbol{B}^{\mathrm{H}}\right)^{\mathrm{H}} = \overline{\boldsymbol{B}}\boldsymbol{A}^{\mathrm{T}} = \boldsymbol{B}\boldsymbol{A}^{\mathrm{H}}$$

This shows the conjugate transpose of the computation performed in "Example 8" on page 403 for CGEMUL, which uses the following calling sequence:

You instead code the calling sequence for  $\mathbf{C} \leftarrow \beta \mathbf{C} + \alpha \mathbf{B} \mathbf{A}^H$ , where  $\beta = 0$ ,  $\alpha = 1$ , and the array  $\mathbf{C}$  has the correct dimensions to receive the transposed matrix.

Because  $\beta$  is zero,  $\beta C = 0$ . For a description of all the matrix identities, see "Special Usage" on page 398.

#### Call Statement and Input

B = 
$$\begin{bmatrix} (1.0, 3.0) & (-3.0, 2.0) \\ (2.0, 5.0) & (4.0, 6.0) \\ (1.0, 1.0) & (-1.0, 9.0) \end{bmatrix}$$

C =(not relevant)

Output

$$C = \begin{bmatrix} (20.0, 1.0) & (18.0, 23.0) & (26.0, 23.0) \\ (12.0, -25.0) & (80.0, 2.0) & (56.0, -37.0) \\ (24.0, -26.0) & (49.0, 37.0) & (76.0, -2.0) \\ & & & & & & \end{bmatrix}$$

**Example 5:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B}^{\mathsf{H}} + \beta \mathbf{C}$  using complex data, where A, B, and C are the same size as the arrays A, B, and C, in which they are contained. Because  $\beta$  is zero,  $\beta C = 0$ . (Based on the dimensions of the matrices, **A** is actually a column vector, and **C** is actually a row vector.)

$$A = \begin{bmatrix} (1.0, 2.0) \\ (2.0, 5.0) \\ (1.0, 6.0) \end{bmatrix}$$

B = 
$$\begin{bmatrix} (1.0, 6.0) & (-3.0, 4.0) & (2.0, 6.0) \\ (2.0, 3.0) & (4.0, 6.0) & (0.0, 3.0) \\ (1.0, 3.0) & (-1.0, 6.0) & (-1.0, 9.0) \end{bmatrix}$$

## SGEMM, DGEMM, CGEMM, and ZGEMM

C =(not relevant)

Output

A = 
$$\begin{bmatrix} (86.0, 44.0) & (58.0, 70.0) & (121.0, 55.0) \end{bmatrix}$$

# SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM—Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian

These subroutines compute one of the following matrix-matrix products, using the scalars  $\alpha$  and  $\beta$  and matrices **A**, **B**, and **C**:

1.  $\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$ 

2.  $C \leftarrow \alpha BA + \beta C$ 

where matrix **A** is stored in either upper or lower storage mode, and:

- For SSYMM and DSYMM, matrix A is real symmetric.
- For CSYMM and ZSYMM, matrix **A** is complex symmetric.
- For CHEMM and ZHEMM, matrix **A** is complex Hermitian.

Table 77. Data Types	
α, <b>A</b> , <b>B</b> , β, <b>C</b>	Subprogram
Short-precision real	SSYMM
Long-precision real	DSYMM
Short-precision complex	CSYMM and CHEMM
Long-precision complex	ZSYMM and ZHEMM

#### Syntax

Fortran	CALL SSYMM   DSYMM   CSYMM   ZSYMM   CHEMM   ZHEMM (side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc)
C and C++	ssymm   dsymm   csymm   zsymm   chemm   zhemm (side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc);
PL/I	CALL SSYMM   DSYMM   CSYMM   ZSYMM   CHEMM   ZHEMM (side, uplo, m, n, alpha, a, lda, b, ldb, beta, c, ldc);

#### On Entry

side

indicates whether matrix  $\boldsymbol{A}$  is located to the left or right of rectangular matrix  $\boldsymbol{B}$  in the equation used for this computation, where:

If side = 'L', **A** is to the left of **B**, resulting in equation 1.

If side = 'R', **A** is to the right of **B**, resulting in equation 2.

Specified as: a single character. It must be 'L' or 'R'. uplo

indicates the storage mode used for matrix **A**, where:

If uplo = 'U', **A** is stored in upper storage mode.

If uplo = 'L', **A** is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

m

is the number of rows in rectangular matrices **B** and **C**, and:

If side = 'L', m is the order of triangular matrix A.

Specified as: a fullword integer;  $0 \le m \le ldb$ ,  $m \le ldc$ , and:

#### SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

```
If side = 'L', m \le Ida.
n
    is the number of columns in rectangular matrices B and C, and:
    If side = 'R', n is the order of triangular matrix A.
    Specified as: a fullword integer; n \ge 0 and:
    If side = 'R', n \le Ida.
alpha
    is the scalar \alpha. Specified as: a number of the data type indicated in Table 77
    on page 420.
а
    is the real symmetric, complex symmetric, or complex Hermitian matrix A,
    where:
    If side = 'L', A is order m.
    If side = 'R', A is order n.
    and where it is stored as follows:
    If uplo = 'U', A is stored in upper storage mode.
    If uplo = 'L', A is stored in lower storage mode.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 77 on page 420, where:
    If side = 'L', its size must be Ida by (at least) m.
    If side = 'R', it size must be Ida by (at least) n.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0 and:
    If side = 'L', Ida \ge m.
    If side = 'R', Ida \ge n.
b
    is the m by n rectangular matrix B. Specified as: an ldb by (at least) n array,
    containing numbers of the data type indicated in Table 77 on page 420.
ldb
    is the leading dimension of the array specified for b. Specified as: a fullword
    integer; ldb > 0 and ldb \ge m.
beta
    is the scalar β. Specified as: a number of the data type indicated in Table 77
    on page 420.
    is the m by n rectangular matrix \boldsymbol{c}. Specified as: an ldc by (at least) n array,
    containing numbers of the data type indicated in Table 77 on page 420.
ldc
    is the leading dimension of the array specified for c. Specified as: a fullword
    integer; ldc > 0 and ldc \ge m.
On Return
    is the m by n matrix \boldsymbol{c}, containing the results of the computation.
```

Returned as: an *ldc* by (at least) *n* array, containing numbers of the data type

indicated in Table 77 on page 420.

#### **Notes**

- 1. These subroutines accept lowercase letters for the *side* and *uplo* arguments.
- 2. Matrices A, B, and C must have no common elements; otherwise, results are unpredictable.
- 3. If matrix **A** is upper triangular (uplo = 'U'), these subroutines use only the data in the upper triangular portion of the array. If matrix **A** is lower triangular, (uplo = 'L'), these subroutines use only the data in the lower triangular portion of the array. In each case, the other portion of the array is altered during the computation, but restored before exit.
- 4. The imaginary parts of the diagonal elements of a complex Hermitian matrix A are assumed to be zero, so you do not have to set these values.
- 5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 70.

Function: These subroutines can perform the following matrix-matrix product computations using matrix A, which is real symmetric for SSYMM and DSYMM, complex symmetric for CSYMM and ZSYMM, and complex Hermitian for CHEMM and ZHEMM:

- 1.  $\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$
- 2.  $C \leftarrow \alpha BA + \beta C$

where:

 $\alpha$  and  $\beta$  are scalars.

A is a matrix of the type indicated above, stored in upper or lower storage mode. It is order *m* for equation 1 and order *n* for equation 2.

**B** and **C** are *m* by *n* rectangular matrices.

See references [32] and [38]. In the following two cases, no computation is performed:

- n or m is 0.
- β is one and α is zero.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors

- 1. m < 0
- 2. m > ldb
- 3. m > ldc
- 4. n < 0
- 5. Ida, Idb,  $Idc \le 0$
- 6. *side* ≠ 'L' or 'R'
- 7. *uplo* ≠ 'L' or 'U'
- 8. side = 'L' and m > Ida
- 9. side = 'R' and n > Ida

**Example 1:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a real symmetric matrix of order 5, stored in upper storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 5 by 4 rectangular matrices.

#### Call Statement and Input

$$B = \begin{bmatrix} 1.0 & -1.0 & 0.0 & 2.0 \\ 2.0 & 2.0 & -1.0 & -2.0 \\ 1.0 & 0.0 & -1.0 & 1.0 \\ -3.0 & -1.0 & 1.0 & -1.0 \\ 4.0 & 2.0 & -1.0 & 1.0 \\ & & & & & & & & \\ \end{bmatrix}$$

$$C = \begin{bmatrix} 23.0 & 12.0 & -6.0 & 2.0 \\ -4.0 & -5.0 & 1.0 & 3.0 \\ 5.0 & 6.0 & -1.0 & -4.0 \\ -4.0 & 1.0 & 0.0 & -5.0 \\ 8.0 & -4.0 & -2.0 & 13.0 \end{bmatrix}$$

#### Output

$$C = \begin{bmatrix} 69.0 & 36.0 & -18.0 & 6.0 \\ -12.0 & -15.0 & 3.0 & 9.0 \\ 15.0 & 18.0 & -3.0 & -12.0 \\ -12.0 & 3.0 & 0.0 & -15.0 \\ 8.0 & -20.0 & -2.0 & 35.0 \end{bmatrix}$$

**Example 2:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{AB} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a real symmetric matrix of order 3, stored in lower storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 3 by 6 rectangular matrices.

#### SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

$$A = \begin{bmatrix} 1.0 & . & . \\ 2.0 & 4.0 & . \\ 1.0 & -1.0 & -1.0 \\ . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 & 2.0 & -1.0 & 2.0 \\ 2.0 & 4.0 & 0.0 & 0.0 & 1.0 & -2.0 \\ 1.0 & -1.0 & -1.0 & -1.0 & -1.0 & 1.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 6.0 & 4.0 & 1.0 & 1.0 & 0.0 & -1.0 \\ 9.0 & 11.0 & 5.0 & 5.0 & 3.0 & -5.0 \\ -2.0 & -6.0 & 3.0 & 3.0 & -1.0 & 32.0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & \vdots \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 24.0 & 16.0 & 4.0 & 4.0 & 0.0 & -4.0 \\ 36.0 & 44.0 & 20.0 & 20.0 & 12.0 & -20.0 \\ -8.0 & -24.0 & 12.0 & 12.0 & -4.0 & 12.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ . & . & . & . & . & . & . \end{bmatrix}$$

**Example 3:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{B} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a real symmetric matrix of order 3, stored in upper storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 2 by 3 rectangular matrices.

$$A = \begin{bmatrix} 1.0 & -3.0 & 1.0 \\ . & 4.0 & -1.0 \\ . & . & 2.0 \\ . & . & . \end{bmatrix}$$

$$B = \begin{vmatrix} 1.0 & -3.0 & 3.0 \\ 2.0 & 4.0 & -1.0 \\ \cdot & \cdot & \cdot \end{vmatrix}$$

$$C = \begin{bmatrix} 13.0 & -18.0 & 10.0 \\ -11.0 & 11.0 & -4.0 \\ \vdots & \vdots & \vdots \\ 0.0 & 0.0 & \vdots \end{bmatrix}$$

Output

**Example 4:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{B} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a real symmetric matrix of order 3, stored in lower storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 3 by 3 square matrices.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & . & . \\ 2.0 & 10.0 & . \\ 1.0 & 11.0 & 4.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -3.0 & 2.0 \\ 2.0 & 4.0 & 0.0 \\ 1.0 & -1.0 & -1.0 \end{bmatrix}$$

$$C = \begin{bmatrix} 1.0 & 5.0 & -9.0 \\ -3.0 & 10.0 & -2.0 \\ -2.0 & 8.0 & 0.0 \end{bmatrix}$$

Output

$$C = \begin{bmatrix} 4.0 & 11.0 & 15.0 \\ -13.0 & -34.0 & -48.0 \\ 0.0 & 27.0 & 14.0 \end{bmatrix}$$

**Example 5:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{B} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a complex symmetric matrix of order 3, stored in upper storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 2 by 3 rectangular matrices.

$$A = \begin{bmatrix} (1.0, 5.0) & (-3.0, 2.0) & (1.0, 6.0) \\ . & (4.0, 5.0) & (-1.0, 4.0) \\ . & . & (2.0, 5.0) \end{bmatrix}$$

B = 
$$\begin{bmatrix} (1.0, 1.0) & (-3.0, 2.0) & (3.0, 3.0) \\ (2.0, 6.0) & (4.0, 5.0) & (-1.0, 4.0) \\ & & & & & & & \\ \end{bmatrix}$$

Output

**Example 6:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{B} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a complex Hermitian matrix of order 3, stored in lower storage mode, and  $\mathbf{B}$  and  $\mathbf{C}$  are 3 by 3 square matrices.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values.

### SSYMM, DSYMM, CSYMM, ZSYMM, CHEMM, and ZHEMM

$$C = \begin{bmatrix} (13.0, 6.0) & (-18.0, 6.0) & (10.0, 7.0) \\ (-11.0, 8.0) & (11.0, 1.0) & (-4.0, 2.0) \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \end{bmatrix}$$

Output

# STRMM, DTRMM, CTRMM, and ZTRMM—Triangular Matrix-Matrix Product

STRMM and DTRMM compute one of the following matrix-matrix products, using the scalar  $\alpha$ , rectangular matrix  $\boldsymbol{B}$ , and triangular matrix  $\boldsymbol{A}$  or its transpose:

1. 
$$\mathbf{B} \leftarrow \alpha \mathbf{A} \mathbf{B}$$
 3.  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}$   
2.  $\mathbf{B} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B}$  4.  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}^{\mathsf{T}}$ 

CTRMM and ZTRMM compute one of the following matrix-matrix products, using the scalar  $\alpha$ , rectangular matrix  $\boldsymbol{B}$ , and triangular matrix  $\boldsymbol{A}$ , its transpose, or its conjugate transpose:

1. 
$$B \leftarrow \alpha AB$$
3.  $B \leftarrow \alpha BA$ 5.  $B \leftarrow \alpha A^{H}B$ 2.  $B \leftarrow \alpha A^{T}B$ 4.  $B \leftarrow \alpha BA^{T}$ 6.  $B \leftarrow \alpha BA^{H}B$ 

Table 78. Data Types	
<b>Α</b> , <b>Β</b> , α	Subroutine
Short-precision real	STRMM
Long-precision real	DTRMM
Short-precision complex	CTRMM
Long-precision complex	ZTRMM

#### Syntax

Fortran	CALL STRMM   DTRMM   CTRMM   ZTRMM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)
C and C++	strmm   dtrmm   ctrmm   ztrmm (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb);
PL/I	CALL STRMM   DTRMM   CTRMM   ZTRMM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb);

On Entry

side

indicates whether the triangular matrix  $\boldsymbol{A}$  is located to the left or right of rectangular matrix  $\boldsymbol{B}$  in the equation used for this computation, where:

If side = 'L', **A** is to the left of **B** in the equation, resulting in either equation 1, 2, or 5.

If side = 'R', **A** is to the right of **B** in the equation, resulting in either equation 3, 4, or 6.

Specified as: a single character. It must be 'L' or 'R'. uplo

indicates whether matrix **A** is an upper or lower triangular matrix, where:

If uplo = 'U', **A** is an upper triangular matrix.

If uplo = 'L', **A** is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'. transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation, resulting in either equation 1 or 3.

```
If transa = T^{\dagger}, A^{\dagger} is used in the computation, resulting in either equation 2 or
    4.
    If transa = 'C', AH is used in the computation, resulting in either equation 5 or
    Specified as: a single character. It must be 'N', 'T', or 'C'.
diag
    indicates the characteristics of the diagonal of matrix A, where:
    If diag = 'U', A is a unit triangular matrix.
    If diag = 'N', A is not a unit triangular matrix.
    Specified as: a single character. It must be 'U' or 'N'.
m
   is the number of rows in rectangular matrix B, and:
    If side = 'L', m is the order of triangular matrix A.
    Specified as: a fullword integer, where:
    If side = L', 0 \le m \le Ida and m \le Idb.
    If side = {}^{\shortmid}R{}^{\shortmid}, 0 \le m \le ldb.
    is the number of columns in rectangular matrix B, and:
    If side = 'R', n is the order of triangular matrix A.
    Specified as: a fullword integer; n \ge 0 and:
    If side = 'R', n \le Ida.
alpha
    is the scalar \alpha. Specified as: a number of the data type indicated in Table 78
    on page 428.
    is the triangular matrix A, of which only the upper or lower triangular portion is
    used, where:
    If side = 'L', A is order m.
    If side = 'R', A is order n.
    Note: No data should be moved to form A^T or A^H; that is, the matrix A should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 78 on page 428, where:
    If side = L', its size must be lda by (at least) m.
    If side = 'R', it size must be Ida by (at least) n.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
   integer; Ida > 0 and:
   If side = L', Ida \ge m.
    If side = 'R', Ida \ge n.
b
    is the m by n rectangular matrix B. Specified as: an ldb by (at least) n array,
```

containing numbers of the data type indicated in Table 78 on page 428.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge m$ .

#### On Return

h

is the m by n matrix  $\mathbf{B}$ , containing the results of the computation. Returned as: an ldb by (at least) n array, containing numbers of the data type indicated in Table 78 on page 428.

#### Notes

- These subroutines accept lowercase letters for the side, uplo, transa, and diag arguments.
- 2. For STRMM and DTRMM, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 3. Matrices **A** and **B** must have no common elements; otherwise, results are unpredictable.
- 4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.
- 5. For a description of triangular matrices and how they are stored, see "Triangular Matrix" on page 73.

**Function:** These subroutines can perform the following matrix-matrix product computations, using the triangular matrix **A**, its transpose, or its conjugate transpose, where **A** can be either upper- or lower-triangular:

```
1. B \leftarrow \alpha AB
```

2.  $\mathbf{B} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B}$ 

3.  $\mathbf{B} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}$  (for CTRMM and ZTRMM only)

where:

 $\alpha$  is a scalar.

**A** is a triangular matrix of order *m*.

**B** is an *m* by *n* rectangular matrix.

4.  $B \leftarrow \alpha BA$ 

5.  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}^{\mathsf{T}}$ 

6.  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}^{\mathsf{H}}$  (for CTRMM and ZTRMM only)

where:

 $\alpha$  is a scalar.

**A** is a triangular matrix of order *n*.

**B** is an *m* by *n* rectangular matrix.

See references [32] and [38]. If *n* or *m* is 0, no computation is performed.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

#### Input-Argument Errors

- 1. m < 0
- 2. n < 0
- 3. Ida,  $Idb \leq 0$
- 4. *side* ≠ 'L' or 'R'
- 5. *uplo* ≠ 'L' or 'U'
- 6. *transa* ≠ 'T', 'N', or 'C'
- 7. *diag* ≠ 'N' or 'U'
- 8. side = 'L' and m > Ida
- 9. m > ldb
- 10. side = 'R' and n > Ida

**Example 1:** This example shows the computation  $\mathbf{B} \leftarrow \alpha \mathbf{AB}$ , where  $\mathbf{A}$  is a 5 by 5 upper triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a 5 by 3 rectangular matrix.

#### Call Statement and Input

$$B = \begin{bmatrix} 2.0 & 3.0 & 1.0 \\ 5.0 & 5.0 & 4.0 \\ 0.0 & 1.0 & 2.0 \\ 3.0 & 1.0 & -3.0 \\ -1.0 & 2.0 & 1.0 \\ & & & & \end{bmatrix}$$

#### Output

$$B = \begin{bmatrix} 6.0 & 10.0 & -2.0 \\ -16.0 & -1.0 & 6.0 \\ -2.0 & 1.0 & -4.0 \\ 14.0 & 0.0 & -14.0 \\ -1.0 & 2.0 & 1.0 \\ & & & & \end{bmatrix}$$

**Example 2:** This example shows the computation  $\mathbf{B} \leftarrow \alpha \mathbf{A}^T \mathbf{B}$ , where  $\mathbf{A}$  is a 5 by 5 upper triangular matrix that is not unit triangular, and **B** is a 5 by 4 rectangular matrix.

#### Call Statement and Input

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 \\ 3.0 & 3.0 & -1.0 & 2.0 \\ -2.0 & -1.0 & 0.0 & 1.0 \\ 4.0 & 4.0 & -3.0 & -3.0 \\ 2.0 & 2.0 & 2.0 & 2.0 \\ & & & & & & & \end{bmatrix}$$

#### Output

$$B = \begin{bmatrix} -1.0 & -2.0 & -3.0 & -4.0 \\ 2.0 & -2.0 & -14.0 & -12.0 \\ 10.0 & 5.0 & -8.0 & -7.0 \\ 14.0 & 15.0 & 1.0 & 8.0 \\ -3.0 & 4.0 & 3.0 & 16.0 \\ & & & & & & & & & & \end{bmatrix}$$

**Example 3:** This example shows the computation  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}$ , where  $\mathbf{A}$  is a 5 by 5 lower triangular matrix that is not unit triangular, and **B** is a 3 by 5 rectangular matrix.

$$B = \begin{bmatrix} 3.0 & 4.0 & -1.0 & -1.0 & -1.0 \\ 2.0 & 1.0 & -1.0 & 0.0 & 3.0 \\ -2.0 & -1.0 & -3.0 & 0.0 & 2.0 \\ & & & & & & & & & & \end{bmatrix}$$

Output

$$B = \begin{bmatrix} 10.0 & 4.0 & 0.0 & 0.0 & 1.0 \\ 10.0 & 14.0 & -4.0 & 6.0 & -3.0 \\ -8.0 & 2.0 & -5.0 & 4.0 & -2.0 \\ & & & & & & & & & & & & \end{bmatrix}$$

**Example 4:** This example shows the computation  $\mathbf{B} \leftarrow \alpha \mathbf{B} \mathbf{A}$ , where  $\mathbf{A}$  is a 6 by 6 upper triangular matrix that is unit triangular, and  $\mathbf{B}$  is a 1 by 6 rectangular matrix.

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

Output

$$B = \begin{bmatrix} 1.0 & 4.0 & -2.0 & 10.0 & 2.0 & -6.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

**Example 5:** This example shows the computation  $\mathbf{B} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{B}$ , where  $\mathbf{A}$  is a 5 by 5 upper triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a 5 by 1 rectangular matrix.

#### STRMM, DTRMM, CTRMM, and ZTRMM

$$B = \begin{bmatrix} (3.0, 4.0) \\ (-4.0, 2.0) \\ (-5.0, 0.0) \\ (1.0, 3.0) \\ (3.0, 1.0) \\ \end{bmatrix}$$

Output

$$B = \begin{bmatrix} (-8.0, -19.0) \\ (8.0, 21.0) \\ (44.0, -8.0) \\ (13.0, -7.0) \\ (19.0, 2.0) \\ . \end{bmatrix}$$

# SSYRK, DSYRK, CSYRK, ZSYRK, CHERK, and ZHERK—Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix

These subroutines compute one of the following rank-k updates, where matrix  $\boldsymbol{\mathcal{C}}$  is stored in either upper or lower storage mode. SSYRK, DSYRK, CSYRK, and ZSYRK use the scalars  $\alpha$  and  $\beta$ , real or complex matrix  $\boldsymbol{\mathcal{A}}$  or its transpose, and real or complex symmetric matrix  $\boldsymbol{\mathcal{C}}$  to compute:

1. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{A}^{\mathsf{T}} + \beta \mathbf{C}$$

2. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{A} + \beta \mathbf{C}$$

CHERK and ZHERK use the scalars  $\alpha$  and  $\beta$ , complex matrix  $\boldsymbol{A}$  or its complex conjugate transpose, and complex Hermitian matrix  $\boldsymbol{C}$  to compute:

3. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{A}^{\mathsf{H}} + \beta \mathbf{C}$$

4. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{A} + \beta \mathbf{C}$$

Table 79. Data Types					
A, C	α, β	Subprogram			
Short-precision real	Short-precision real	SSYRK			
Long-precision real	Long-precision real	DSYRK			
Short-precision complex	Short-precision complex	CSYRK			
Long-precision complex	Long-precision complex	ZSYRK			
Short-precision complex	Short-precision real	CHERK			
Long-precision complex	Long-precision real	ZHERK			

#### Syntax

Fortran	CALL SSYRK   DSYRK   CSYRK   ZSYRK   CHERK   ZHERK (uplo, trans, n, k, alpha, a, lda, beta, c, ldc)
C and C++	ssyrk   dsyrk   csyrk   zsyrk   cherk   zherk (uplo, trans, n, k, alpha, a, lda, beta, c, ldc);
PL/I	CALL SSYRK   DSYRK   CSYRK   ZSYRK   CHERK   ZHERK (uplo, trans, n, k, alpha, a, lda, beta, c, ldc);

On Entry

uplo

indicates the storage mode used for matrix *C*, where:

If uplo = 'U', C is stored in upper storage mode.

If *uplo* = 'L', **C** is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

trans

indicates the form of matrix **A** to use in the computation, where:

If trans = 'N', **A** is used, resulting in equation 1 or 3.

If  $trans = {}^{\mathsf{T}}\mathsf{T}$ ,  $A^{\mathsf{T}}$  is used, resulting in equation 2.

If trans = 'C', AH is used, resulting in equation 4.

Specified as: a single character, where:

```
For SSYRK and DSYRK, it must be 'N', 'T', or 'C'.
   For CSYRK and ZSYRK, it must be 'N' or 'T'.
   For CHERK and ZHERK, it must be 'N' or 'C'.
n
   is the order of matrix C. Specified as: a fullword integer; 0 \le n \le ldc and:
   If trans = 'N', then n \le Ida.
k
   has the following meaning, where:
   If trans = 'N', it is the number of columns in matrix A.
   If trans = 'T' or 'C', it is the number of rows in matrix A.
    Specified as: a fullword integer; k \ge 0 and:
   If trans = 'T' or 'C', then k \le Ida.
alpha
   is the scalar \alpha. Specified as: a number of the data type indicated in Table 79
   on page 435.
   is the rectangular matrix A, where:
   If trans = 'N', A is n by k.
   If trans = 'T' or 'C', A is k by n.
   Note: No data should be moved to form A^T or A^H; that is, the matrix A should
           always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
   indicated in Table 79 on page 435, where:
   If trans = 'N', its size must be lda by (at least) k.
   If trans = 'T' or 'C', its size must be lda by (at least) n.
lda
   is the leading dimension of the array specified for a. Specified as: a fullword
   integer; Ida > 0 and:
   If trans = 'N', Ida \ge n.
   If trans = 'T' \text{ or } 'C', Ida \ge k.
beta
   is the scalar β. Specified as: a number of the data type indicated in Table 79
   on page 435.
С
   is matrix C of order n, which is real symmetric, complex symmetric, or complex
   Hermitian, where:
   If uplo = 'U', C is stored in upper storage mode.
   If uplo = 'L', C is stored in lower storage mode.
   Specified as: an ldc by (at least) n array, containing numbers of the data type
   indicated in Table 79 on page 435.
ldc
   is the leading dimension of the array specified for c. Specified as: a fullword
   integer; ldc > 0 and ldc \ge n.
```

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On Return

С

is matrix C of order n, which is real symmetric, complex symmetric, or complex Hermitian, containing the results of the computation, where:

If *uplo* = 'U', **C** is stored in upper storage mode.

If *uplo* = 'L', **C** is stored in lower storage mode.

Returned as: an *ldc* by (at least) *n* array, containing numbers of the data type indicated in Table 79 on page 435.

#### Notes

- 1. These subroutines accept lowercase letters for the *uplo* and *trans* arguments.
- 2. For SSYRK and DSYRK, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
- 3. Matrices **A** and **C** must have no common elements; otherwise, results are unpredictable.
- 4. The imaginary parts of the diagonal elements of a complex Hermitian matrix  $\boldsymbol{A}$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero, except when  $\beta$  is one and  $\alpha$  or k is zero, in which case no computation is performed.
- 5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines can perform the following rank-k updates. For SSYRK and DSYRK, matrix  $\boldsymbol{c}$  is real symmetric. For CSYRK and ZSYRK, matrix  $\boldsymbol{c}$  is complex symmetric. They perform:

- 1.  $\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{A}^{\mathsf{T}} + \beta \mathbf{C}$
- 2.  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{A} + \beta \mathbf{C}$

For CHERK and ZHERK, matrix *C* is complex Hermitian. They perform:

- 3.  $\boldsymbol{C} \leftarrow \alpha \boldsymbol{A} \boldsymbol{A}^{\mathsf{H}} + \beta \boldsymbol{C}$
- 4.  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{A} + \beta \mathbf{C}$

#### where:

 $\alpha$  and  $\beta$  are scalars.

 $\boldsymbol{A}$  is a rectangular matrix, which is n by k for equations 1 and 3, and is k by n for equations 2 and 4.

 ${\it C}$  is a matrix of order n of the type indicated above, stored in upper or lower storage mode.

See references [32] and [38]. In the following two cases, no computation is performed:

- n is 0.
- $\beta$  is one, and  $\alpha$  is zero or k is zero.

Assuming the above conditions do not exist, if  $\beta$  is not one, and  $\alpha$  is zero or k is zero, then  $\beta$  C is returned.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

#### Input-Argument Errors

- 1. Ida,  $Idc \le 0$
- 2. Idc < n
- 3. k, n < 0
- 4. *uplo* ≠ 'U' or 'L'
- 5. trans ≠ 'N', 'T', or 'C' for SSYRK and DSYRK
- 6. trans ≠ 'N' or 'T' for CSYRK and ZSYRK
- 7. trans ≠ 'N' or 'C' for CHERK and ZHERK
- 8. trans = 'N' and lda < n
- 9. trans = 'T' or 'C' and Ida < k

**Example 1:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{A}^\mathsf{T} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is an 8 by 2 real rectangular matrix, and  $\mathbf{C}$  is a real symmetric matrix of order 8, stored in upper storage mode.

#### Call Statement and Input

Output

**Example 2:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a 3 by 8 real rectangular matrix, and  $\mathbf{C}$  is a real symmetric matrix of order 8, stored in lower storage mode.

Call Statement and Input

$$A = \begin{bmatrix} 0.0 & 3.0 & 6.0 & 9.0 & 12.0 & 15.0 & 18.0 & 21.0 \\ 1.0 & 4.0 & 7.0 & 10.0 & 13.0 & 16.0 & 19.0 & 22.0 \\ 2.0 & 5.0 & 8.0 & 11.0 & 14.0 & 17.0 & 20.0 & 23.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \end{bmatrix}$$

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} 0.0 \\ 1.0 \\ 8.0 \\ 2.0 \\ 9.0 \\ 15.0 \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\ \\ \\ \end{array} & \begin{array}{c} \\ \\$$

Output

**Example 3:** This example shows the computation  $C \leftarrow \alpha AA^T + \beta C$ , where A is a 3 by 5 complex rectangular matrix, and C is a complex symmetric matrix of order 3, stored in upper storage mode.

Output

$$C = \begin{bmatrix} (-57.0, 13.0) & (-63.0, 79.0) & (-24.0, 70.0) \\ . & (-28.0, 90.0) & (-55.0, 103.0) \\ . & . & (13.0, 75.0) \\ . & . & . \end{bmatrix}$$

**Example 4:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{H}} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  is a 5 by 3 complex rectangular matrix, and  $\mathbf{C}$  is a complex Hermitian matrix of order 3, stored in lower storage mode.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

Call Statement and Input

$$A = \begin{bmatrix} (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (6.0, .) & . & . & . \\ (3.0, 4.0) & (10.0, .) & . \\ (9.0, 1.0) & (12.0, 2.0) & (3.0, .) \\ . & . & . \end{bmatrix}$$

Output

$$C = \begin{bmatrix} (138.0, 0.0) & . & . & . \\ (65.0, 80.0) & (165.0, 0.0) & . \\ (134.0, 46.0) & (88.0, -88.0) & (199.0, 0.0) \\ . & . & . & . \end{bmatrix}$$

# SSYR2K, DSYR2K, CSYR2K, ZSYR2K, CHER2K, and ZHER2K—Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix

These subroutines compute one of the following rank-2k updates, where matrix C is stored in upper or lower storage mode. SSYR2K, DSYR2K, CSYR2K, and ZSYR2K use the scalars  $\alpha$  and  $\beta$ , real or complex matrices **A** and **B** or their transposes, and real or complex symmetric matrix  $\boldsymbol{c}$  to compute:

1. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathsf{T}} + \alpha \mathbf{B} \mathbf{A}^{\mathsf{T}} + \beta \mathbf{C}$$

2. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B} + \alpha \mathbf{B}^{\mathsf{T}} \mathbf{A} + \beta \mathbf{C}$$

CHER2K and ZHER2K use the scalars  $\alpha$  and  $\beta$ , complex matrices **A** and **B** or their complex conjugate transposes, and complex Hermitian matrix *C* to compute:

3. 
$$C \leftarrow \alpha A B^{H} + \overline{\alpha} B A^{H} + \beta C$$

4. 
$$C \leftarrow \alpha A^{\mathrm{H}} B + \overline{\alpha} B^{\mathrm{H}} A + \beta C$$

Table 80. Data Types					
<b>Α</b> , <b>Β</b> , <b>C</b> , α	β	Subprogram			
Short-precision real	Short-precision real	SSYR2K			
Long-precision real	Long-precision real	DSYR2K			
Short-precision complex	Short-precision complex	CSYR2K			
Long-precision complex	Long-precision complex	ZSYR2K			
Short-precision complex	Short-precision real	CHER2K			
Long-precision complex	Long-precision real	ZHER2K			

#### **Syntax**

Fortran	CALL SSYR2K   DSYR2K   CSYR2K   ZSYR2K   CHER2K   ZHER2K (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc)
C and C++	ssyr2k   dsyr2k   csyr2k   zsyr2k   cher2k   zher2k ( <i>uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc</i> );
PL/I	CALL SSYR2K   DSYR2K   CSYR2K   ZSYR2K   CHER2K   ZHER2K (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc);

On Entry

indicates the storage mode used for matrix  $\boldsymbol{c}$ , where:

If uplo = 'U', C is stored in upper storage mode.

If *uplo* = 'L', *C* is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

trans

indicates the form of matrices **A** and **B** to use in the computation, where:

If trans = 'N', **A** and **B** are used, resulting in equation 1 or 3.

```
If trans = {}^{\mathsf{T}}\mathsf{T}, \mathbf{A}^{\mathsf{T}} and \mathbf{B}^{\mathsf{T}} are used, resulting in equation 2.
    If trans = 'C', A^H and B^H are used, resulting in equation 4.
    Specified as: a single character, where:
    For SSYR2K and DSYR2K, it must be 'N', 'T', or 'C'.
    For CSYR2K and ZSYR2K, it must be 'N' or 'T'.
    For CHER2K and ZHER2K, it must be 'N' or 'C'.
n
    is the order of matrix C. Specified as: a fullword integer; 0 \le n \le ldc and:
    If trans = 'N', then n \le Ida and n \le Idb.
k
    has the following meaning, where:
    If trans = 'N', it is the number of columns in matrices A and B.
    If trans = 'T' or 'C', it is the number of rows in matrices A and B.
    Specified as: a fullword integer; k \ge 0 and:
    If trans = 'T' or 'C', then k \le Ida and k \le Idb.
    is the scalar \alpha. Specified as: a number of the data type indicated in Table 80
    on page 442.
а
    is the rectangular matrix A, where:
    If trans = 'N', A is n by k.
    If trans = 'T' or 'C', A is k by n.
    Note: No data should be moved to form A^T or A^H; that is, the matrix A should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 80 on page 442, where:
    If trans = 'N', its size must be lda by (at least) k.
    If trans = 'T' or 'C', its size must be lda by (at least) n.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0 and:
    If trans = 'N', lda \ge n.
    If trans = 'T' \text{ or } 'C', Ida \ge k.
b
    is the rectangular matrix B, where:
    If trans = 'N', B is n by k.
    If trans = 'T' \text{ or } 'C', B is k \text{ by } n.
    Note: No data should be moved to form B^{T} or B^{H}; that is, the matrix B should
            always be stored in its untransposed form.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 80 on page 442, where:
```

If trans = 'N', its size must be ldb by (at least) k.

If trans = 'T' or 'C', its size must be ldb by (at least) n.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and:

If trans = 'N',  $ldb \ge n$ .

If  $trans = 'T' \text{ or } 'C', Idb \ge k.$ 

beta

is the scalar  $\beta$ . Specified as: a number of the data type indicated in Table 80 on page 442.

С

is matrix  $\boldsymbol{C}$  of order n, which is real symmetric, complex symmetric, or complex Hermitian. where:

If uplo = 'U', C is stored in upper storage mode.

If *uplo* = 'L', *C* is stored in lower storage mode.

Specified as: an *ldc* by (at least) *n* array, containing numbers of the data type indicated in Table 80 on page 442.

ldc

is the leading dimension of the array specified for c. Specified as: a fullword integer; ldc > 0 and  $ldc \ge n$ .

#### On Return

С

is matrix C of order n, which is real symmetric, complex symmetric, or complex Hermitian, containing the results of the computation, where:

If uplo = 'U', C is stored in upper storage mode.

If uplo = 'L', C is stored in lower storage mode.

Returned as: an ldc by (at least) n array, containing numbers of the data type indicated in Table 80 on page 442.

#### **Notes**

- 1. These subroutines accept lowercase letters for the *uplo* and *trans* arguments.
- 2. For SSYR2K and DSYR2K, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
- 3. Matrices **A** and **B** must have no common elements with matrix **C**; otherwise, results are unpredictable.
- 4. The imaginary parts of the diagonal elements of a complex Hermitian matrix  $\boldsymbol{A}$  are assumed to be zero, so you do not have to set these values. On output, they are set to zero, except when  $\beta$  is one and  $\alpha$  or k is zero, in which case no computation is performed.
- 5. For a description of how symmetric matrices are stored in upper and lower storage mode, see "Symmetric Matrix" on page 65. For a description of how complex Hermitian matrices are stored in upper and lower storage mode, see "Complex Hermitian Matrix" on page 70.

**Function:** These subroutines can perform the following rank-2k updates. For SSYR2K and DSYR2K, matrix **C** is real symmetric. For CSYR2K and ZSYR2K, matrix **C** is complex symmetric. They perform:

1. 
$$C \leftarrow \alpha AB^{T} + \alpha BA^{T} + \beta C$$
  
2.  $C \leftarrow \alpha A^{T}B + \alpha B^{T}A + \beta C$ 

For CHER2K and ZHER2K, matrix *C* is complex Hermitian. They perform:

3. 
$$\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathrm{H}} + \overline{\alpha} \mathbf{B} \mathbf{A}^{\mathrm{H}} + \beta \mathbf{C}$$

4. 
$$C \leftarrow \alpha A^{\mathrm{H}} B + \overline{\alpha} B^{\mathrm{H}} A + \beta C$$

where:

 $\alpha$  and  $\beta$  are scalars.

**A** and **B** are rectangular matrices, which are n by k for equations 1 and 3, and are *k* by *n* for equations 2 and 4.

C is a matrix of order n of the type indicated above, stored in upper or lower storage mode.

See references [32], [38], and [66]. In the following two cases, no computation is performed:

- n is 0.
- $\beta$  is one, and  $\alpha$  is zero or k is zero.

Assuming the above conditions do not exist, if  $\beta$  is not one, and  $\alpha$  is zero or k is zero, then  $\beta C$  is returned.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors

- 1. Ida, Idb,  $Idc \leq 0$
- 2. Idc < n
- 3. k, n < 0
- 4. *uplo* ≠ 'U' or 'L'
- 5. trans ≠ 'N', 'T', or 'C' for SSYR2K and DSYR2K
- 6. trans ≠ 'N' or 'T' for CSYR2K and ZSYR2K
- 7. trans ≠ 'N' or 'C' for CHER2K and ZHER2K
- 8. trans = 'N' and lda < n
- 9. trans = 'T' or 'C' and Ida < k
- 10. trans = 'N' and ldb < n
- 11. trans = 'T' or 'C' and ldb < k

**Example 1:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^{\mathsf{T}} + \alpha \mathbf{B} \mathbf{A}^{\mathsf{T}} + \beta \mathbf{C}$ , where **A** and **B** are 8 by 2 real rectangular matrices, and **C** is a real symmetric matrix of order 8, stored in upper storage mode.

Output

**Example 2:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A}^{\mathsf{T}} \mathbf{B} + \alpha \mathbf{B}^{\mathsf{T}} \mathbf{A} + \beta \mathbf{C}$ , where  $\mathbf{A}$  and  $\mathbf{B}$  are 3 by 8 real rectangular matrices, and  $\mathbf{C}$  is a real symmetric matrix of order 8, stored in lower storage mode.

$$A = \begin{bmatrix} 0.0 & 3.0 & 6.0 & 9.0 & 12.0 & 15.0 & 18.0 & 21.0 \\ 1.0 & 4.0 & 7.0 & 10.0 & 13.0 & 16.0 & 19.0 & 22.0 \\ 2.0 & 5.0 & 8.0 & 11.0 & 14.0 & 17.0 & 20.0 & 23.0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \end{bmatrix}$$

Output

**Example 3:** This example shows the computation  $\mathbf{C} \leftarrow \alpha \mathbf{A} \mathbf{B}^T + \alpha \mathbf{B} \mathbf{A}^T + \beta \mathbf{C}$ , where  $\mathbf{A}$  and  $\mathbf{B}$  are 3 by 5 complex rectangular matrices, and  $\mathbf{C}$  is a complex symmetric matrix of order 3, stored in lower storage mode.

$$B = \begin{bmatrix} (1.0, 5.0) & (6.0, 2.0) & (3.0, 1.0) & (2.0, 0.0) & (1.0, 0.0) \\ (2.0, 4.0) & (7.0, 5.0) & (2.0, 5.0) & (2.0, 4.0) & (0.0, 0.0) \\ (3.0, 5.0) & (8.0, 1.0) & (1.0, 5.0) & (1.0, 0.0) & (1.0, 1.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (2.0, 3.0) & . & . \\ (1.0, 9.0) & (3.0, 3.0) & . \\ (4.0, 5.0) & (6.0, 7.0) & (8.0, 3.0) \\ . & . & . \end{bmatrix}$$

Output

$$C = \begin{bmatrix} (-101.0, 121.0) & . & . \\ (-182.0, 192.0) & (-274.0, 248.0) & . \\ (-98.0, 146.0) & (-163.0, 205.0) & (-151.0, 115.0) \\ . & . & . & . \end{bmatrix}$$

**Example 4:** This example shows the computation:

$$C \leftarrow \alpha A^{\mathrm{H}} B + \overline{\alpha} B^{\mathrm{H}} A + \beta C$$

where  $\boldsymbol{A}$  and  $\boldsymbol{B}$  are 5 by 3 complex rectangular matrices, and  $\boldsymbol{C}$  is a complex Hermitian matrix of order 3, stored in upper storage mode.

**Note:** The imaginary parts of the diagonal elements of a complex Hermitian matrix are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

$$ALPHA = (1.0, 1.0)$$

$$A = \begin{bmatrix} (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (4.0, 5.0) & (6.0, 7.0) & (8.0, 0.0) \\ (1.0, 9.0) & (3.0, 0.0) & (6.0, 7.0) \\ (3.0, 3.0) & (8.0, 0.0) & (2.0, 5.0) \\ (1.0, 3.0) & (2.0, 1.0) & (6.0, 0.0) \\ (2.0, 0.0) & (3.0, 2.0) & (4.0, 1.0) \end{bmatrix}$$

$$C = \begin{bmatrix} (6.0, ..) & (3.0, 4.0) & (9.0, 1.0) \\ .. & (10.0, ..) & (12.0, 2.0) \\ .. & .. & (3.0, ..) \end{bmatrix}$$

Output

$$C = \begin{bmatrix} (102.0, 0.0) & (56.0, -143.0) & (244.0, -96.0) \\ & & (174.0, & 0.0) & (238.0, & 78.0) \\ & & & & & & & & \\ & & & & & & & & \end{bmatrix}$$

# SGETMI, DGETMI, CGETMI, and ZGETMI—General Matrix Transpose (In-Place)

These subroutines transpose an n by n matrix A in place—that is, in matrix A:

$$A \leftarrow A^{\mathsf{T}}$$

Table 81. Data Types			
Α	Subroutine		
Short-precision real	SGETMI		
Long-precision real	DGETMI		
Short-precision complex	CGETMI		
Long-precision complex	ZGETMI		

#### Syntax

Fortran	CALL SGETMI   DGETMI   CGETMI   ZGETMI (a, lda, n)
C and C++	sgetmi   dgetmi   cgetmi   zgetmi (a, Ida, n);
PL/I	CALL SGETMI   DGETMI   CGETMI   ZGETMI (a, lda, n);

#### On Entry

а

is the matrix  $\mathbf{A}$  having n rows and n columns. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 81.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

is the number of rows and columns in matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

#### On Return

а

is the n by n matrix  $A^T$ , containing the results of the matrix transpose operation Returned as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 81.

#### Notes

- 1. To achieve optimal performance in these subroutines, specify an even value for *lda*. An odd value may degrade performance.
- 2. To achieve optimal performance in CGETMI, align the array specified for *a* on a doubleword boundary.

**Function:** Matrix **A** is transposed in place; that is, the *n* rows and *n* columns in matrix **A** are exchanged. For matrix **A** with elements  $a_{ij}$ , where i, j = 1, n, the in-place transpose is expressed as  $a_{ij} = a_{ij}$  for i, j = 1, n.

For the following input matrix A:

#### SGETMI, DGETMI, CGETMI, and ZGETMI

$$\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ & & & \\ & & & \\ & & & \\ a_{n1} & \dots & a_{nn} \end{bmatrix}$$

the in-place matrix transpose operation  $\mathbf{A} \leftarrow \mathbf{A}^{\mathsf{T}}$  is expressed as:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \vdots & & \vdots \\ a_{1n} & \dots & a_{nn} \end{bmatrix}$$

If n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. 
$$n < 0$$
 or  $n > Ida$ 

2. Ida ≤ 0

**Example:** This example shows an in-place matrix transpose of matrix **A** having 5 rows and 5 columns.

Call Statement and Input

Output

### SGETMI, DGETMI, CGETMI, and ZGETMI

		Γ						7
		•	•	•	•	•	•	•
		.		1.0	2.0	3.0	4.0	5.0
		.		6.0	7.0	8.0	9.0	10.0
		.		11.0	12.0	13.0	14.0	15.0
Α	=	.		16.0	17.0	18.0	19.0	20.0
		.		21.0	22.0	23.0	24.0	25.0
		.	•	•	•	•	•	
		•	•	•	•	•	•	
		•	•	•	•	•	•	
		•	•	•	•	•	•	
		1						

# SGETMO, DGETMO, CGETMO, and ZGETMO—General Matrix Transpose (Out-of-Place)

These subroutines transpose an m by n matrix  $\boldsymbol{A}$  out of place, returning the result in matrix  $\boldsymbol{B}$ :

$$B \leftarrow A^{\mathsf{T}}$$

Table 82. Data Types			
А, В	Subroutine		
Short-precision real	SGETMO		
Long-precision real	DGETMO		
Short-precision complex	CGETMO		
Long-precision complex	ZGETMO		

#### Syntax

Fortran	CALL SGETMO   DGETMO   CGETMO   ZGETMO (a, lda, m, n, b, ldb)
C and C++	sgetmo   dgetmo   cgetmo   zgetmo (a, lda, m, n, b, ldb);
PL/I	CALL SGETMO   DGETMO   CGETMO   ZGETMO (a, lda, m, n, b, ldb);

#### On Entry

а

is the matrix  $\bf A$  having  $\bf m$  rows and  $\bf n$  columns. Specified as: an  $\bf lda$  by (at least)  $\bf n$  array, containing numbers of the data type indicated in Table 82.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

m

is the number of rows in matrix  $\bf{A}$  and the number of columns in matrix  $\bf{B}$ . Specified as: a fullword integer;  $m \ge 0$ .

n

is the number of columns in matrix  $\bf{A}$  and the number of rows in matrix  $\bf{B}$ . Specified as: a fullword integer;  $n \ge 0$ .

b

See "On Return."

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

#### On Return

b

is the matrix  $\boldsymbol{B}$  having n rows and m columns, containing the results of the matrix transpose operation,  $\boldsymbol{A}^{\mathsf{T}}$ . Returned as: an ldb by (at least) m array, containing numbers of the data type indicated in Table 82.

#### Notes

1. The matrix **B** must have no common elements with matrix **A**; otherwise, results are unpredictable. See "Concepts" on page 55.

#### SGETMO, DGETMO, CGETMO, and ZGETMO

2. To achieve optimal performance in CGETMO, align the arrays specified for *a* and *b* on doubleword boundaries.

**Function:** Matrix  $\bf{A}$  is transposed out of place; that is, the m rows and n columns in matrix  $\bf{A}$  are stored in n rows and m columns of matrix  $\bf{B}$ . For matrix  $\bf{A}$  with elements  $a_{ij}$ , where i=1, m and j=1, n, the out-of-place transpose is expressed as  $b_{ij}=a_{ij}$  for i=1, m and j=1, n.

For the following input matrix **A**:

$$\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

the out-of-place matrix transpose operation  $\mathbf{B} \leftarrow \mathbf{A}^{\mathsf{T}}$  is expressed as:

$$\begin{bmatrix} b_{11} & \dots & b_{1m} \\ \vdots & & \vdots \\ \vdots & & \vdots \\ b_{n1} & \dots & b_{nm} \end{bmatrix} \leftarrow \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \vdots & & \vdots \\ a_{1n} & \dots & a_{mn} \end{bmatrix}$$

If m or n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. m < 0 or m > Ida
- 2. n < 0 or n > ldb
- 3.  $Ida \leq 0$
- $4. Idb \leq 0$

**Example 1:** This example shows an out-of-place matrix transpose of matrix **A**, having 5 rows and 4 columns, with the result going into matrix **B**.

Output

$$B = \begin{bmatrix} . & . & . & . & . & . & . & . & . \\ . & 1.0 & 2.0 & 3.0 & 4.0 & 5.0 & . \\ . & 6.0 & 7.0 & 8.0 & 9.0 & 10.0 & . \\ . & 11.0 & 12.0 & 13.0 & 14.0 & 15.0 & . \\ . & 16.0 & 17.0 & 18.0 & 19.0 & 20.0 & . \\ . & . & . & . & . & . & . & . \end{bmatrix}$$

**Example 2:** This example uses the same input matrix **A** as in Example 1 to show that transposes can be achieved in the same array as long as the input and output data do not overlap. On output, the input data is not overwritten in the array.

### SGETMO, DGETMO, CGETMO, and ZGETMO

# **Chapter 10. Linear Algebraic Equations**

The linear algebraic equation subroutines, provided in four areas, are described in this chapter.

# **Overview of the Linear Algebraic Equation Subroutines**

This section describes the subroutines in each of the four linear algebraic equation areas:

- Dense linear algebraic equations (Table 83)
- Banded linear algebraic equations (Table 84)
- Sparse linear algebraic equations (Table 85)
- Linear least squares (Table 86)

**Note:** Some of the linear algebraic equations were designed in accordance with the Level 2 BLAS, Level 3 BLAS, and LAPACK de facto standard. If these subprograms do not comply with the standard as approved, IBM will consider updating them to do so. If IBM updates these subprograms, the updates could require modifications of the calling application program. For details on the Level 2 and 3 BLAS, see references [32] and [34]. For details on the LAPACK routines, see reference [8].

# **Dense Linear Algebraic Equation Subroutines**

The dense linear algebraic equation subroutines provide solutions to linear systems of equations for both real and complex general matrices and their transposes, positive definite real symmetric and complex Hermitian matrices, and triangular matrices. Some of these subroutines correspond to the Level 2 BLAS, Level 3 BLAS, and LAPACK routines described in references [32], [34], and [8].

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
General Matrix Factorization	SGEF CGEF SGETRF∆ CGETRF∆	DGEF ZGEF DGETRF ZGETRF DGEFP§	466 479
General Matrix, Its Transpose, or Its Conjugate Transpose Solve	SGES CGES	DGES ZGES	469
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGESM CGESM SGETRS∆ CGETRS∆	DGESM ZGESM DGETRS <sup>A</sup> ZGETRS <sup>A</sup>	473 483
General Matrix Factorization, Condition Number Reciprocal, and Determinant	SGEFCD	DGEFCD	488
Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization	SPPF SPOF CPOF	DPPF DPOF ZPOF DPPFP§	492

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Table 83 (Page 2 of 2). List of Dense Linear Algebraic Equation Se	ubroutines		
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Positive Definite Real Symmetric Matrix Solve	SPPS	DPPS	500
Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve	SPOSM CPOSM	DPOSM ZPOSM	503
Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant	SPPFCD SPOFCD	DPPFCD DPOFCD	508
General Matrix Inverse, Condition Number Reciprocal, and Determinant	SGEICD	DGEICD	514
Positive Definite Real Symmetric Matrix Inverse, Condition Number Reciprocal, and Determinant	SPPICD SPOICD	DPPICD DPOICD	519
Solution of a Triangular System of Equations with a Single Right-Hand Side	STRSV4 CTRSV4 STPSV4 CTPSV4	DTRSV4 ZTRSV4 DTPSV4 ZTPSV4	526
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM◆ CTRSM◆	DTRSM◆ ZTRSM◆	532
Triangular Matrix Inverse	STRI STPI	DTRI DTPI	540

<sup>◆</sup> Level 2 BLAS

# **Banded Linear Algebraic Equation Subroutines**

The banded linear algebraic equation subroutines provide solutions to linear systems of equations for real general band matrices, real positive definite symmetric band matrices, real or complex general tridiagonal matrices, real positive definite symmetric tridiagonal matrices, and real or complex triangular band matrices.

Table 84 (Page 1 of 2). List of Banded Linear Algebraic Equation Subroutines					
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page		
General Band Matrix Factorization	SGBF	DGBF	546		
General Band Matrix Solve	SGBS	DGBS	550		
Positive Definite Symmetric Band Matrix Factorization	SPBF SPBCHF	DPBF DPBCHF	553		
Positive Definite Symmetric Band Matrix Solve	SPBS SPBCHS	DPBS DPBCHS	557		
General Tridiagonal Matrix Factorization	SGTF	DGTF	560		
General Tridiagonal Matrix Solve	SGTS	DGTS	563		

<sup>◆</sup> Level 3 BLAS

<sup>△</sup> LAPACK

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use is new programs. Documentation for this subroutine is no longer provided.

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting	SGTNP CGTNP	DGTNP ZGTNP	565
General Tridiagonal Matrix Factorization with No Pivoting	SGTNPF CGTNPF	DGTNPF ZGTNPF	568
General Tridiagonal Matrix Solve with No Pivoting	SGTNPS CGTNPS	DGTNPS ZGTNPS	571
Positive Definite Symmetric Tridiagonal Matrix Factorization	SPTF	DPTF	574
Positive Definite Symmetric Tridiagonal Matrix Solve	SPTS	DPTS	576
Triangular Band Equation Solve	STBSV⁴ CTBSV⁴	DTBSV⁴ ZTBSV⁴	578

# **Sparse Linear Algebraic Equation Subroutines**

The sparse linear algebraic equation subroutines provide direct and iterative solutions to linear systems of equations both for general sparse matrices and their transposes and for sparse symmetric matrices.

	Long- Precision	
Descriptive Name	Subroutine	Page
General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns	DGSF	585
General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns	DGSS	591
General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode	DGKFS	595
Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode	DSKFS	613
Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows	DSRIS	632
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMCG§	643
Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDCG	651
General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode	DSMGCG§	659
General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode	DSDGCG	666
§ These subroutines are provided only for migration from earlier releases of ESSL new programs. Use DSRIS instead.	and are not intended	for use in

### **Linear Least Squares Subroutines**

The linear least squares subroutines provide least squares solutions to linear systems of equations for real general matrices. Two methods are provided: one that uses the singular value decomposition and another that uses a QR decomposition with column pivoting.

Table 86. List of Linear Least Squares Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Singular Value Decomposition for a General Matrix	SGESVF	DGESVF	674
Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition	SGESVS	DGESVS	682
Linear Least Squares Solution for a General Matrix Using a QR Decomposition with Column Pivoting	SGELLS	DGELLS	687

# **Dense and Banded Linear Algebraic Equation Considerations**

This section provides some key points about using the dense and banded linear algebraic equation subroutines.

#### **Use Considerations**

- To solve a system of equations, you need to use both the factorization and solve subroutines for the type of matrix you have. Each factorization subroutine should be followed in your program by the corresponding solve subroutine. The output from the factorization subroutine should be used as input to the solve subroutine.
- 2. To solve a system of equations with one or more right-hand sides, follow the call to the factorization subroutine with one or more calls to a solve subroutine or one call to a multiple solve subroutine.
- 3. The ESSL naming conventions for the dense and banded linear algebraic equation subroutines are similar to those used in the LAPACK documentation. (LAPACK, as well as its documentation, is available from the sources listed in reference [8].) The following ESSL subroutines correspond to the LAPACK subroutines: SGETRF, DGETRF, CGETRF, ZGETRF, SGETRS, DGETRS, CGETRS, and ZGETRS.

- Except in a few instances, the \_GTNP subroutines provide better performance than the \_GTNPF and \_GTNPS subroutines. For details, see the subroutine descriptions.
- 2. The general subroutines (dense and banded) use partial pivoting for accuracy and fast performance.
- 3. The short-precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.

4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Sparse Matrix Direct Solver Considerations**

This section provides some key points about using the sparse matrix direct solver subroutines.

### **Use Considerations**

- To solve a sparse system of equations by a direct method, you must use both
  the factorization and solve subroutines. The factorization subroutine should be
  followed in your program by the corresponding solve subroutine; that is, the
  output from the factorization subroutine should be used as input to the solve
  subroutine.
- 2. To solve a system of equations with one or more right-hand sides, follow the call to the factorization subroutine with one or more calls to the solve subroutine.
- 3. The amount of storage required for the arrays depends on the sparsity pattern of the matrix. The requirement that *lna* > 2*nz* on entry to DGSF does not guarantee a successful run of the program. Some programs may be terminated because of the large number of fill-ins generated upon factorization. Fill-ins generated in a program depend on the structure of each matrix. If a large number of fill-ins is anticipated when factoring a matrix, the value of *lna* should be large enough to accommodate your problem.

- To make the subroutine more efficient, an input matrix comprised of all nonzero elements is preferable. See the syntax description of each subroutine for details.
- 2. DGSF optionally checks the validity of the indices and pointers of the input matrix. Use of this option is suggested; however, it may affect performance. For details, see the syntax description for DGSF.
- 3. In DGSS, if there are multiple sparse right-hand sides to be solved, you should take advantage of the sparsity by selecting a proper value for *jopt* (such as *jopt* = 10 or 11). If there is only one right-hand side to be solved, it is suggested that you do not exploit the sparsity.
- 4. In DGSF, the value you enter for the lower bound of all elements in the matrix (RPARM(1)) affects the accuracy of the result. Specifying a larger number allows you to gain some performance; however, you may lose some accuracy in the solution.
- 5. In DGSF, the threshold pivot tolerance (RPARM(2)) is used to select pivots. A value that is close to 0.0 approaches no pivoting. A value close to 1.0 approaches partial pivoting. A value of 0.1 is considered to be a good compromise between numerical stability and sparsity.
- 6. If the ESSL subroutine performs storage compressions, you receive an attention message. When this occurs, the performance of this subroutine is

affected. You can improve the performance by increasing the value specified for Ina.

7. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Sparse Matrix Skyline Solver Considerations**

This section provides some key points about using the sparse matrix skyline solver subroutines.

#### **Use Considerations**

- 1. To solve a system of equations with one or more right-hand sides, where the matrix is stored in skyline storage mode, you can use either of the following methods. The factored output matrix is the same for both of these methods.
  - Call the skyline subroutine with the combined factor-and-solve option.
  - Call the skyline subroutine with the factor-only option, followed in your program by a call to the same subroutine with the solve-only option. The factored output matrix resulting from the factorization should be used as input to the same subroutine to do the solve. You can solve for the right-hand sides in a single call or in individual calls.

You also have the option of doing a partial factorization, where the subroutine assumes that the initial part of the input matrix is already factored. It then factors the remaining rows and columns. If you want, you can factor a very large matrix progressively by using this option.

- 2. Forward elimination can be done with or without scaling the right-hand side by the diagonal matrix elements. To perform the computation without scaling, call DGKFS with the normal solve-only option, and define the upper triangular skyline matrix (AU) as a diagonal. To perform the computation with scaling, call DGKFS with the transpose solve-only, option and define the lower triangular skyline matrix (AL) as a diagonal.
- 3. Back substitution can be done with or without scaling the right-hand side by the diagonal matrix elements. To perform the computation without scaling, call DGKFS with the transpose solve-only option, and define the upper triangular skyline matrix (AU) as a diagonal. To perform the computation with scaling, call DGKFS with the normal solve-only option, and define the lower triangular skyline matrix (AL) as a diagonal.

- 1. For optimal performance, use diagonal-out skyline storage mode for both your input and output matrices. If you specify profile-in skyline storage mode for your input matrix, and either you do not plan to use the factored output or you plan to do a solve only, it is more efficient to specify diagonal-out skyline storage mode for your output matrix. These rules apply to all the computations.
- 2. In some cases, elapsed time may be reduced significantly by using the combined factor-and-solve option to solve for all right-hand sides at once, in conjunction with the factorization, rather than doing the factorization and solve separately.

- 3. If you do a solve only, and you solve for more than one right-hand side, it is most efficient to call the skyline subroutine once with all right-hand sides, rather than once for each right-hand side.
- 4. The skyline subroutines allow some control over processing of the pivot (diagonal) elements of the matrix during the factorization phase. Pivot processing is controlled by IPARM(10) through IPARM(15) and RPARM(10) through RPARM(15). If a pivot occurs within a range that is designated to be fixed (IPARM(0) = 1, IPARM(10) = 1, and the appropriate element IPARM(11) through IPARM(15) = 1), it is replaced with the corresponding element of RPARM(11) through RPARM(15). Should this pivot fix-up occur, you receive an attention message. This message indicates that the matrix being factored may be unstable (singular or not definite). The results produced in this situation may be inaccurate, and you should review them carefully.

# **Sparse Matrix Iterative Solver Considerations**

This section provides some key points about using the sparse matrix iterative solver subroutines.

#### **Use Considerations**

If you need to solve linear systems with different right-hand sides but with the same matrix using the preconditioned algorithms, you can reuse the incomplete factorization computed during the first call to the subroutine.

- The DSMCG and DSMGCG subroutines are provided for migration purposes from earlier releases of ESSL. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
- 2. To select the sparse matrix subroutine that provides the best performance, you must consider the sparsity pattern of the matrix. From this, you can determine the most efficient storage mode for your sparse matrix. ESSL provides a number of versions of the sparse matrix iterative solve subroutines. They operate on sparse matrices stored in row-wise, diagonal, and compressed-matrix storage modes. These storage modes are described in "Sparse Matrix" on page 92.
  - Storage-by-rows is generally applicable. You should use this storage mode unless your matrices are already set up in one of the other storage modes. If, however, your matrix has a regular sparsity pattern—that is, where the nonzero elements are concentrated along a few diagonals—you may want to use compressed-diagonal storage mode. This can save some storage space. Compressed-matrix storage mode is provided for migration purposes from earlier releases of ESSL and is not intended for use. (You get better performance and a wider choice of algorithms if you use the DSRIS subroutine, which uses storage-by-rows.)
- 3. The performance achieved in the sparse matrix iterative solver subroutines depends on the value specified for the relative accuracy  $\epsilon$ . For details, see Notes for each subroutine.
- You can select the iterative algorithm you want to use to solve your linear system. The methods include conjugate gradient (CG), conjugate gradient squared (CGS), generalized minimum residual (GMRES), more smoothly

- converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR).
- 5. For a general sparse or positive definite symmetric matrix, the iterative algorithm may fail to converge for one of the following reasons:
  - The value of  $\varepsilon$  is too small, asking for too much precision.
  - The maximum number of iterations is too small, allowing too few iterations for the algorithm to converge.
  - The matrix is not positive real; that is, the symmetric part, (A+AT)/2, is not
    positive definite.
  - The matrix is ill-conditioned, which may cause overflows during the computation.
- These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

# **Linear Least Squares Considerations**

This section provides some key points about using the linear least squares subroutines.

#### **Use Considerations**

If you want to use a singular value decomposition method to compute the minimal norm linear least squares solution of  $AX \cong B$ , calls to SGESVF or DGESVF should be followed by calls to SGESVS or DGESVS, respectively.

- Least squares solutions obtained by using a singular value decomposition require more storage and run time than those obtained using a QR decomposition with column pivoting. The singular value decomposition method, however, is a more reliable way to handle rank deficiency.
- 2. The short-precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.
- 3. The accuracy of the resulting singular values and singular vectors varies between the short- and long-precision versions of each subroutine. The degree of difference depends on the size and conditioning of the matrix computation.
- 4. There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Dense Linear Algebraic Equation Subroutines**

This section contains the dense linear algebraic equation subroutine descriptions.

# SGEF, DGEF, CGEF, and ZGEF—General Matrix Factorization

This subroutine factors a square general matrix **A** using Gaussian elimination with partial pivoting. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGES/SGESM, DGES/DGESM, CGES/CGESM, or ZGES/ZGESM, respectively. To compute the inverse of matrix **A**, follow the call to these subroutines with a call to SGEICD or DGEICD, respectively.

Table 87. Data Types	
Α	Subroutine
Short-precision real	SGEF
Long-precision real	DGEF
Short-precision complex	CGEF
Long-precision complex	ZGEF

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGES/SGESM/SGEICD, DGES/DGESM/DGEICD, CGES/CGESM, and ZGES/ZGESM, respectively.

#### **Syntax**

Fortran	CALL SGEF   DGEF   CGEF   ZGEF (a, lda, n, ipvt)
C and C++	sgef   dgef   cgef   zgef (a, lda, n, ipvt);
PL/I	CALL SGEF   DGEF   CGEF   ZGEF (a, lda, n, ipvt);

#### On Entry

а

is the n by n general matrix  $\mathbf{A}$  to be factored. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 87.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le Ida$ .

ipvt

See "On Return."

#### On Return

а

is the n by n transformed matrix  $\mathbf{A}$ , containing the results of the factorization. See "Function" on page 467. Returned as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 87.

ipvt

is the integer vector *ipvt* of length *n*, containing the pivot indices. Returned as: a one-dimensional array of (at least) length *n*, containing fullword integers.

Notes

 Calling SGEFCD or DGEFCD with iopt = 0 is equivalent to calling SGEF or DGEF.

2. On both input and output, matrix **A** conforms to LAPACK format.

**Function:** The matrix A is factored using Gaussian elimination with partial pivoting (**ipvt**) to compute the **LU** factorization of A, where (A = PLU):

L is a unit lower triangular matrix.

**U** is an upper triangular matrix.

**P** is the permutation matrix.

On output, the transformed matrix A contains U in the upper triangle and L in the strict lower triangle where ipvt contains the pivots representing permutation P, such that A = PLU.

If *n* is 0, no computation is performed. See references [36] and [38].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: Matrix A is singular.

- One or more columns of L and the corresponding diagonal of U contain all zeros (all columns of L are checked). The first column, i, of L with a corresponding U = 0 diagonal element is identified in the computational error message.
- The return code is set to 1.
- *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. n < 0
- 3. n > Ida

**Example 1:** This example shows a factorization of a real general matrix **A** of order 9.

$$A = \begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 4.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 6.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 7.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 8.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 9.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 10.0 & 11.0 & 12.0 \end{bmatrix}$$

#### Output

```
4.0000
                                                                0.0000
                                                                         0.0000
        1.0000
                1.0000
                         1.0000
                                   1.0000
                                            1.0000
                                                      0.0000
0.0000
        5.0000
                1.0000
                         1.0000
                                   1.0000
                                            1.0000
                                                      1.0000
                                                               0.0000
                                                                         0.0000
0.0000
        0.0000
                 6.0000
                         1.0000
                                   1.0000
                                            1.0000
                                                      1.0000
                                                               1.0000
                                                                         0.0000
0.0000
        0.0000
                 0.0000
                         7.0000
                                            1.0000
                                                      1.0000
                                                               1.0000
                                   1.0000
                                                                         1.0000
0.0000
        0.0000
                                            1.0000
                                                               1.0000
                 0.0000
                         0.0000
                                   8.0000
                                                      1.0000
                                                                         1.0000
0.0000
        0.0000
                 0.0000
                         0.0000
                                  0.0000
                                            9.0000
                                                     1.0000
                                                               1.0000
                                                                         1.0000
0.0000
        0.0000
                 0.0000
                         0.0000
                                  0.0000
                                            0.0000
                                                     10.0000
                                                              11.0000
                                                                        12.0000
0.2500
        0.1500
                 0.1000
                         0.0714
                                   0.0536
                                           -0.0694
                                                     -0.0306
                                                                0.1806
                                                                         0.3111
0.2500
        0.1500
                 0.1000
                         0.0714
                                 -0.0714
                                           -0.0556
                                                     -0.0194
                                                               0.9385
                                                                        -0.0031
```

IPVT = 
$$(3, 4, 5, 6, 7, 8, 9, 8, 9)$$

**Example 2:** This example shows a factorization of a complex general matrix **A** of order 4.

#### Call Statement and Input

$$A = \begin{pmatrix} (1.0, 2.0) & (1.0, 7.0) & (2.0, 4.0) & (3.0, 1.0) \\ (2.0, 0.0) & (1.0, 3.0) & (4.0, 4.0) & (2.0, 3.0) \\ (2.0, 1.0) & (5.0, 0.0) & (3.0, 6.0) & (0.0, 0.0) \\ (8.0, 5.0) & (1.0, 9.0) & (6.0, 6.0) & (8.0, 1.0) \end{pmatrix}$$

#### Output

IPVT

$$A = \begin{bmatrix} (8.0000, 5.0000) & (1.0000, 9.0000) & (6.0000, 6.0000) & (8.0000, 1.0000) \\ (0.2022, 0.1236) & (1.9101, 5.0562) & (1.5281, 2.0449) & (1.5056, -0.1910) \\ (0.2360, -0.0225) & (-0.0654, -0.9269) & (-0.3462, 6.2692) & (-1.6346, 1.3269) \\ (0.1798, -0.1124) & (0.2462, 0.1308) & (0.4412, -0.3655) & (0.2900, 2.3864) \end{bmatrix}$$

= (4, 4, 3, 4)

## SGES, DGES, CGES, and ZGES—General Matrix, Its Transpose, or Its Conjugate Transpose Solve

These subroutines solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  for  $\mathbf{x}$ , where  $\mathbf{A}$  is a general matrix and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. Using the *iopt* argument, they can also solve the real system  $\mathbf{A}^T\mathbf{x} = \mathbf{b}$  or the complex system  $\mathbf{A}^H\mathbf{x} = \mathbf{b}$  for  $\mathbf{x}$ . These subroutines use the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFPDGEFCD, CGEF, or ZGEF, respectively.

Table 88. Data Types	
A, b, x	Subroutine
Short-precision real	SGES
Long-precision real	DGES
Short-precision complex	CGES
Long-precision complex	ZGES

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.

#### Syntax

Fortran	CALL SGES   DGES   CGES   ZGES (a, Ida, n, ipvt, bx, iopt)
C and C++	sges   dges   cges   zges (a, lda, n, ipvt, bx, iopt);
PL/I	CALL SGES   DGES   CGES   ZGES (a, Ida, n, ipvt, bx, iopt);

#### On Entry

а

is the factorization of matrix  $\boldsymbol{A}$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. Specified as: an *Ida* by (at least)  $\boldsymbol{n}$  array, containing numbers of the data type indicated in Table 88.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le lda$ .

is the integer vector *ipvt* of length n, containing the pivot indices produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFCD, CGEF, or ZGEF, respectively. Specified as: a one-dimensional array of (at least) length n, containing fullword integers.

bx

is the vector  $\mathbf{b}$  of length n, containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 88.

iopt

determines the type of computation to be performed, where:

If iopt = 0, **A** is used in the computation.

If iopt = 1,  $A^{T}$  is used in SGES and DGES.  $A^{H}$  is used in CGES and ZGES.

**Note:** No data should be moved to form  $A^T$  or  $A^H$ ; that is, the matrix A should always be stored in its untransposed form.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

bx

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 88 on page 469.

#### **Notes**

- The scalar data specified for input arguments *Ida* and *n* for these subroutines must be the same as the corresponding input arguments specified for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
- 2. The array data specified for input arguments *a* and *ipvt* for these subroutines must be the same as the corresponding output arguments for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
- 3. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  is solved for  $\mathbf{x}$ , where  $\mathbf{A}$  is a general matrix and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. Using the *iopt* argument, this subroutine can also solve the real system  $\mathbf{A}^T\mathbf{x} = \mathbf{b}$  or the complex system  $\mathbf{A}^H\mathbf{x} = \mathbf{b}$  for  $\mathbf{x}$ . These subroutines use the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. For a description of how  $\mathbf{A}$  is factored, see "SGEF, DGEF, CGEF, and ZGEF—General Matrix Factorization" on page 466.

If *n* is 0, no computation is performed. See references [36 ] and [38 ].

#### **Error Conditions**

Computational Errors: None

**Note:** If the factorization performed by SGEF, DGEF, CGEF, ZGEF, SGEFCD, DGEFCD, or DGEFP failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

#### Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. n < 0
- 3. n > Ida
- 4.  $iopt \neq 0$  or 1

#### Example 1

*Part 1:* This part of the example shows how to solve the system Ax = b, where matrix A is the same matrix factored in the "Example 1" on page 467 for SGEF and DGEF.

Call Statement and Input

*Part 2:* This part of the example shows how to solve the system  $A^Tx = b$ , where matrix A is the input matrix factored in "Example 1" on page 467 for SGEF and DGEF. Most of the input is the same in Part 2 as in Part 1.

Call Statement and Input

#### Example 2

Part 1: This part of the example shows how to solve the system Ax = b, where matrix A is the same matrix factored in the "Example 2" on page 468 for CGEF and ZGEF.

Call Statement and Input

A LDA N IPVT BX IOPT

| | | | | | | | | |

CALL CGES(A, 4, 4, 4, IPVT, BX, 0)

IPVT = 
$$(4, 4, 3, 4)$$

BX =  $((-10.0, 85.0), (-6.0, 61.0), (10.0, 38.0), (58.0, 168.0))$ 

A = (same as output A in "Example 1" on page 467)

Output

BX =  $((9.0, 0.0), (5.0, 1.0), (1.0, 6.0), (3.0, 4.0))$ 

*Part 2:* This part of the example shows how to solve the system  $A^Hx = b$ , where matrix A is the input matrix factored in "Example 2" on page 468 for CGEF and ZGEF. Most of the input is the same in Part 2 as in Part 1.

```
A LDA N IPVT
                             BX IOPT
CALL CGES( A , 4 , 4 , IPVT , BX , 1 )
IPVT
        = (4, 4, 3, 4)
ВХ
        = ((71.0, 12.0), (61.0, -70.0), (123.0, -34.0),
            (68.0, 7.0)
        = (same as output A in "Example 1" on page 467)
Output
ВХ
        = ((9.0, 0.0), (5.0, 1.0), (1.0, 6.0), (3.0, 4.0))
```

# SGESM, DGESM, CGESM, and ZGESM—General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve

These subroutines solve the following systems of equations for multiple right-hand sides, where **A**, **X**, and **B** are general matrices. SGESM and DGESM solve one of the following:

- 1. AX = B
- 2.  $A^{T}X = B$

CGESM and ZGESM solve one of the following:

- 1. AX = B
- 2.  $\mathbf{A}^{\mathsf{T}}\mathbf{X} = \mathbf{B}$
- 3.  $A^{H}X = B$

These subroutines use the results of the factorization of matrix **A**, produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFCD, CGEF, or ZGEF, respectively.

Table 89. Data Types	
A, B, X	Subroutine
Short-precision real	SGESM
Long-precision real	DGESM
Short-precision complex	CGESM
Long-precision complex	ZGESM

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.

#### Syntax

Fortran	Fortran CALL SGESM   DGESM   CGESM   ZGESM (trans, a, Ida, n, ipvt, b, Idb, nrhs)	
C and C++ sgesm   dgesm   cgesm   zgesm (trans, a, Ida, n, ipvt, b, Idb, nrhs);		
PL/I	CALL SGESM   DGESM   CGESM   ZGESM (trans, a, Ida, n, ipvt, b, Idb, nrhs);	

#### On Entry

trans

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation, resulting in equation 1.

If  $transa = {}^{t}T^{t}$ ,  $A^{T}$  is used in the computation, resulting in equation 2.

If  $transa = {}^{t}C^{t}$ ,  $A^{H}$  is used in the computation, resulting in equation 3.

Specified as: a single character. It must be 'N', 'T', or 'C'.

а

is the factorization of matrix **A**, produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le lda$ .

ipvt

is the integer vector *ipvt* of length *n*, containing the pivot indices produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, or ZGEF, respectively. Specified as: a one-dimensional array of (at least) length *n*, containing fullword integers.

b

is the matrix  $\mathbf{B}$ , containing the *nrhs* right-hand sides of the system. The right-hand sides, each of length n, reside in the columns of matrix  $\mathbf{B}$ . Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 89 on page 473.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

nrhs

is the number of right-hand sides in the system to be solved. Specified as: a fullword integer;  $nrhs \ge 0$ .

#### On Return

b

is the matrix **B**, containing the *nrhs* solutions to the system in the columns of **B**. Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 89 on page 473.

#### Notes

- 1. For SGESM and DGESM, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
- 2. The scalar data specified for input arguments *Ida* and *n* for these subroutines must be the same as the corresponding input arguments specified for SGEF/SGEFCD, DGEF/DGEFP/DGEFCD, CGEF, and ZGEF, respectively.
- 3. The array data specified for input arguments *a* and *ipvt* for these subroutines must be the same as the corresponding output arguments for SGEF/SGEFCD, DGEF/DGEFCD, CGEF, and ZGEF, respectively.
- 4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** One of the following systems of equations is solved for multiple right-hand sides:

- 1. AX = B
- 2.  $A^{T}X = B$
- 3.  $A^HX = B$  (only for CGESM and ZGESM)

where A, B, and X are general matrices. These subroutines use the results of the factorization of matrix A, produced by a preceding call to SGEF/SGEFCD, DGEF/DGEFCD, CGEF, or ZGEF, respectively. For a description of how A

is factored, see "SGEF, DGEF, CGEF, and ZGEF—General Matrix Factorization" on page 466.

If *n* or *nrhs* is 0, no computation is performed. See references [36] and [38].

#### **Error Conditions**

Computational Errors: None

**Note:** If the factorization performed by SGEF, DGEF, CGEF, ZGEF, SGEFCD, DGEFCD, or DGEFP failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

#### Input-Argument Errors

- 1. trans ≠ 'N', 'T', or 'C'
- 2. Ida,  $Idb \le 0$
- 3. n < 0
- 4. n > Ida, Idb
- 5. nrhs < 0

#### Example 1

Part 1: This part of the example shows how to solve the system AX = B for two right-hand sides, where matrix A is the same matrix factored in the "Example 1" on page 467 for SGEF and DGEF.

#### Call Statement and Input

=(same as output A in "Example 1" on page 467)

$$B = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

Part 2: This part of the example shows how to solve the system  $A^TX = B$  for two right-hand sides, where matrix **A** is the input matrix factored in "Example 1" on page 467 for SGEF and DGEF.

Call Statement and Input

TRANS A LDA N IPVT B LDB NRHS

| | | | | | | | | | | | | | |

CALL SGESM('T', A, 9, 9, 1PVT, B, 9, 2)

IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)

= (same as output A in "Example 1" on page 467)

$$\begin{bmatrix}
6.0 & 15.0 \\
8.0 & 26.0 \\
10.0 & 40.0
\end{bmatrix}$$

Output

$$B = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

#### Example 2

Part 1: This part of the example shows how to solve the system AX = B for two right-hand sides, where matrix **A** is the same matrix factored in the "Example 2" on page 468 for CGEF and ZGEF.

B = 
$$\begin{bmatrix} (-10.0, 85.0) & (-11.0, 53.0) \\ (-6.0, 61.0) & (-6.0, 54.0) \\ (10.0, 38.0) & (2.0, 40.0) \\ (58.0, 168.0) & (15.0, 105.0) \end{bmatrix}$$

Output

B = 
$$\begin{bmatrix} (9.0, 0.0) & (1.0, 1.0) \\ (5.0, 1.0) & (2.0, 2.0) \\ (1.0, 6.0) & (3.0, 3.0) \\ (3.0, 4.0) & (4.0, 4.0) \end{bmatrix}$$

*Part 2:* This part of the example shows how to solve the system  $A^TX = B$  for two right-hand sides, where matrix A is the input matrix factored in "Example 2" on page 468 for CGEF and ZGEF.

Call Statement and Input

$$B = \begin{bmatrix} (71.0, 12.0) & (18.0, 68.0) \\ (61.0, -70.0) & (-27.0, 71.0) \\ (123.0, -34.0) & (-11.0, 97.0) \\ (68.0, 7.0) & (28.0, 50.0) \end{bmatrix}$$

Output

$$B = \begin{bmatrix} (9.0, 0.0) & (1.0, 1.0) \\ (5.0, 1.0) & (2.0, 2.0) \\ (1.0, 6.0) & (3.0, 3.0) \\ (3.0, 4.0) & (4.0, 4.0) \end{bmatrix}$$

*Part 3:* This part of the example shows how to solve the system  $A^HX = B$  for two right-hand sides, where matrix A is the input matrix factored in "Example 2" on page 468 for CGEF and ZGEF.

#### SGESM, DGESM, CGESM, and ZGESM

TRANS A LDA N IPVT B LDB NRHS

| | | | | | | | | | | | | | |

CALL CGESM('C', A, 4, 4, 1PVT, B, 4, 2)

IPVT = (4, 4, 3, 4)
= (same as output A in "Example 2" on page 468)

B = 
$$\begin{bmatrix}
(58.0, -3.0) & (45.0, 20.0) \\
(68.0, -31.0) & (83.0, -20.0) \\
(89.0, -22.0) & (98.0, 1.0) \\
(53.0, 15.0) & (45.0, 25.0)
\end{bmatrix}$$

$$B = \begin{bmatrix} (1.0, 4.0) & (4.0, 5.0) \\ (2.0, 3.0) & (3.0, 4.0) \\ (3.0, 2.0) & (2.0, 3.0) \\ (4.0, 1.0) & (1.0, 2.0) \end{bmatrix}$$

### SGETRF, DGETRF, CGETRF and ZGETRF—General Matrix Factorization

These subroutines factor general matrix  $\boldsymbol{A}$  using Gaussian elimination with partial pivoting. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGETRS, DGETRS CGETRS, or ZGETRS, respectively. To compute the inverse of matrix  $\boldsymbol{A}$ , follow the call to these subroutines with a call to SGEICD or DGEICD, respectively.

Table 90. Data Types	
Α	Subroutine
Short-precision real	SGETRF
Long-precision real	DGETRF
Short-precision complex	CGETRF
Long-precision complex	ZGETRF

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGETRS, DGETRS, CGETRS, ZGETRS, SGEICD or DGEICD respectively.

#### Syntax

Fortran	CALL SGETRF   DGETRF   CGETRF   ZGETRF (m, n, a, lda, ipvt, info)
C and C++	sgetrf   dgetrf   cgetrf   zgetrf (m, n, a, lda, ipvt, info);
PL/I	CALL SGETRF   DGETRF   CGETRF   ZGETRF (m, n, a, lda, ipvt, info);

#### On Entry

m

the number of rows in general matrix  $\boldsymbol{A}$  used in the computation. Specified as: a fullword integer;  $0 \le m \le lda$ .

the number of columns in general matrix  $\mathbf{A}$  used in the computation. Specified as: a fullword integer;  $n \ge 0$ .

is the *m* by *n* general matrix **A** to be factored. Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 90.

is the leading dimension of matrix **A**. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

ipvt

lda

See "On Return."

info

See "On Return."

#### On Return

а

is the m by n transformed matrix A, containing the results of the factorization. See "Function" on page 480. Returned as: an lda by (at least) n array, containing numbers of the data type indicated in Table 90.

ipvt

is the integer vector *ipvt* of length  $\min(m,n)$ , containing the pivot indices. Returned as: a one-dimensional array of (at least) length  $\min(m,n)$ , containing fullword integers, where  $1 \le ipvt(i) \le m$ .

info

has the following meaning:

If info = 0, the factorization of general matrix **A** completed successfully.

If info > 0, info is set equal to the first i, where  $U_{ii}$  is singular and its inverse could not be computed.

Specified as: a fullword integer;  $info \ge 0$ .

#### **Notes**

- 1. In your C program, argument info must be passed by reference.
- 2. The matrix **A** and vector **ipvt** must have no common elements; otherwise results are unpredictable.
- The way these subroutines handle singularity differs from LAPACK. These subroutines us the *info* argument to provide information about the singularity of A, like LAPACK, but also provide an error message.
- 4. On both input and output, matrix **A** conforms to LAPACK format.

**Function:** The matrix **A** is factored using Gaussian elimination with partial pivoting (**ipvt**) to compute the **LU** factorization of **A**, where (**A=PLU**):

L is a unit lower triangular matrix.

U is an upper triangular matrix.

**P** is the permutation matrix.

On output, the transformed matrix A contains U in the upper triangle (if  $m \ge n$ ) or upper trapezoid (if m < n) and L in the strict lower triangle (if  $m \le n$ ) or lower trapezoid (if m > n). *ipvt* contains the pivots representing permutation P, such that A = PLU.

If m or n is 0, no computation is performed and the subroutine returns after doing some parameter checking. See references [36] and [59].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: Matrix A is singular.

- The first column, i, of L with a corresponding U<sub>ii</sub> = 0 diagonal element is identified in the computational error message.
- The computational error message may occur multiple times with processing continuing after each error, because the default for the number of allowable errors for error code 2146 is set to be unlimited in the ESSL error option table.

#### Input-Argument Errors

- 1. m < 0
- 2. n < 0
- 3. m > Ida
- $4. Ida \leq 0$

**Example 1:** This example shows a factorization of a real general matrix **A** of order 9.

#### Call Statement and Input

#### Output

INF0

$$A = \begin{bmatrix} 2.6 & 2.4 & 2.2 & 2.0 & 1.8 & 1.6 & 1.4 & 1.2 & 1.0 \\ 0.4 & 0.3 & 0.6 & 0.8 & 1.1 & 1.4 & 1.7 & 1.9 & 2.2 \\ 0.5 & -0.4 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 & 2.8 \\ 0.5 & -0.3 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 & 2.4 \\ 0.6 & -0.3 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 \\ 0.7 & -0.2 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 & 2.0 \\ 0.8 & -0.2 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 & 1.6 \\ 0.8 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 & 1.2 \\ 0.9 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.8 \\ 0.9 & -0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 \end{bmatrix}$$

$$IPVT = (9, 9, 9, 9, 9, 9, 9, 9, 9, 9, 9)$$

**Example 2:** This example shows a factorization of a complex general matrix **A** of order 9.

#### Call Statement and Input

= 0

```
 \begin{pmatrix} (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) & (4.8, -1.0) & (5.2, -1.0) \\ (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) & (4.8, -1.0) \\ (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) & (4.4, -1.0) \\ (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) & (4.0, -1.0) \\ (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (3.2, -1.0) & (3.6, -1.0) \\ (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.8, -1.0) & (2.8, -1.0) \\ (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) & (2.4, -1.0) \\ (4.8, 1.0) & (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.4, -1.0) \\ (5.2, 1.0) & (4.8, 1.0) & (4.4, 1.0) & (4.0, 1.0) & (3.6, 1.0) & (3.2, 1.0) & (3.2, 1.0) & (2.8, 1.0) & (2.4, 1.0) & (2.0, 1.0) & (2.0, 1.0) \\ \end{pmatrix}
```

#### SGETRF, DGETRF, CGETRF and ZGETRF

```
(3.6, 1.0) (3.2, 1.0) (2.8, 1.0) (2.4, 1.0) (2.0, 1.0)
  (5.2, 1.0) (4.8, 1.0) (4.4, 1.0)
                                      (4.0, 1.0)
  (0.4, 0.1) (0.6, -2.0) (1.1, -1.9)
                                      (1.7, -1.9)
                                                    (2.3, -1.8)
                                                                (2.8,-1.8) (3.4,-1.7) (3.9,-1.7) (4.5,-1.6)
 (0.5, 0.1) (0.0, -0.1) (0.6, -1.9)
                                      (1.2, -1.8)
                                                    (1.8, -1.7)
                                                                (2.5,-1.6) (3.1,-1.5) (3.7,-1.4) (4.3,-1.3)
 (0.6, 0.1) (0.0, -0.1) (-0.1, -0.1)
                                     (0.7, -1.9)
                                                    (1.3, -1.7)
                                                                (2.0,-1.6) (2.7,-1.5) (3.4,-1.4) (4.0,-1.2)
(0.6, 0.1) (0.0, -0.1) (-0.1, -0.1) (-0.1, 0.0)
                                                    (0.7, -1.9)
                                                                (1.5,-1.7) (2.2,-1.6) (2.9,-1.5) (3.7,-1.3)
 (0.7, 0.1) (0.0, -0.1)
                          (0.0, 0.0) (-0.1, 0.0)
                                                   (-0.1, 0.0)
                                                                (0.8,-1.9) (1.6,-1.8) (2.4,-1.6) (3.2,-1.5)
 (0.8, 0.0) (0.0, 0.0)
                          (0.0, 0.0)
                                      (0.0, 0.0)
                                                    (0.0, 0.0)
                                                                (0.0, 0.0) (0.8, -1.9) (1.7, -1.8) (2.5, -1.8)
 (0.9, 0.0) (0.0, 0.0)
                         (0.0, 0.0)
                                      (0.0, 0.0)
                                                    (0.0, 0.0)
                                                                (0.0, 0.0) (0.0, 0.0) (0.8, -2.0) (1.7, -1.9)
 (0.9, 0.0) (0.0, 0.0) (0.0, 0.0)
                                     (0.0, 0.0)
                                                    (0.0, 0.0)
                                                                (0.0, 0.0) (0.0, 0.0) (0.0, 0.0) (0.8, -2.0)
```

= (9, 9, 9, 9, 9, 9, 9, 9, 9)IPVT INF0 0

### SGETRS, DGETRS, CGETRS, and ZGETRS—General Matrix Multiple Right-Hand Side Solve

SGETRS and DGETRS solve one of the following systems of equations for multiple right-hand sides:

- 1. AX = B
- 2.  $A^{T}X = B$

CGETRS and ZGETRS solve one of the following systems of equations for multiple right-hand sides:

- 1. AX = B
- 2.  $A^TX = B$
- 3.  $A^H X = B$

In the formulas above:

**A** represents the general matrix **A** containing the **LU** factorization.

 ${\it B}$  represents the general matrix  ${\it B}$  containing the right-hand sides in its columns.

 ${\it X}$  represents the general matrix  ${\it B}$  containing the solution vectors in its columns.

These subroutines use the results of the factorization of matrix **A**, produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively.

Table 91. Data Types	
A, B	Subroutine
Short-precision real	SGETRS
Long-precision real	DGETRS
Short-precision complex	CGETRS
Long-precision complex	ZGETRS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGETRF, DGETRF, CGETRF and ZGETRF, respectively.

#### Syntax

Fortran	CALL SGETRS   DGETRS   CGETRS   ZGETRS (transa, n, nrhs, a, Ida, ipvt, bx, Idb, info)
C and C++	sgetrs   dgetrs   cgetrs   zgetrs (transa, n, nrhs, a, lda, ipvt, bx, ldb, info);
PL/I	CALL SGETRS   DGETRS   CGETRS   ZGETRS (transa, n, nrhs, a, lda, ipvt, bx, ldb, info);

On Entry

transa

indicates the form of matrix **A** to use in the computation, where:

If transa = 'N', **A** is used in the computation, resulting in solution 1.

If  $transa = {}^{t}T^{t}$ ,  $A^{T}$  is used in the computation, resulting in solution 2.

If  $transa = {}^{\mathsf{L}}C^{\mathsf{L}}$ ,  $A^{\mathsf{H}}$  is used in the computation, resulting in solution 3.

n

is the order of factored matrix  $\mathbf{A}$  and the number of rows in matrix  $\mathbf{B}$ . Specified as: a fullword integer;  $n \ge 0$ .

nrhs

the number of right-hand sides—that is, the number of columns in matrix  $\boldsymbol{B}$  used in the computation. Specified as: a fullword integer;  $nrhs \ge 0$ .

а

is the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively. Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 91 on page 483.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

ipvt

is the integer vector *ipvt* of length n, containing the pivot indices produced by a preceding call to SGETRF, DGETRF, CGETRF, or ZGETRF, respectively. Specified as: a one-dimensional array of (at least) length n, containing fullword integers, where  $1 \le ipvt(i) \le n$ .

bx

is the general matrix **B** containing the right-hand side of the system. Specified as: an *Idb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 91 on page 483.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

info

See "On Return."

#### On Return

bx

is the solution **X** containing the results of the computation. Returned as: an *Idb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 91 on page 483.

info

info has the following meaning:

If info = 0, the solve of general matrix **A** completed successfully.

#### Notes

- 1. In your C program, argument *info* must be passed by reference.
- 2. These subroutines accept lower case letters for the *transa* argument.
- 3. For SGETRS and DGETRS, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 4. The scalar data specified for input argument *n* must be the same for both \_GETRF and \_GETRS. In addition, the scalar data specified for input argument *m* in \_GETRF **must be the same** as input argument *n* in both \_GETRF and GETRS.

If, however, you do **not** plan to call \_GETRS after calling \_GETRF, then input arguments m and n in \_GETRF do not need to be equal.

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- The array data specified for input arguments a and ipvt for these subroutines must be the same as the corresponding output arguments for SGETRF, DGETRF, CGETRF, and ZGETRF, respectively.
- 6. The matrices and vector used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 7. On both input and output, matrices **A** and **B** conform to LAPACK format.

**Function:** One of the following systems of equations is solved for multiple right-hand sides:

- 1. AX = B
- 2.  $A^{T}X = B$
- 3.  $A^HX = B$  (only for CGETRS and ZGETRS)

where **A**, **B**, and **X** are general matrices. These subroutines uses the results of the factorization of matrix **A**, produced by a preceding call to SGETRF, DGETRF, CGETRF or ZGETRF, respectively. For details on the factorization, see "SGETRF, DGETRF, CGETRF and ZGETRF—General Matrix Factorization" on page 479.

If n = 0 or nrhs = 0, no computation is performed and the subroutine returns after doing some parameter checking. See references [36] and [59].

#### **Error Conditions**

Computational Errors: None

**Note:** If the factorization performed by SGETRF, DGETRF, CGETRF or ZGETRF failed because a pivot element is zero, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

Input-Argument Errors

- 1. *transa* ≠ 'N', 'T', or 'C'
- 2. n < 0
- 3. nrhs < 0
- 4. n > Ida
- 5. n > ldb
- 6. Ida ≤ 0
- 7.  $ldb \leq 0$

**Example 1:** This example shows how to solve the system AX = B, where matrix A is the same matrix factored in the "Example 1" on page 481 for DGETRF.

#### Output

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 & 5.0 \\ 2.0 & 4.0 & 6.0 & 8.0 & 10.0 \\ 3.0 & 6.0 & 9.0 & 12.0 & 15.0 \\ 4.0 & 8.0 & 12.0 & 16.0 & 20.0 \\ 5.0 & 10.0 & 15.0 & 20.0 & 25.0 \\ 6.0 & 12.0 & 18.0 & 24.0 & 30.0 \\ 7.0 & 14.0 & 21.0 & 28.0 & 35.0 \\ 8.0 & 16.0 & 24.0 & 32.0 & 40.0 \\ 9.0 & 18.0 & 27.0 & 36.0 & 45.0 \end{bmatrix}$$

INFO = 0

**Example 2:** This example shows how to solve the system AX = b, where matrix A is the same matrix factored in the "Example 2" on page 481 for ZGETRF.

#### Call Statement and Input

```
(221.0, 119.0)
(193.0, -10.6)
                (200.0, 21.8)
                                 (207.0, 54.2)
                                                 (214.0, 86.6)
(173.8, -9.4)
                (178.8, 20.2)
                                 (183.8, 49.8)
                                                 (188.8, 79.4)
                                                                 (193.8, 109.0)
                (159.2, 22.2)
                                 (162.2, 49.8)
                                                 (165.2, 77.4)
(156.2, -5.4)
                                                                 (168.2, 105.0)
(141.0,
        1.4)
                (142.0, 27.8)
                                 (143.0, 54.2)
                                                 (144.0, 80.6)
                                                                 (145.0, 107.0)
(129.0, 11.0)
                (128.0, 37.0)
                                 (127.0, 63.0)
                                                 (126.0, 89.0)
                                                                 (125.0, 115.0)
(121.0, 23.4)
                (118.0, 49.8)
                                 (115.0, 76.2)
                                                 (112.0, 102.6)
                                                                 (109.0, 129.0)
(117.8, 38.6)
                (112.8, 66.2)
                                 (107.8, 93.8)
                                                 (102.8, 121.4)
                                                                  (97.8,149.0)
(120.2, 56.6)
                (113.2, 86.2)
                                 (106.2, 115.8)
                                                  (99.2,145.4)
                                                                   (92.2,175.0)
(129.0, 77.4)
                (120.0, 109.8)
                                (111.0,142.2). (102.0,174.6)
                                                                  (93.0,207.0)
```

```
(1.0,3.0) (1.0,4.0) (1.0,5.0)
          (1.0, 1.0)
                      (1.0,2.0)
          (2.0, 1.0)
                      (2.0, 2.0)
                                  (2.0,3.0) (2.0,4.0) (2.0,5.0)
          (3.0,1.0)
                      (3.0,2.0)
                                  (3.0,3.0) (3.0,4.0) (3.0,5.0)
          (4.0, 1.0)
                      (4.0, 2.0)
                                  (4.0,3.0) (4.0,4.0) (4.0,5.0)
В
          (5.0,1.0)
                      (5.0,2.0)
                                  (5.0,3.0) (5.0,4.0) (5.0,5.0)
          (6.0, 1.0)
                      (6.0,2.0)
                                  (6.0,3.0) (6.0,4.0) (6.0,5.0)
          (7.0, 1.0)
                                  (7.0,3.0) (7.0,4.0) (7.0,5.0)
                      (7.0,2.0)
          (8.0, 1.0)
                      (8.0,2.0)
                                 (8.0,3.0) (8.0,4.0) (8.0,5.0)
          (9.0,1.0) (9.0,2.0) (9.0,3.0) (9.0,4.0) (9.0,5.0)
```

INFO = 0

### SGEFCD and DGEFCD—General Matrix Factorization, Condition Number Reciprocal, and Determinant

These subroutines factor general matrix  $\mathbf{A}$  using Gaussian elimination. An estimate of the reciprocal of the condition number and the determinant of matrix  $\mathbf{A}$  can also be computed. To solve a system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGES/SGESM or DGES/DGESM, respectively. To compute the inverse of matrix  $\mathbf{A}$ , follow the call to these subroutines with a call to SGEICD and DGEICD, respectively.

Table 92. Data Types	
A, aux, rcond, det	Subroutine
Short-precision real	SGEFCD
Long-precision real	DGEFCD

**Note:** The output from these factorization subroutines should be used only as input to the following subroutines for performing a solve or inverse: SGES/SGESM/SGEICD and DGES/DGESM/DGEICD, respectively.

#### Syntax

Fortran	CALL SGEFCD   DGEFCD (a, Ida, n, ipvt, iopt, rcond, det, aux, naux)
C and C++	sgefcd   dgefcd (a, Ida, n, ipvt, iopt, rcond, det, aux, naux);
PL/I	CALL SGEFCD   DGEFCD (a, Ida, n, ipvt, iopt, rcond, det, aux, naux);

#### On Entry

а

is a general matrix  $\mathbf{A}$  of order n, whose factorization, reciprocal of condition number, and determinant are computed. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 92.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le lda$ . *ipvt* 

See "On Return" on page 489.

iopt

indicates the type of computation to be performed, where:

If iopt = 0, the matrix is factored.

If iopt = 1, the matrix is factored, and the reciprocal of the condition number is computed.

If iopt = 2, the matrix is factored, and the determinant is computed.

If iopt = 3, the matrix is factored, and the reciprocal of the condition number and the determinant are computed.

Specified as: a fullword integer; iopt = 0, 1, 2, or 3. rcond

See "On Return" on page 489.

det

See "On Return" on page 489.

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 92 on page 488.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SGEFCD and DGEFCD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n$ .

#### On Return

а

is the transformed matrix  $\bf{\it A}$  of order  $\it n$ , containing the results of the factorization. See "Function" on page 490. Returned as: an  $\it lda$  by (at least)  $\it n$  array, containing numbers of the data type indicated in Table 92 on page 488.

ipvt

is the integer vector *ipvt* of length *n*, containing the pivot indices. Returned as: a one-dimensional array of (at least) length *n*, containing fullword integers. *rcond* 

is an estimate of the reciprocal of the condition number, rcond, of matrix **A**. Returned as: a number of the data type indicated in Table 92 on page 488;  $rcond \ge 0$ .

det

is the vector det, containing the two components,  $det_1$  and  $det_2$ , of the determinant of matrix A. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \le det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 92 on page 488.

#### Notes

- 1. In your C program, argument rcond must be passed by reference.
- 2. When *iopt* = 0, these subroutines provide the same function as a call to SGEF or DGEF, respectively.
- 3. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.
- 4. On both input and output, matrix **A** conforms to LAPACK format.

**Function:** Matrix **A** is factored using Gaussian elimination with partial pivoting (**ipvt**) to compute the **LU** factorization of **A**, where (**A=PLU**):

L is a unit lower triangular matrix.

**U** is an upper triangular matrix.

**P** is the permutation matrix.

On output, the transformed matrix A contains U in the upper triangle and L in the strict lower triangle where ipvt contains the pivots representing permutation P, such that A = PLU.

An estimate of the reciprocal of the condition number, *rcond*, and the determinant, *det*, can also be computed by this subroutine. The estimate of the condition number uses an enhanced version of the algorithm described in references [63] and [64].

If *n* is 0, no computation is performed. See reference [36].

These subroutines call SGEF and DGEF, respectively, to perform the factorization. *ipvt* is an output vector of SGEF and DGEF. It is returned for use by SGES/SGESM and DGES/DGESM, the solve subroutines.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: Matrix A is singular.

- If your program is not terminated by SGEF and DGEF, then SGEFCD and DGEFCD, respectively, return 0 for rcond and det.
- One or more columns of L and the corresponding diagonal of U contain all zeros (all columns of L are checked). The first column, i, of L with a corresponding U = 0 diagonal element is identified in the computational error message, issued by SGEF or DGEF, respectively.
- *i* can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SGEF or DGEF, respectively, when this error occurs. If your program is not terminated by SGEF or DGEF, respectively, the return code is set to 2. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

- 1. Ida ≤ 0
- 2. n < 0
- 3. n > Ida
- 4.  $iopt \neq 0, 1, 2, or 3$
- Error 2015 is recoverable or naux≠0, and naux is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example shows a factorization of matrix **A** of order 9. The input is the same as used in SGEF and DGEF. See "Example 1" on page 467. The reciprocal of the condition number and the determinant of matrix **A** are also

computed. The values used to estimate the reciprocal of the condition number in this example are obtained with the following values:

$$\|\mathbf{A}\|_{1} = \max(6.0, 8.0, 10.0, 12.0, 13.0, 14.0, 15.0, 15.0, 15.0) = 15.0$$

Estimate of 
$$\|\mathbf{A}^{-1}\|_1 = 1091.87$$

This estimate is equal to the actual *rcond* of 5.436(10-5), which is computed by SGEICD and DGEICD. (See "Example 1" on page 517.) On output, the value in det, |A|, is equal to 336.

#### Call Statement and Input

A =(same as input A in "Example 1" on page 467)

```
A =(same as output A in "Example 1" on page 467)

IPVT = (3, 4, 5, 6, 7, 8, 9, 8, 9)

RCOND = 0.00005436

DET = (3.36, 2.00)
```

# SPPF, DPPF, SPOF, DPOF, CPOF, and ZPOF—Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization

The SPPF and DPPF subroutines factor positive definite symmetric matrix  $\mathbf{A}$ , stored in lower-packed storage mode, using Gaussian elimination ( $\mathbf{LDL}^T$ ) or the Cholesky factorization method. To solve a system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPPS or DPPS, respectively. To find the inverse of matrix  $\mathbf{A}$ , follow the call to these subroutines, performing Cholesky factorization, with a call to SPPICD or DPPICD, respectively.

The SPOF, DPOF, CPOF, and ZPOF subroutines factor matrix **A** stored in upper or lower storage mode, where:

- For SPOF and DPOF, **A** is a positive definite symmetric matrix.
- For CPOF and ZPOF, **A** is a positive definite complex Hermitian matrix.

Matrix  $\boldsymbol{A}$  is factored using Cholesky factorization, ( $\boldsymbol{LL^{T}}$  or  $\boldsymbol{U^{T}U}$  for SPOF and DPOF and  $\boldsymbol{LL^{H}}$  or  $\boldsymbol{U^{H}U}$  for CPOF and ZPOF). To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with a call to SPOSM, DPOSM, CPOSM, or ZPOSM. To find the inverse of matrix  $\boldsymbol{A}$ , follow the call to SPOF or DPOF with a call to SPOICD or DPOICD.

Table 93. Data Types	
Α	Subroutine
Short-precision real	SPPF and SPOF
Long-precision real	DPPF and DPOF
Short-precision complex	CPOF
Long-precision complex	ZPOF

**Note:** The output from SPPF and DPPF should be used only as input to the following subroutines for performing a solve or inverse: SPPS/SPPICD and DPPS/DPPICD, respectively. The output from SPOF, DPOF, CPOF, and ZPOF should be used only as input to the following subroutines for performing a solve or inverse: SPOSM/SPOICD, DPOSM/DPOICD, CPOSM, and ZPOSM, respectively.

#### Syntax

Fortran	CALL SPPF   DPPF (ap, n, iopt)
	CALL SPOF   DPOF   CPOF   ZPOF (uplo, a, lda, n)
C and C++	sppf   dppf (ap, n, iopt);
	spof   dpof   cpof   zpof (uplo, a, lda, n);
PL/I	CALL SPPF   DPPF (ap, n, iopt);
	CALL SPOF   DPOF   CPOF   ZPOF (uplo, a, lda, n);

On Entry

### uplo indicates whether matrix **A** is stored in upper or lower storage mode, where: If uplo = 'U', **A** is stored in upper storage mode. If uplo = 'L', **A** is stored in lower storage mode. Specified as: a single character. It must be 'U' or 'L'. is array, referred to as AP, in which matrix A, to be factored, is stored in lower-packed storage mode. Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 93 on page 492. See Notes. If iopt = 0, the array must have at least n(n+1)/2+n elements. If iopt = 1, the array must have at least n(n+1)/2 elements. is the positive definite matrix $\boldsymbol{A}$ , to be factored. Specified as: an *Ida* by (at least) n array, containing numbers of the data type indicated in Table 93 on page 492.

lda

а

is the leading dimension of the array specified for a.

Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

is the order n of matrix A.

Specified as: a fullword integer;  $n \ge 0$ .

iopt

determines the type of computation to be performed, where:

If iopt = 0, the matrix is factored using the **LDL**<sup>T</sup> method.

If iopt = 1, the matrix is factored using Cholesky factorization.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

ap

is the transformed matrix  $\bf{A}$  of order n, containing the results of the factorization. See "Notes" and "Function" on page 494.

Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 93 on page 492.

If *iopt* = 0, the array contains n(n+1)/2+n elements.

If iopt = 1, the array contains n(n+1)/2 elements.

is the transformed matrix  $\bf{A}$  of order n, containing the results of the factorization. See "Function" on page 494.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 93 on page 492.

#### Notes

- 1. All subroutines accept lowercase letters for the *uplo* argument.
- 2. In the input and output arrays specified for ap, the first n(n+1)/2 elements are

#### SPPF, DPPF, SPOF, DPOF, CPOF, and ZPOF

matrix elements. The additional n locations, required in the array when iopt = 0, are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.

- 3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values. On output, they are set to zero.
- 4. For a description of the storage modes used for the matrices, see:
  - For positive definite symmetric matrices, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.
  - For positive definite complex Hermitian matrices, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 71.

**Function:** The functions for these subroutines are described in the sections below.

For SPPF and DPPF: If iopt = 0, the positive definite symmetric matrix  $\boldsymbol{A}$ , stored in lower-packed storage mode, is factored using Gaussian elimination, where  $\boldsymbol{A}$  is expressed as:

 $A = LDL^{T}$ 

where:

L is a unit lower triangular matrix.

 $L^{T}$  is the transpose of matrix L.

**D** is a diagonal matrix.

If iopt = 1, the positive definite symmetric matrix  $\boldsymbol{A}$  is factored using Cholesky factorization, where  $\boldsymbol{A}$  is expressed as:

 $A = LL^{T}$ 

where **L** is a lower triangular matrix.

If *n* is 0, no computation is performed. See references [36 ] and [38 ].

For SPOF, DPOF, CPOF, and ZPOF: The positive definite matrix **A**, stored in upper or lower storage mode, is factored using Cholesky factorization, where **A** is expressed as:

 $A = LL^{T}$  or  $A = U^{T}U$  for SPOF and DPOF  $A = LL^{H}$  or  $A = U^{H}U$  for CPOF and ZPOF

where:

L is a lower triangular matrix.

 $L^{T}$  is the transpose of matrix L.

**L**<sup>H</sup> is the conjugate transpose of matrix **L**.

**U** is an upper triangular matrix.

 $U^{T}$  is the transpose of matrix U.

 $U^{H}$  is the conjugate transpose of matrix U.

If *n* is 0, no computation is performed. See references [8], [64], and [36].

**Error Conditions** 

Resource Errors: Unable to allocate internal work area.

#### Computational Errors

- 1. Matrix  $\mathbf{A}$  is not positive definite (for SPPF and DPPF when iopt = 0).
  - · Processing continues to the end of the matrix.
  - One or more elements of *D* contain values less than or equal to 0; all elements of *D* are checked. The index *i* of the **last** nonpositive element encountered is identified in the computational error message.
  - The return code is set to 1.
  - *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2104 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.
- 2. Matrix **A** is not positive definite (for SPPF and DPPF when *iopt* = 1 and for SPOF, DPOF, CPOF, and ZPOF).
  - Processing stops at the first occurrence of a nonpositive definite diagonal element.
  - The order *i* of the **first** minor encountered having a nonpositive determinant is identified in the computational error message.
  - The return code is set to 1.
  - *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

```
1. n < 0

2. iopt \neq 0 \text{ or } 1

3. uplo \neq 'U' \text{ or } 'L'

4. Ida \leq 0

5. n > Ida
```

**Example 1:** This example shows a factorization of positive definite symmetric matrix **A** of order 9, stored in lower-packed storage mode, where on input matrix **A** is:

```
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
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      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
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      1.0
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      1.0
      1.0
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      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1.0
      1
```

On output, all elements of this matrix **A** are 1.0.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

#### Call Statement and Input

#### Output

**Example 2:** This example shows a factorization of the same positive definite symmetric matrix **A** of order 9 used in Example 1, stored in lower-packed storage mode.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

#### Call Statement and Input

**Example 3:** This example shows a factorization of the same positive definite symmetric matrix **A** of order 9 used in Example 1, but stored in lower storage mode.

Call Statement and Input

Output

**Example 4:** This example shows a factorization of the same positive definite symmetric matrix **A** of order 9 used in Example 1, but stored in upper storage mode.

Output

**Example 5:** This example shows a factorization of positive definite complex Hermitian matrix **A** of order 3, stored in lower storage mode, where on input matrix **A** is:

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

Call Statement and Input

UPLO A LDA N

| | | | |
| CALL CPOF('L', A, 3, 3)

$$A = \begin{bmatrix} (25.0, .) & . & . \\ (-5.0, 5.0) & (51.0, .) & . \\ (10.0, -5.0) & (4.0, 6.0) & (71.0, .) \end{bmatrix}$$

$$A = \begin{bmatrix} (5.0, 0.0) & . & . \\ (-1.0, 1.0) & (7.0, 0.0) & . \\ (2.0, -1.0) & (1.0, 1.0) & (8.0, 0.0) \end{bmatrix}$$

**Example 6:** This example shows a factorization of positive definite complex Hermitian matrix **A** of order 3, stored in upper storage mode, where on input matrix **A** is:

**Note:** On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values. On output, they are set to zero.

Call Statement and Input

$$A = \begin{bmatrix} (9.0, .) & (3.0,3.0) & (3.0,-3.0) \\ . & (18.0, .) & (8.0,-6.0) \\ . & . & (43.0, .) \end{bmatrix}$$

$$A = \begin{bmatrix} (3.0, 0.0) & (1.0, 1.0) & (1.0, -1.0) \\ . & (4.0, 0.0) & (2.0, -1.0) \\ . & . & (6.0, 0.0) \end{bmatrix}$$

### SPPS and DPPS—Positive Definite Real Symmetric Matrix Solve

These subroutines solve the system Ax = b for x, where A is a positive definite symmetric matrix, and x and b are vectors. The subroutines use the results of the factorization of matrix A, produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFPDPFCD, respectively.

Table 94. Data Types	
A, b, x	Subroutine
Short-precision real	SPPS
Long-precision real	DPPS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.

#### Syntax

Fortran	CALL SPPS   DPPS (ap, n, bx, iopt)
C and C++	spps   dpps (ap, n, bx, iopt);
PL/I	CALL SPPS   DPPS (ap, n, bx, iopt);

#### On Entry

ар

is the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFCD, respectively. Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 94, where:

If iopt = 0, the array must contain n(n+1)/2+n elements.

If iopt = 1, the array must contain n(n+1)/2 elements.

n

is the order of matrix  $\boldsymbol{A}$  used in the factorization, and the lengths of vectors  $\boldsymbol{b}$  and  $\boldsymbol{x}$ . Specified as: a fullword integer;  $n \ge 0$ .

bx

is the vector  $\boldsymbol{b}$  of length n, containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 94.

iopt

indicates the type of factorization that was performed on matrix **A**, where:

If iopt = 0, the matrix was factored using the **LDL**<sup>T</sup> method.

If *iopt* = 1, the matrix was factored using Cholesky factorization.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

bx

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 94.

#### Notes

- 1. The array data specified for input argument *ap* for these subroutines must be the same as the corresponding output argument for SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.
- The scalar data specified for input argument n for these subroutines must be the same as that specified for SPPF/SPPFCD and DPPF/DPPFP/DPPFCD, respectively.
- 3. When you call these subroutines after calling SPPF or DPPF, the value of input argument *iopt* must be the same as that specified for SPPF and DPPF.
- 4. When you call these subroutines after calling SPPFCD or DPPFCD, the value of input argument *iopt* must be 0.
- 5. When you call these subroutines after calling DPPFP, the value of input argument *iopt* must be 1.
- 6. In the input array specified for ap, the first n(n+1)/2 elements are matrix elements. The additional n locations, required in the array when iopt = 0, are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.
- 7. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 8. For a description of how a positive definite symmetric matrix is stored in lower-packed storage mode in an array, see "Symmetric Matrix" on page 65.

**Function:** The system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  is solved for  $\mathbf{x}$ , where  $\mathbf{A}$  is a positive definite symmetric matrix, stored in lower-packed storage mode in array AP, and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. These subroutines use the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SPPF/SPPFCD or DPPF/DPPFP/DPPFCD, respectively.

If *n* is 0, no computation is performed. See references [36 ] and [38 ].

#### **Error Conditions**

Computational Errors: None

**Note:** If a call to SPPF, DPPF, SPPFCD, DPPFCD, or DPPFP resulted in a nonpositive definite matrix, error 2104 or 2115, SPPS or DPPS results may be unpredictable or numerically unstable.

Input-Argument Errors

- 1. n < 0
- 2.  $iopt \neq 0$  or 1

**Example 1:** This example shows how to solve the system Ax = b, where matrix A is the same matrix factored in the "Example 1" on page 495 for SPPF and DPPF.

**Example 2:** This example shows how to solve the same system as in Example 1, where matrix A is the same matrix factored in the "Example 2" on page 496 for SPPF and DPPF.

# SPOSM, DPOSM, CPOSM, and ZPOSM—Positive Definite Real Symmetric or Complex Hermitian Matrix Multiple Right-Hand Side Solve

These subroutines solve the system AX = B for X, using multiple right-hand sides, where X and B are general matrices and:

- For SPOSM and DPOSM, **A** is a positive definite symmetric matrix.
- For CPOSM and ZPOSM, **A** is a positive definite complex Hermitian matrix.

These subroutines use the results of the factorization of matrix **A**, produced by a preceding call to SPOF/SPOFCD, DPOF/DPOFCD, CPOF, or ZPOF, respectively.

Table 95. Data Types		
A, B, X	Subroutine	
Short-precision real	SPOSM	
Long-precision real	DPOSM	
Short-precision complex	CPOSM	
Long-precision complex	ZPOSM	

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SPOF/SPOFCD, DPOF/DPOFCD, CPOF, and ZPOF, respectively.

## Syntax

Fortran	CALL SPOSM   DPOSM   CPOSM   ZPOSM (uplo, a, lda, n, b, ldb, nrhs)	
C and C++	C and C++ sposm   dposm   cposm   zposm (uplo, a, lda, n, b, ldb, nrhs);	
PL/I	CALL SPOSM   DPOSM   CPOSM   ZPOSM (uplo, a, lda, n, b, ldb, nrhs);	

On Entry

uplo

indicates whether the original matrix  $\boldsymbol{A}$  is stored in upper or lower storage mode, where:

If uplo = 'U', **A** is stored in upper storage mode.

If *uplo* = 'L', **A** is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

а

is the factorization of positive definite matrix A, produced by a preceding call to SPOF/SPOFCD, DPOF/DPOFCD, CPOF, or ZPOF, respectively. Specified as: an *Ida* by (at least) n array, containing numbers of the data type indicated in Table 95.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le Ida$ .

b

is the matrix  $\mathbf{B}$ , containing the *nrhs* right-hand sides of the system. The right-hand sides, each of length n, reside in the columns of matrix  $\mathbf{B}$ . Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 95.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

nrhs

is the number of right-hand sides in the system to be solved. Specified as: a fullword integer;  $nrhs \ge 0$ .

#### On Return

b

is the matrix **B**, containing the *nrhs* solutions to the system in the columns of **B**. Specified as: an *ldb* by (at least) *nrhs* array, containing numbers of the data type indicated in Table 95 on page 503.

#### **Notes**

- 1. All subroutines accept lowercase letters for the *uplo* argument.
- 2. The scalar data specified for input arguments *uplo*, *lda*, and *n* for these subroutines must be the same as the corresponding input arguments specified for SPOF/SPOFCD, DPOF/DPOFCD, CPOF, and ZPOF, respectively.
- The array data specified for input argument a for these subroutines must be the same as the corresponding output arguments for SPOF/SPOFCD, DPOF/DPOFCD, CPOF, and ZPOF, respectively.
- 4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 5. For a description of how the matrices are stored:
  - For positive definite symmetric matrices, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.
  - For positive definite complex Hermitian matrices, see "Positive Definite or Negative Definite Complex Hermitian Matrix" on page 71.

**Function:** The system  $\mathbf{AX} = \mathbf{B}$  is solved for  $\mathbf{X}$ , using multiple right-hand sides, where  $\mathbf{X}$  and  $\mathbf{B}$  are general matrices, and  $\mathbf{A}$  is a positive definite symmetric matrix for SPOSM and DPOSM and a positive definite complex Hermitian matrix for CPOSM and ZPOSM. These subroutines use the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SPOF/SPOFCD, DPOF/DPOFCD, CPOF, or ZPOF, respectively. For a description of how  $\mathbf{A}$  is factored, see "SPPF, DPPF, SPOF, DPOF, CPOF, and ZPOF—Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization" on page 492.

If *n* or *nrhs* is 0, no computation is performed. See references [8] and [36].

# **Error Conditions**

Computational Errors: None

**Note:** If the factorization performed by SPOF, DPOF, CPOF, ZPOF, SPOFCD, or DPOFCD failed because matrix **A** was not positive definite, the results

returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

Input-Argument Errors

2. 
$$Ida$$
,  $Idb \leq 0$ 

3. 
$$n < 0$$

5. 
$$n > ldb$$

**Example 1:** This example shows how to solve the system AX = B for two right-hand sides, where matrix A is the same matrix factored in the "Example 3" on page 497 for SPOF.

Call Statement and Input

A =(same as output A in "Example 3" on page 497)

Output

$$B = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \\ 1.0 & 3.0 \\ 1.0 & 4.0 \\ 1.0 & 5.0 \\ 1.0 & 6.0 \\ 1.0 & 7.0 \\ 1.0 & 8.0 \\ 1.0 & 9.0 \end{bmatrix}$$

**Example 2:** This example shows how to solve the system  $A^TX = B$  for two right-hand sides, where matrix A is the input matrix factored in "Example 4" on page 497 for SPOF.

A =(same as output A in "Example 4" on page 497)

Output

**Example 3:** This example shows how to solve the system AX = B for two right-hand sides, where matrix A is the same matrix factored in the "Example 5" on page 498 for CPOF.

Call Statement and Input

A =(same as output A in "Example 5" on page 498)

B = 
$$\begin{bmatrix} (60.0, -55.0) & (70.0, 10.0) \\ (34.0, 58.0) & (-51.0, 110.0) \\ (13.0, -152.0) & (75.0, 63.0) \end{bmatrix}$$

Output

$$B = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, 1.0) & (-1.0, 2.0) \\ (0.0, -2.0) & (1.0, 1.0) \end{bmatrix}$$

**Example 4:** This example shows how to solve the system AX = B for two right-hand sides, where matrix A is the input matrix factored in "Example 6" on page 499 for CPOF.

Call Statement and Input

=(same as output A in "Example 6" on page 499)

B = 
$$\begin{bmatrix} (33.0, -18.0) & (15.0, -3.0) \\ (45.0, -45.0) & (8.0, -2.0) \\ (152.0, 1.0) & (43.0, -29.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (2.0, -1.0) & (2.0, 0.0) \\ (1.0, -1.0) & (0.0, 1.0) \\ (3.0, 0.0) & (1.0, -1.0) \end{bmatrix}$$

# SPPFCD, DPPFCD, SPOFCD, and DPOFCD—Positive Definite Real Symmetric Matrix Factorization, Condition Number Reciprocal, and Determinant

The SPPFCD and DPPFCD subroutines factor positive definite symmetric matrix  $\mathbf{A}$ , stored in lower-packed storage mode, using Gaussian elimination ( $\mathbf{LDL}^{\mathsf{T}}$ ). The reciprocal of the condition number and the determinant of matrix  $\mathbf{A}$  can also be computed. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPPS or DPPS, respectively.

The SPOFCD and DPOFCD subroutines factor positive definite symmetric matrix  $\mathbf{A}$ , stored in upper or lower storage mode, using Cholesky factorization ( $\mathbf{L}\mathbf{L}^T$  or  $\mathbf{U}^T\mathbf{U}$ ). The reciprocal of the condition number and the determinant of matrix  $\mathbf{A}$  can also be computed. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with a call to SPOSM or DPOSM, respectively. To find the inverse of matrix  $\mathbf{A}$ , follow the call to these subroutines with a call to SPOICD or DPOICD, respectively.

Table 96. Data Types	
A, aux, rcond, det	Subroutine
Short-precision real	SPPFCD and SPOFCD
Long-precision real	DPPFCD and DPOFCD

**Note:** The output factorization from SPPFCD and DPPFCD should be used only as input to the solve subroutines SPPS and DPPS, respectively. The output from SPOFCD and DPOFCD should be used only as input to the following subroutines for performing a solve or inverse: SPOSM/SPOICD and DPOSM/DPOICD, respectively.

#### **Syntax**

Fortran	CALL SPPFCD   DPPFCD (ap, n, iopt, rcond, det, aux, naux)
	CALL SPOFCD   DPOFCD (uplo, a, Ida, n, iopt, rcond, det, aux, naux)
C and C++	sppfcd   dppfcd (ap, n, iopt, rcond, det, aux, naux);
	spofcd   dpofcd (uplo, a, lda, n, iopt, rcond, det, aux, naux);
PL/I	CALL SPPFCD   DPPFCD (ap, n, iopt, rcond, det, aux, naux);
	CALL SPOFCD   DPOFCD (uplo, a, Ida, n, iopt, rcond, det, aux, naux);

On Entry

uplo

indicates whether matrix **A** is stored in upper or lower storage mode, where:

If uplo = 'U', **A** is stored in upper storage mode.

If uplo = 'L', **A** is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

ap

is the array, referred to as AP, in which the matrix A, to be factored, is stored in lower-packed storage mode. Specified as: a one-dimensional array of (at least) length n(n+1)/2+n, containing numbers of the data type indicated in Table 96.

а

is the positive definite symmetric matrix A, to be factored. Specified as: an *Ida* by (at least) n array, containing numbers of the data type indicated in Table 96 on page 508.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order n of matrix A. Specified as: a fullword integer, where:

For SPPFCD and DPPFCD,  $n \ge 0$ .

For SPOFCD and DPOFCD,  $0 \le n \le Ida$ .

iopt

indicates the type of computation to be performed, where:

If iopt = 0, the matrix is factored.

If iopt = 1, the matrix is factored, and the reciprocal of the condition number is computed.

If iopt = 2, the matrix is factored, and the determinant is computed.

If iopt = 3, the matrix is factored and the reciprocal of the condition number and the determinant are computed.

Specified as: a fullword integer; iopt = 0, 1, 2, or 3.

rcond

See "On Return."

det

See "On Return."

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, is the storage work area used by these subroutines. Its size is specified by *naux*. Specified as: an area of storage, containing numbers of the data type indicated in Table 96 on page 508.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SPPFCD, DPPFCD, SPOFCD, and DPOFCD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n$ .

On Return

ар

is the transformed matrix A of order n, containing the results of the factorization. See "Function" on page 510. Returned as: a one-dimensional array of (at least) length n(n+1)/2+n, containing numbers of the data type indicated in Table 96 on page 508.

а

is the transformed matrix  $\mathbf{A}$  of order n, containing the results of the factorization. See "Function" on page 510. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 96 on page 508.

rcond

is the estimate of the reciprocal of the condition number, rcond, of matrix **A**. Returned as: a number of the data type indicated in Table 96 on page 508;  $rcond \ge 0$ .

det

is the vector det, containing the two components  $det_1$  and  $det_2$  of the determinant of matrix A. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \le det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 96 on page 508.

#### Notes

- 1. All subroutines accept lowercase letters for the uplo argument.
- 2. In your C program, argument *rcond* must be passed by reference.
- 3. When *iopt* = 0, SPPFCD and DPPFCD provide the same function as a call to SPPF or DPPF, respectively. When *iopt* = 0, SPOFCD and DPOFCD provide the same function as a call to SPOF or DPOF, respectively.
- 4. See "Notes" on page 501 for information on specifying a value for *iopt* in the SPPS and DPPS subroutines after calling SPPFCD and DPPFCD, respectively.
- 5. In the input and output arrays specified for *ap*, the first *n*(*n*+1)/2 elements are matrix elements. The additional *n* locations in the array are used for working storage by this subroutine and should not be altered between calls to the factorization and solve subroutines.
- 6. For a description of how a positive definite symmetric matrix is stored in lower-packed storage mode in an array, see "Symmetric Matrix" on page 65. For a description of how a positive definite symmetric matrix is stored in upper or lower storage mode, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The functions for these subroutines are described in the sections below.

For SPPFCD and DPPFCD: The positive definite symmetric matrix **A**, stored in lower-packed storage mode, is factored using Gaussian elimination, where **A** is expressed as:

$$A = LDL^{T}$$

where:

L is a unit lower triangular matrix.

 $L^{T}$  is the transpose of matrix L. D is a diagonal matrix.

An estimate of the reciprocal of the condition number, *rcond*, and the determinant, *det*, can also be computed by this subroutine. The estimate of the condition number uses an enhanced version of the algorithm described in references [63] and [64].

If *n* is 0, no computation is performed. See references [36] and [38].

These subroutines call SPPF and DPPF, respectively, to perform the factorization using Gaussian elimination ( $LDL^{T}$ ). If you want to use the Cholesky factorization method, you must call SPPF and DPPF directly.

For SPOFCD and DPOFCD: The positive definite symmetric matrix **A**, stored in upper or lower storage mode, is factored using Cholesky factorization, where **A** is expressed as:

$$A = LL \top \text{ or } A = U \top U$$

where:

 $\boldsymbol{L}$  is a lower triangular matrix.  $\boldsymbol{L}^{\mathsf{T}}$  is the transpose of matrix  $\boldsymbol{L}$ .  $\boldsymbol{U}$  is an upper triangular matrix.

 $U^{T}$  is the transpose of matrix U.

If specified, the estimate of the reciprocal of the condition number and the determinant can also be computed. The estimate of the condition number uses an enhanced version of the algorithm described in references [63] and [64].

If *n* is 0, no computation is performed. See references [8] and [36].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors

- 1. Matrix **A** is not positive definite (for SPPFCD and DPPFCD).
  - If matrix **A** is singular (at least one of the diagonal elements are 0), then *rcond* and *det*, if you requested them, are set to 0.
  - If matrix **A** is nonsingular and nonpositive definite (none of the diagonal elements are 0 and at least one diagonal element is negative), then *rcond* and *det*, if you requested them, are computed.
  - One or more elements of *D* contain values less than or equal to 0; all elements of *D* are checked. The index *i* of the last nonpositive element encountered is identified in the computational error message, issued by SPPF or DPPF, respectively.
  - i can be determined at run time by using the ESSL error-handling facilities.
    To obtain this information, you must use ERRSET to change the number of
    allowable errors for error code 2104 in the ESSL error option table;
    otherwise, the default value causes your program to be terminated by
    SPPF or DPPF, respectively, when this error occurs. If your program is not
    terminated by SPPF or DPPF, respectively, the return code is set to 2. For

details, see "What Can You Do about ESSL Computational Errors?" on page 48.

- 2. Matrix **A** is not positive definite (for SPOFCD and DPOFCD).
  - If matrix **A** is singular (at least one of the diagonal elements are 0), then rcond and det, if you requested them, are set to 0.
  - If matrix A is nonsingular and nonpositive definite (none of the diagonal elements are 0 and at least one diagonal element is negative), then rcond and *det*, if you requested them, are computed.
  - · Processing stops at the first occurrence of a nonpositive definite diagonal element.
  - The order i of the first minor encountered having a nonpositive determinant is identified in the computational error message.
  - *i* can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SPPF or DPPF, respectively, when this error occurs. If your program is not terminated by SPPF or DPPF, respectively, the return code is set to 2. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

## Input-Argument Errors

- 1. *uplo* ≠ 'U' or 'L'
- $2. Ida \leq 0$
- 3. Ida < n
- 4. n < 0
- 5.  $iopt \neq 0, 1, 2, or 3$
- 6. Error 2015 is recoverable or naux≠0, and naux is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example computes the factorization, reciprocal of the condition number, and determinant of matrix A. The input is the same as used in "Example 1" on page 495 for SPPF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|\mathbf{A}\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$
 Estimate of  $\|\mathbf{A}\| = 4.0$ 

On output, the value in det, |A|, is equal to 1.

#### Call Statement and Input

=(same as input AP in "Example 1" on page 495) AP

# Output

```
AP = (same as output AP in "Example 1" on page 495)

RCOND = 0.0055555

DET = (1.0, 0.0)
```

**Example 2:** This example computes the factorization, reciprocal of the condition number, and determinant of matrix **A**. The input is the same as used in "Example 3" on page 497 for SPOF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|\mathbf{A}\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$
  
Estimate of  $\|\mathbf{A}\| = 4.0$ 

On output, the value in det, |A|, is equal to 1.

Call Statement and Input

# Output

A = (same as output A in "Example 3" on page 497)  
RCOND = 
$$0.0055555$$
  
DET =  $(1.0, 0.0)$ 

**Example 3:** This example computes the factorization, reciprocal of the condition number, and determinant of matrix **A**. The input is the same as used in "Example 4" on page 497 for SPOF.

The values used to estimate the reciprocal of the condition number are obtained with the following values:

$$\|\mathbf{A}\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$
  
Estimate of  $\|\mathbf{A}\| = 4.0$ 

On output, the value in det, |A|, is equal to 1.

Call Statement and Input

A =(same as input A in "Example 4" on page 497)

```
A = (same as output A in "Example 4" on page 497)

RCOND = 0.0055555

DET = (1.0, 0.0)
```

# SGEICD and DGEICD—General Matrix Inverse, Condition Number Reciprocal, and Determinant

These subroutines find the inverse, the reciprocal of the condition number, and the determinant of matrix A.

Table 97. Data Types		
A, aux, rcond, det	Subroutine	
Short-precision real	SGEICD	
Long-precision real	DGEICD	

**Note:** If you call these subroutines with iopt = 0, 1, 2, or 3 the input must be the output from the factorization subroutines SGEF/SGEFCD/SGETRF or DGEF/DGEFCD/DGEFP/DGETRF, respectively.

# Syntax

Fortran	CALL SGEICD   DGEICD (a, Ida, n, iopt, rcond, det, aux, naux)
C and C++	sgeicd   dgeicd (a, Ida, n, iopt, rcond, det, aux, naux);
PL/I	CALL SGEICD   DGEICD (a, Ida, n, iopt, rcond, det, aux, naux);

# On Entry

has the following meaning, where:

If iopt = 0, 1, 2, or 3, it is matrix **A** of order n, whose inverse, reciprocal of condition number, and determinant are computed.

If iopt = 4, it is the transformed matrix **A** of order *n*, resulting from the factorization performed in a previous call to SGEF/SGEFCD or DGEF/DGEFCD/DGEFP, respectively, whose inverse is computed.

Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 97.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $0 \le n \le Ida$ . iopt

indicates the type of computation to be performed, where:

If iopt = 0, the inverse is computed for matrix **A**.

If *iopt* = 1, the inverse and the reciprocal of the condition number are computed for matrix A.

If iopt = 2, the inverse and the determinant are computed for matrix **A**.

If iopt = 3, the inverse, the reciprocal of the condition number, and the determinant are computed for matrix A.

If iopt = 4, the inverse is computed using the factored matrix **A**.

Specified as: a fullword integer; iopt = 0, 1, 2, 3, 4.

rcond

See "On Return" on page 515.

det

See "On Return."

aux

has the following meaning, and its size is specified by naux:

If iopt = 0, 1, 2, or 3, then if naux = 0 and error 2015 is unrecoverable, aux is ignored. Otherwise, it is the storage work area used by this subroutine.

If iopt = 4, aux has the following meaning:

- For SGEICD, the first n locations in aux must contain the ipvt integer vector of length n, resulting from a previous call to SGEF, SGETRF, or SGEFCD.
- For DGEICD, the first ceiling(n/2) locations in aux must contain the ipvt integer vector of length n, resulting from a previous call to DGEF, DGETRF, DGEFCD, or DGEFP.

Specified as: an area of storage, containing numbers of the data type indicated in Table 97 on page 514.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If  $iopt \neq 4$ , then if naux = 0 and error 2015 is unrecoverable, SGEICD and DGEICD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise naux must have the following value:

For the RS/6000 POWER, POWER3, or PowerPC processors,  $naux \ge 100n$ .

For the RS/6000 POWER2 processors,  $naux \ge 200n$ .

**Note:** *naux* values specified for releases prior to ESSL Version 2 Release 2 will still work, but you may not achieve optimal performance.

On Return

а

is the resulting inverse of matrix  $\bf{A}$  of order  $\bf{n}$ . Returned as: an  $\bf{lda}$  by (at least)  $\bf{n}$  array, containing numbers of the data type indicated in Table 97 on page 514.

rcond

is the reciprocal of the condition number, rcond, of matrix **A**. Returned as: a real number of the data type indicated in Table 97 on page 514;  $rcond \ge 0$ . det

is the vector det, containing the two components  $det_1$  and  $det_2$  of the determinant of matrix A. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \le det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 97 on page 514.

#### Notes

- 1. In your C program, argument *rcond* must be passed by reference.
- 2. If *iopt* = 4, the following input arguments for SGEICD and DGEICD must be set to the same values in the previous call to SGEF/SGEFCD or DGEF/DGEFCD/DGEFP, respectively:

For _GEF_	For _GEICD
Input arguments n and Ida	Input arguments n and Ida
Output arguments a and ipvt	Input arguments a and aux

3. You have the option of having the value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The inverse, the reciprocal of the condition number, and the determinant of a general square matrix **A** are computed using partial pivoting to preserve accuracy, where:

- $A^{-1}$  is the inverse of matrix A, where  $AA^{-1} = A^{-1}A = I$ , and I is the identity matrix.
- $1/(\|\mathbf{A}\|_1)(\|\mathbf{A}^{-1}\|_1)$  is the reciprocal of the condition number, where  $\|\mathbf{A}\|_1$  is the one-norm of matrix  $\mathbf{A}$ .
- |A| is the determinant of matrix A, where |A| is expressed as:

$$det_1(10^{det_2})$$

The *iopt* argument is used to determine the combination of output items produced by this subroutine: the inverse, the reciprocal of the condition number, and the determinant.

If *n* is 0, no computation is performed. See references [36], [38], and [44].

## **Error Conditions**

Resource Errors: If iopt = 0, 1, 2, or 3, then error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: Matrix A is singular or nearly singular.

- The index *i* of the first pivot element having a value equal to 0, is identified in the computational error message.
- These subroutines return 0 for rcond and det, if you requested them.
- The return code is set to 2.
- *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2105 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. n < 0
- 3. n > Ida
- 4.  $iopt \neq 0, 1, 2, 3, or 4$
- 5. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example computes the inverse, the reciprocal of the condition number, and the determinant of matrix **A**. The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|\mathbf{A}\|_1 = \max(6.0, 8.0, 10.0, 12.0, 13.0, 14.0, 15.0, 15.0, 15.0) = 15.0$$
  
 $\|\mathbf{A}^{-1}\|_1 = 1226.33$ 

On output, the value in **det**, |A|, is equal to 336.

Call Statement and Input

Output

$$\mathsf{A} \quad = \quad \begin{bmatrix} 0.333 & -0.667 & 0.333 & 0.000 & 0.000 & 0.000 & 0.042 & -0.042 & 0.000 \\ 56.833 & -52.167 & -1.167 & -0.500 & -0.500 & -0.357 & 6.836 & -0.479 & -0.500 \\ -55.167 & 51.833 & 0.833 & 0.500 & 0.500 & 0.214 & -6.735 & 0.521 & 0.500 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.143 & -0.143 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ -1.000 & 1.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 & 0.000 \\ -226.000 & 206.000 & 5.000 & 3.000 & 2.000 & 1.429 & -27.179 & 1.750 & 2.000 \\ 560.000 & -520.000 & -10.000 & -6.000 & -4.000 & -2.857 & 67.857 & -5.000 & -5.000 \\ -325.000 & 305.000 & 5.000 & 3.000 & 2.000 & 1.429 & -39.554 & 3.125 & 3.000 \end{bmatrix}$$

RCOND = 0.00005436DET = (3.36, 2.00)

**Example 2:** This example computes the inverse of matrix  $\mathbf{A}$ , where *iopt* = 4 and matrix  $\mathbf{A}$  is the transformed matrix factored in "Example 1" on page 467 by SGEF. The input contents of AUX, shown here, is the same as the output contents of IPVT in that example.

# Call Statement and Input

```
0.000
  0.333
           -0.667
                   0.333 0.000 0.000
                                         0.000
                                                 0.042 -0.042
 56.833
          -52.167
                   -1.167 -0.500 -0.500 -0.357
                                                 6.836 -0.479 -0.500
           51.833
                                                        0.521 0.500
 -55.167
                   0.833 0.500 0.500
                                         0.214
                                                -6.735
 -1.000
           1.000
                    0.000
                          0.000 \quad 0.000
                                         0.143
                                                -0.143
                                                        0.000
                                                               0.000
 -1.000
           1.000
                    0.000
                           0.000
                                  0.000
                                         0.000
                                                 0.000
                                                        0.000
                                                               0.000
 -1.000
           1.000
                    0.000
                           0.000
                                  0.000
                                         0.000
                                                -0.125
                                                        0.125
                                                               0.000
-226.000
         206.000
                    5.000
                           3.000
                                 2.000
                                        1.429 -27.179
                                                        1.750
                                                               2.000
 560.000 -520.000 -10.000 -6.000 -4.000 -2.857
                                                67.857 -5.000 -5.000
-325.000
         305.000
                    5.000 3.000 2.000 1.429 -39.554 3.125 3.000
```

# SPPICD, DPPICD, SPOICD, and DPOICD—Positive Definite Real Symmetric Matrix Inverse, Condition Number Reciprocal, and Determinant

These subroutines find the inverse, the reciprocal of the condition number, and the determinant of positive definite symmetric matrix **A** using Cholesky factorization, where:

- For SPPICD and DPPICD, A is stored in lower-packed storage mode.
- For SPOICD and DPOICD, A is stored in upper or lower storage mode.

Table 98. Data Types	
A, aux, rcond, det	Subroutine
Short-precision real	SPPICD and SPOICD
Long-precision real	DPPICD and DPOICD

**Note:** If you call these subroutines with *iopt* = 4, the input must be the output from the factorization subroutines SPPF, DPPF, SPOF/SPOFCD, or DPOF/DPOFCD, respectively, where Cholesky factorization was performed.

# Syntax

Fortran	CALL SPPICD   DPPICD (ap, n, iopt, rcond, det, aux, naux)
	CALL SPOICD   DPOICD (uplo, a, Ida, n, iopt, rcond, det, aux, naux)
C and C++	sppicd   dppicd (ap, n, iopt, rcond, det, aux, naux);
	spoicd   dpoicd (uplo, a, lda, n, iopt, rcond, det, aux, naux);
PL/I	CALL SPPICD   DPPICD (ap, n, iopt, rcond, det, aux, naux);
	CALL SPOICD   DPOICD (uplo, a, Ida, n, iopt, rcond, det, aux, naux);

On Entry

uplo

indicates whether matrix  $\boldsymbol{A}$  is stored in upper or lower storage mode, where:

If uplo = 'U', **A** is stored in upper storage mode.

If uplo = 'L', **A** is stored in lower storage mode.

Specified as: a single character. It must be 'U' or 'L'.

ар

is the array, referred to as AP, where:

If iopt = 0, 1, 2, or 3, then AP contains the positive definite real symmetric matrix  $\mathbf{A}$ , whose inverse, condition number reciprocal, and determinant are computed, where matrix  $\mathbf{A}$  is stored in lower-packed storage mode.

If iopt = 4, then AP contains the transformed matrix **A** of order n, resulting from the Cholesky factorization performed in a previous call to SPPF or DPPF, respectively, whose inverse is computed.

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 98.

а

has the following meaning, where:

If iopt = 0, 1, 2, or 3, it is the positive definite real symmetric matrix  $\mathbf{A}$ , whose inverse, condition number reciprocal, and determinant are computed, where matrix  $\mathbf{A}$  is stored in upper or lower storage mode.

If iopt = 4, it is the transformed matrix **A** of order *n*, containing results of the factorization from a previous call to SPOF/SPOFCD or DPOF/DPOFCD, respectively, whose inverse is computed.

Specified as: an n by (at least) n array, containing numbers of the data type indicated in Table 98 on page 519.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

n

is the order n of matrix A. Specified as: a fullword integer;  $n \ge 0$ . iont

indicates the type of computation to be performed, where:

If iopt = 0, the inverse is computed for matrix **A**.

If iopt = 1, the inverse and the reciprocal of the condition number are computed for matrix **A**.

If iopt = 2, the inverse and the determinant are computed for matrix **A**.

If iopt = 3, the inverse, the reciprocal of the condition number, and the determinant are computed for matrix A.

If iopt = 4, the inverse is computed for the (Cholesky) factored matrix **A**.

Specified as: a fullword integer; iopt = 0, 1, 2, 3, or 4.

rcond

See "On Return."

det

See "On Return."

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*. Specified as: an area of storage, containing numbers of the data type indicated in Table 98 on page 519.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SPPICD, DPPICD, SPOICD, AND DPOICD dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n$ .

On Return

ар

is the resulting array, referred to as AP, containing the inverse of the matrix in lower-packed storage mode. Returned as: a one-dimensional array of (at least)

length n(n+1)/2, containing numbers of the data type indicated in Table 98 on page 519.

а

is the transformed matrix A of order n, containing the inverse of the matrix in upper or lower storage mode. Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 98 on page 519.

#### rcond

is the reciprocal of the condition number, rcond, of matrix **A**. Returned as: a real number of the data type indicated in Table 98 on page 519;  $rcond \ge 0$ . det

is the vector det, containing the two components  $det_1$  and  $det_2$  of the determinant of matrix A. The determinant is:

$$det_1(10^{det_2})$$

where  $1 \le det_1 < 10$ . Returned as: an array of length 2, containing numbers of the data type indicated in Table 98 on page 519.

#### Notes

- 1. For these subroutines, when you specify iopt = 4, you must do the following:
  - For SPPICD and DPPICD, use Cholesky factorization in the previous call to SPPF and DPPF, respectively.
  - For SPOICD and DPOICD, specify the same storage mode for matrix A
    that was specified in the previous call to SPOF/SPOFCD and
    DPOF/DPOFCD, respectively.
  - The scalar data specified for input arguments *uplo*, *lda*, and *n* for these subroutines must be the same as the corresponding input arguments specified for SPOF/SPOFCD and DPOF/DPOFCD, respectively.
- 2. All subroutines accept lowercase letters for the uplo argument.
- 3. In your C program, argument *rcond* must be passed by reference.
- 4. For a description of how a positive definite symmetric matrix is stored in lower-packed storage mode in an array, see "Symmetric Matrix" on page 65. For a description of how a positive definite symmetric matrix is stored in upper or lower storage mode, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** These subroutines find the inverse, the reciprocal of the condition number, and the determinant of positive definite symmetric matrix **A** using Cholesky factorization, where:

- $A^{-1}$  is the inverse of matrix A, where  $AA^{-1} = A^{-1}A = I$ , and I is the identity matrix.
- $1/(\|\mathbf{A}\|_1)(\|\mathbf{A}^{-1}\|_1)$  is the reciprocal of the condition number, where  $\|\mathbf{A}\|_1$  is the one-norm of matrix  $\mathbf{A}$ .
- |A| is the determinant of matrix A, where |A| is expressed as:

$$det_1(10^{det_2})$$

The *iopt* argument is used to determine the combination of output items produced by this subroutine: the inverse, the reciprocal of the condition number, and the determinant.

If *n* is 0, no computation is performed. See references [36], [38], and [44].

#### **Error Conditions**

#### Resource Errors

- Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.
- Unable to allocate internal work area.

Computational Errors: Matrix A is not positive definite.

- These subroutines do not perform the inverse, determinant, and reciprocal of the condition number computations.
- For *iopt* = 1, 2, or 3, the leading minor of order *i* has a nonpositive determinant. The order *i* is identified in the computational error message, issued by SPPF, DPPF, SPOF, or DPOF, respectively.

For *iopt* = 4 for SPPICD and DPPICD, if the Cholesky factorization performed by SPPF or DPPF, respectively, failed due to a nonpositive definite matrix A, the results from STPI or DTPI, respectively, are unpredictable, and a computational error message may be issued.

For *iopt* = 4 for SPOICD and DPOICD, if the factorization performed by SPOF/SPOFCD or DPOF/DPOFCD, respectively, failed due to a nonpositive definite matrix A, the results from STRI or DTRI, respectively, are unpredictable, and a computational error message may be issued.

 i can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to be terminated by SPPF, DPPF, SPOF, or DPOF, respectively, when this error occurs. If your program is not terminated by SPPF, DPPF, SPOF, or DPOF, respectively, the return code is set to 2. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

### Input-Argument Errors

- 1. *uplo* ≠ 'U' or 'L'
- 2. n < 0
- 3.  $Ida \leq 0$
- 4. Ida < n
- 5.  $iopt \neq 0, 1, 2, 3, or 4$
- 6. Error 2015 is recoverable or naux≠0, and naux is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

Example 1: This example uses SPPICD to compute the inverse, reciprocal of the condition number, and determinant of matrix A. Where A is:

```
1.0 1.0
       1.0 1.0 1.0 1.0
                         1.0
1.0 2.0
       2.0 2.0 2.0
                     2.0
                          2.0
                              2.0
                                  2.0
1.0 2.0
       3.0
            3.0
                3.0
                     3.0
                         3.0
                              3.0
                                  3.0
1.0 2.0
        3.0 4.0
                4.0
                     4.0 4.0
                              4.0
                                  4.0
1.0 2.0
        3.0 4.0
                 5.0
                     5.0 5.0
                              5.0
                                  5.0
1.0 2.0
        3.0 4.0 5.0
                                  6.0
                     6.0 6.0
                              6.0
1.0 2.0
       3.0 4.0 5.0 6.0 7.0
                              7.0
                                  7.0
1.0 2.0 3.0 4.0 5.0
                     6.0 7.0 8.0
                                  8.0
1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
                                  9.0
```

The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|\mathbf{A}\|_1 = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$
  
 $\|\mathbf{A}^{-1}\|_1 = 4.0$ 

On output, the value in det, |A|, is equal to 1, and RCOND = 1/180.

N IOPT RCOND

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

DET

AUX NAUX

Call Statement and Input

ΑP

```
CALL SPPICD(AP, 9, 3, RCOND, DET, AUX, 9)
AP
        2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0,
         3.0, 3.0, 3.0, 3.0, 3.0, 3.0, 3.0,
         4.0, 4.0, 4.0, 4.0, 4.0, 4.0,
         5.0, 5.0, 5.0, 5.0, 5.0,
         6.0, 6.0, 6.0, 6.0,
         7.0, 7.0, 7.0,
         8.0, 8.0,
         9.0)
Output
AΡ
        (2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
         2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0,
         2.0, -1.0, 0.0, 0.0, 0.0, 0.0, 0.0,
         2.0, -1.0, 0.0, 0.0, 0.0, 0.0,
         2.0, -1.0, 0.0, 0.0, 0.0,
         2.0, -1.0, 0.0, 0.0,
         2.0, -1.0, 0.0,
         2.0, -1.0,
         1.0)
        = 0.005556
RCOND
DET
        = (1.0, 0.0)
```

**Example 2:** This example uses SPPICD to compute the inverse of matrix  $\boldsymbol{A}$ , where iopt = 4, and matrix  $\boldsymbol{A}$  is the transformed matrix factored in "Example 1" on page 495 by SPPF.

**Note:** The AP arrays are formatted in a triangular arrangement for readability; however, they are stored in lower-packed storage mode.

Call Statement and Input

AP =(same as output AP in "Example 2" on page 496 for SPPF)

# Output

**Example 3:** This example uses SPOICD to compute the inverse, reciprocal of the condition number, and determinant of the same matrix **A** used in Example 1; however, matrix **A** is stored in upper storage mode in this example.

The values used to compute the reciprocal of the condition number in this example are obtained with the following values:

$$\|\mathbf{A}\|_{1} = \max(9.0, 17.0, 24.0, 30.0, 35.0, 39.0, 42.0, 44.0, 45.0) = 45.0$$
  
 $\|\mathbf{A}^{-1}\|_{1} = 4.0$ 

On output, the value in det, |A|, is equal to 1, and RCOND = 1/180.

### Call Statement and Input

RCOND = 0.005555556DET = (1.0, 0.0)

**Example 4:** This example uses SPOICD to compute the inverse of matrix  $\boldsymbol{A}$ , where iopt = 4, and matrix  $\boldsymbol{A}$  is the transformed matrix factored in "Example 1" on page 495 by SPOF.

Call Statement and Input

A =(same as output A in "Example 4" on page 497 for SPOF)

# STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV—Solution of a Triangular System of Equations with a Single Right-Hand Side

STRSV, DTRSV, STPSV, and DTPSV perform one of the following solves for a triangular system of equations with a single right-hand side, using the vector  $\mathbf{x}$  and triangular matrix  $\mathbf{A}$  or its transpose:

Solution	Equation	
1. $x \leftarrow A^{-1}x$	Ax = b	
2. $\mathbf{x} \leftarrow \mathbf{A}^{-T}\mathbf{x}$	$A^{T}x = b$	

CTRSV, ZTRSV, CTPSV, and ZTPSV perform one of the following solves for a triangular system of equations with a single right-hand side, using the vector  $\mathbf{x}$  and and triangular matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

Solution	Equation	
1. $x \leftarrow A^{-1}x$	Ax = b	
2. $\mathbf{x} \leftarrow \mathbf{A}^{-T}\mathbf{x}$	$A^{T}x = b$	
3. $\mathbf{x} \leftarrow \mathbf{A}^{-H}\mathbf{x}$	$A^{H}x = b$	

Matrix **A** can be either upper or lower triangular, where:

- For the \_TRSV subroutines, it is stored in upper- or lower-triangular storage mode, respectively.
- For the \_TPSV subroutines, it is stored in upper- or lower-triangular-packed storage mode, respectively.

**Note:** The term **b** used in the systems of equations listed above represents the right-hand side of the system. It is important to note that in these subroutines the right-hand side of the equation is actually provided in the input-output argument *x*.

Table 99. Data Types		
A, x	Subroutine	
Short-precision real	STRSV and STPSV	
Long-precision real	DTRSV and DTPSV	
Short-precision complex	CTRSV and CTPSV	
Long-precision complex	ZTRSV and ZTPSV	

### Syntax

Fortran	CALL STRSV   DTRSV   CTRSV   ZTRSV (uplo, transa, diag, n, a, lda, x, incx)	
	CALL STPSV   DTPSV   CTPSV   ZTPSV (uplo, transa, diag, n, ap, x, incx)	
C and C++	strsv   dtrsv   ctrsv   ztrsv (uplo, transa, diag, n, a, lda, x, incx);	
	stpsv   dtpsv   ctpsv   ztpsv (uplo, transa, diag, n, ap, x, incx);	
PL/I	CALL STRSV   DTRSV   CTRSV   ZTRSV (uplo, transa, diag, n, a, lda, x, incx);	
	CALL STPSV   DTPSV   CTPSV   ZTPSV (uplo, transa, diag, n, ap, x, incx);	

On Entry

# STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV

```
uplo
    indicates whether matrix A is an upper or lower triangular matrix, where:
    If uplo = 'U', A is an upper triangular matrix.
    If uplo = 'L', A is a lower triangular matrix.
    Specified as: a single character. It must be 'U' or 'L'.
transa
    indicates the form of matrix A used in the system of equations, where:
    If transa = 'N', A is used, resulting in solution 1.
    If transa = {}^{\mathsf{T}}\mathsf{T}, \mathbf{A}^{\mathsf{T}} is used, resulting in solution 2.
    If transa = 'C', AH is used, resulting in solution 3.
    Specified as: a single character. It must be 'N', 'T', or 'C'.
diag
    indicates the characteristics of the diagonal of matrix \boldsymbol{A}, where:
    If diag = 'U', A is a unit triangular matrix.
    If diag = 'N', A is not a unit triangular matrix.
    Specified as: a single character. It must be 'U' or 'N'.
n
    is the order of triangular matrix A. Specified as: a fullword integer; n \ge 0 and
    n \leq Ida.
а
    is the upper or lower triangular matrix \mathbf{A} of order n, stored in upper- or
    lower-triangular storage mode, respectively. Specified as: an Ida by (at least) n
    array, containing numbers of the data type indicated in Table 99 on page 526.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0 and Ida \ge n.
ap
    is the upper or lower triangular matrix \boldsymbol{A} of order n, stored in upper- or
    lower-triangular-packed storage mode, respectively. Specified as: a
    one-dimensional array of (at least) length n(n+1)/2, containing numbers of the
    data type indicated in Table 99 on page 526.
Х
    is the vector x of length n, containing the right-hand side of the triangular
    system to be solved. Specified as: a one-dimensional array of (at least) length
    1+(n-1)|incx|, containing numbers of the data type indicated in Table 99 on
    page 526.
incx
    is the stride for vector \mathbf{x}. Specified as: a fullword integer; incx > 0 or incx < 0.
On Return
Х
    is the solution vector \mathbf{x} of length \mathbf{n}, containing the results of the computation.
    Returned as: a one-dimensional array, containing numbers of the data type
```

# Notes

indicated in Table 99 on page 526.

1. These subroutines accept lowercase letters for the *uplo*, *transa*, and *diag* arguments.

- 2. For STRSV, DTRSV, STPSV, and DTPSV, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 3. Matrix **A** and vector **x** must have no common elements; otherwise, results are unpredictable.
- 4. ESSL assumes certain values in your array for parts of a triangular matrix. As a result, you do not have to set these values. For unit diagonal matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices. When using upper- or lower-triangular storage, the unreferenced elements in the lower and upper triangular part, respectively, are assumed to be zero.
- 5. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see "Triangular Matrix" on page 73.

**Function:** These subroutines solve a triangular system of equations with a single right-hand side. The solution x may be any of the following, where triangular matrix A, its transpose, or its conjugate transpose is used, and where A can be either upper- or lower-triangular:

```
1. \mathbf{x} \leftarrow \mathbf{A}^{-1}\mathbf{x}
```

2.  $\mathbf{X} \leftarrow \mathbf{A}^{-\mathsf{T}}\mathbf{X}$ 

3.  $x \leftarrow A^{-H}x$  (only for CTRSV, ZTRSV, CTPSV, and ZTPSV)

where:

x is a vector of length n.

**A** is an upper or lower triangular matrix of order *n*. For \_TRSV, it is stored in upper- or lower-triangular storage mode, respectively. For \_TPSV, it is stored in upper- or lower-triangular-packed storage mode, respectively.

If *n* is 0, no computation is performed. See references [32], [36], and [38].

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

```
1. uplo ≠ 'L' or 'U'
```

2. transa ≠ 'T', 'N', or 'C'

3. *diag* ≠ 'N' or 'U'

4. n < 0

5.  $Ida \leq 0$ 

6. Ida < n

7. incx = 0

**Example 1:** This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix A is a real 4 by 4 lower unit triangular matrix, stored in lower-triangular storage mode. Vector x is a vector of length 4.

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

$$A = \begin{bmatrix} . & . & . & . \\ 1.0 & . & . & . \\ 2.0 & 3.0 & . & . \\ 3.0 & 4.0 & 3.0 & . \end{bmatrix}$$

$$X = (1.0, 3.0, 11.0, 24.0)$$

Output

$$X = (1.0, 2.0, 3.0, 4.0)$$

**Example 2:** This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix A is a real 4 by 4 upper nonunit triangular matrix, stored in upper-triangular storage mode. Vector x is a vector of length 4.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 2.0 \\ . & 2.0 & 2.0 & 5.0 \\ . & . & 3.0 & 3.0 \\ . & . & . & 1.0 \end{bmatrix}$$

$$X = (5.0, 18.0, 32.0, 41.0)$$

Output

$$X = (5.0, 4.0, 3.0, 2.0)$$

**Example 3:** This example shows the solution  $x \leftarrow A^{-H}x$ . Matrix A is a complex 4 by 4 upper unit triangular matrix, stored in upper-triangular storage mode. Vector x is a vector of length 4.

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

# STRSV, DTRSV, CTRSV, ZTRSV, STPSV, DTPSV, CTPSV, and ZTPSV

CALL CTRSV('U', 'C', 'U', 4, A, 4, X, 1)

$$A = \begin{bmatrix} . & (2.0, 2.0) & (3.0, 3.0) & (2.0, 2.0) \\ . & . & (2.0, 2.0) & (5.0, 5.0) \\ . & . & (3.0, 3.0) \end{bmatrix}$$

$$X = ((5.0, 5.0), (24.0, 4.0), (49.0, 3.0), (80.0, 2.0))$$

Output
$$X = ((5.0, 5.0), (4.0, 4.0), (3.0, 3.0), (2.0, 2.0))$$

**Example 4:** This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix A is a real 4 by 4 lower unit triangular matrix, stored in lower-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

**Example 5:** This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix A is a real 4 by 4 upper nonunit triangular matrix, stored in upper-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

**Example 6:** This example shows the solution  $x \leftarrow A^{-H}x$ . Matrix A is a complex 4 by 4 upper unit triangular matrix, stored in upper-triangular-packed storage mode. Vector x is a vector of length 4. Matrix A is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of (1.0, 0.0) for the diagonal elements.

# STRSM, DTRSM, CTRSM, and ZTRSM—Solution of Triangular Systems of Equations with Multiple Right-Hand **Sides**

STRSM and DTRSM perform one of the following solves for a triangular system of equations with multiple right-hand sides, using scalar  $\alpha$ , rectangular matrix **B**, and triangular matrix A or its transpose:

Solution	Equation	
1. $\boldsymbol{B} \leftarrow \alpha(\boldsymbol{A}^{-1})\boldsymbol{B}$	$\mathbf{AX} = \alpha \mathbf{B}$	
2. $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-T})\mathbf{B}$	$\mathbf{A}^{T}\mathbf{X} = \alpha \mathbf{B}$	
3. $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$	$XA = \alpha B$	
4. $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-T})$	$\mathbf{X}\mathbf{A}^{T} = \alpha \mathbf{B}$	

CTRSM and ZTRSM perform one of the following solves for a triangular system of equations with multiple right-hand sides, using scalar  $\alpha$ , rectangular matrix **B**, and triangular matrix **A**, its transpose, or its conjugate transpose:

Solution	Equation	
1. $\boldsymbol{B} \leftarrow \alpha(\boldsymbol{A}^{-1})\boldsymbol{B}$	$\mathbf{AX} = \alpha \mathbf{B}$	
2. $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-T})\mathbf{B}$	$\mathbf{A}^{T}\mathbf{X} = \alpha \mathbf{B}$	
3. $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$	$XA = \alpha B$	
4. $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-T})$	$XA^{T} = \alpha B$	
5. $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-H})\mathbf{B}$	$\mathbf{A}^{H}\mathbf{X} = \alpha \mathbf{B}$	
6. $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-H})$	$XAH = \alpha B$	

**Note:** The term **X** used in the systems of equations listed above represents the output solution matrix. It is important to note that in these subroutines the solution matrix is actually returned in the input-output argument b.

Table 100. Data Types			
<b>Α</b> , <b>Β</b> , α	Subroutine		
Short-precision real	STRSM		
Long-precision real	DTRSM		
Short-precision complex	CTRSM		
Long-precision complex	ZTRSM		

# Syntax

Fortran	CALL STRSM   DTRSM   CTRSM   ZTRSM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb)	
C and C++	strsm   dtrsm   ctrsm   ztrsm (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb);	
PL/I	CALL STRSM   DTRSM   CTRSM   ZTRSM (side, uplo, transa, diag, m, n, alpha, a, lda, b, ldb);	

On Entry

side

indicates whether the triangular matrix A is located to the left or right of rectangular matrix **B** in the system of equations, where:

If side = L', **A** is to the left of **B**, resulting in solution 1, 2, or 5.

If side = 'R', **A** is to the right of **B**, resulting in solution 3, 4, or 6.

```
Specified as: a single character. It must be 'L' or 'R'.
uplo
    indicates whether matrix A is an upper or lower triangular matrix, where:
    If uplo = 'U', A is an upper triangular matrix.
    If uplo = 'L', A is a lower triangular matrix.
    Specified as: a single character. It must be 'U' or 'L'.
transa
    indicates the form of matrix A used in the system of equations, where:
    If transa = 'N', A is used, resulting in solution 1 or 3.
    If transa = {}^{\mathsf{T}}\mathsf{T}, A^{\mathsf{T}} is used, resulting in solution 2 or 4.
    If transa = 'C', A^H is used, resulting in solution 5 or 6.
    Specified as: a single character. It must be 'N', 'T', or 'C'.
diag
    indicates the characteristics of the diagonal of matrix A, where:
    If diag = 'U', A is a unit triangular matrix.
    If diag = 'N', A is not a unit triangular matrix.
    Specified as: a single character. It must be 'U' or 'N'.
m
    is the number of rows in rectangular matrix B, and:
    If side = 'L', m is the order of triangular matrix A.
    Specified as: a fullword integer, where:
    If side = L', 0 \le m \le Ida and m \le Idb.
    If side = {}^{\shortmid}R{}^{\shortmid}, 0 \le m \le ldb.
n
    is the number of columns in rectangular matrix B, and:
    If side = 'R', n is the order of triangular matrix A.
    Specified as: a fullword integer; n \ge 0, and:
    If side = 'R', n \le Ida.
alpha
    is the scalar \alpha. Specified as: a number of the data type indicated in Table 100
    on page 532.
    is the triangular matrix A, of which only the upper or lower triangular portion is
    used, where:
    If side = 'L', A is order m.
    If side = 'R', A is order n.
    Specified as: a two-dimensional array, containing numbers of the data type
    indicated in Table 100 on page 532, where:
    If side = L', its size must be Ida by (at least) m.
    If side = 'R', it size must be Ida by (at least) n.
lda
    is the leading dimension of the array specified for a. Specified as: a fullword
    integer; Ida > 0, and:
```

```
If side = ^{\mathsf{L}}\mathsf{L}^{\mathsf{L}}, Ida \ge m.

If side = ^{\mathsf{L}}\mathsf{R}^{\mathsf{L}}, Ida \ge n.
```

b

is the m by n rectangular matrix  $\mathbf{B}$ , which contains the right-hand sides of the triangular system to be solved. Specified as: an ldb by (at least) n array, containing numbers of the data type indicated in Table 100 on page 532.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge m$ .

#### On Return

h

is the m by n matrix  $\boldsymbol{B}$ , containing the results of the computation.

Returned as: an *ldb* by (at least) *n* array, containing numbers of the data type indicated in Table 100 on page 532.

#### Notes

- 1. These subroutines accept lowercase letters for the *transa*, *side*, *diag*, and *uplo* arguments.
- 2. For STRSM and DTRSM, if you specify 'C' for the *transa* argument, it is interpreted as though you specified 'T'.
- 3. Matrices A and B must have no common elements or results are unpredictable.
- 4. If matrix **A** is upper triangular (*uplo* = 'U'), these subroutines refer to only the upper triangular portion of the matrix. If matrix **A** is lower triangular, (*uplo* = 'L'), these subroutines refer to only the lower triangular portion of the matrix. The unreferenced elements are assumed to be zero.
- The elements of the diagonal of a unit triangular matrix are always one, so you do not need to set these values. The ESSL subroutines always assume that the values in these positions are 1.0 for STRSM and DTRSM and (1.0, 0.0) for CTRSM and ZTRSM.
- 6. For a description of triangular matrices and how they are stored, see "Triangular Matrix" on page 73.

**Function:** These subroutines solve a triangular system of equations with multiple right-hand sides. The solution **B** may be any of the following, where **A** is a triangular matrix and **B** is a rectangular matrix:

```
1. \mathbf{B} \leftarrow \alpha(\mathbf{A}^{-1})\mathbf{B}
```

2.  $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-\mathsf{T}})\mathbf{B}$ 

3.  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$ 

4.  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-\mathsf{T}})$ 

5.  $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-H})\mathbf{B}$  (only for CTRSM and ZTRSM)

6.  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-H})$  (only for CTRSM and ZTRSM)

# where:

 $\alpha$  is a scalar.

**B** is an *m* by *n* rectangular matrix.

A is an upper or lower triangular matrix, where:

If side = L', it has order m, and equation 1, 2, or 5 is performed.

If side = 'R', it has order n, and equation 3, 4, or 6 is performed.

If *n* or *m* is 0, no computation is performed. See references [32] and [36].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

**Note:** If the triangular matrix **A** is singular, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

# Input-Argument Errors

- 1. m < 0
- 2. n < 0
- 3. Ida,  $Idb \leq 0$
- 4. *side* ≠ 'L' or 'R'
- 5. *uplo* ≠ 'L' or 'U'
- 6. transa ≠ 'T', 'N', or 'C'
- 7. *diag* ≠ 'N' or 'U'
- 8. side = 'L' and m > Ida
- 9. m > ldb
- 10. side = 'R' and n > Ida

**Example 1:** This example shows the solution  $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-1})\mathbf{B}$ , where  $\mathbf{A}$  is a real 5 by 5 upper triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a real 5 by 3 rectangular matrix.

Call Statement and Input

$$B = \begin{bmatrix} 6.0 & 10.0 & -2.0 \\ -16.0 & -1.0 & 6.0 \\ -2.0 & 1.0 & -4.0 \\ 14.0 & 0.0 & -14.0 \\ -1.0 & 2.0 & 1.0 \\ & & & & \end{bmatrix}$$

$$B = \begin{bmatrix} 2.0 & 3.0 & 1.0 \\ 5.0 & 5.0 & 4.0 \\ 0.0 & 1.0 & 2.0 \\ 3.0 & 1.0 & -3.0 \\ -1.0 & 2.0 & 1.0 \\ & & & & & & \end{bmatrix}$$

**Example 2:** This example shows the solution  $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-\mathsf{T}})\mathbf{B}$ , where  $\mathbf{A}$  is a real 5 by 5 upper triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a real 5 by 4 rectangular matrix.

# Call Statement and Input

$$A = \begin{bmatrix} -1.0 & -4.0 & -2.0 & 2.0 & 3.0 \\ . & -2.0 & 2.0 & 2.0 & 2.0 \\ . & . & -3.0 & -1.0 & 4.0 \\ . & . & . & 1.0 & 0.0 \\ . & . & . & . & -2.0 \\ . & . & . & . & . & . \end{bmatrix}$$

# Output

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 & 4.0 \\ 3.0 & 3.0 & -1.0 & 2.0 \\ -2.0 & -1.0 & 0.0 & 1.0 \\ 4.0 & 4.0 & -3.0 & -3.0 \\ 2.0 & 2.0 & 2.0 & 2.0 \\ & & & & & & & & \\ \end{bmatrix}$$

**Example 3:** This example shows the solution  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$ , where  $\mathbf{A}$  is a real 5 by 5 lower triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a real 3 by 5 rectangular matrix.

$$A = \begin{bmatrix} 2.0 & . & . & . & . \\ 2.0 & 3.0 & . & . & . \\ 2.0 & 1.0 & 1.0 & . & . \\ 0.0 & 3.0 & 0.0 & -2.0 & . \\ 2.0 & 4.0 & -1.0 & 2.0 & -1.0 \\ . & . & . & . & . \end{bmatrix}$$

$$B = \begin{bmatrix} 10.0 & 4.0 & 0.0 & 0.0 & 1.0 \\ 10.0 & 14.0 & -4.0 & 6.0 & -3.0 \\ -8.0 & 2.0 & -5.0 & 4.0 & -2.0 \\ & & & & & & & & \end{bmatrix}$$

Output

$$B = \begin{bmatrix} 3.0 & 4.0 & -1.0 & -1.0 & -1.0 \\ 2.0 & 1.0 & -1.0 & 0.0 & 3.0 \\ -2.0 & -1.0 & -3.0 & 0.0 & 2.0 \\ & & & & & & & & \end{bmatrix}$$

**Example 4:** This example shows the solution  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$ , where  $\mathbf{A}$  is a real 6 by 6 upper triangular matrix that is unit triangular, and  $\mathbf{B}$  is a real 1 by 6 rectangular matrix.

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal element.

Call Statement and Input

$$B = \begin{bmatrix} 1.0 & 4.0 & -2.0 & 10.0 & 2.0 & -6.0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 1.0 & 3.0 & -1.0 & -2.0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \end{bmatrix}$$

**Example 5:** This example shows the solution  $\mathbf{B} \leftarrow \alpha \mathbf{B}(\mathbf{A}^{-1})$ , where  $\mathbf{A}$  is a complex 5 by 5 lower triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a complex 3 by 5 rectangular matrix.

Call Statement and Input

$$ALPHA = (1.0, 0.0)$$

Output

**Example 6:** This example shows the solution  $\mathbf{B} \leftarrow \alpha(\mathbf{A}^{-H})\mathbf{B}$ , where  $\mathbf{A}$  is a complex 5 by 5 upper triangular matrix that is not unit triangular, and  $\mathbf{B}$  is a complex 5 by 1 rectangular matrix.

$$ALPHA = (1.0, 0.0)$$

$$A = \begin{bmatrix} (-4.0, 1.0) & (4.0, -3.0) & (-1.0, 3.0) & (0.0, 0.0) & (-1.0, 0.0) \\ & & (-2.0, 0.0) & (-3.0, -1.0) & (-2.0, -1.0) & (4.0, 3.0) \\ & & & & (-5.0, 3.0) & (-3.0, -3.0) & (-5.0, -5.0) \\ & & & & & & (4.0, -4.0) & (2.0, 0.0) \\ & & & & & & & & (2.0, -1.0) \end{bmatrix}$$

$$B = \begin{bmatrix} (-8.0, -19.0) \\ (8.0, 21.0) \\ (44.0, -8.0) \\ (13.0, -7.0) \\ (19.0, 2.0) \\ & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} (3.0, 4.0) \\ (-4.0, 2.0) \\ (-5.0, 0.0) \\ (1.0, 3.0) \\ (3.0, 1.0) \end{bmatrix}$$

## STRI, DTRI, STPI, and DTPI—Triangular Matrix Inverse

These subroutines find the inverse of triangular matrix A:

 $\mathbf{A} \leftarrow \mathbf{A}^{-1}$ 

Matrix **A** can be either upper or lower triangular, where:

- For the \_TRI subroutines, it is stored in upper- or lower-triangular storage mode, respectively.
- For the \_TPI subroutines, it is stored in upper- or lower-triangular-packed storage mode, respectively.

Table 101. Data Types	
Α	Subroutine
Short-precision real	STRI and STPI
Long-precision real	DTRI and DTPI

## **Syntax**

Fortran	CALL STRI   DTRI (uplo, diag, a, lda, n)
	CALL STPI   DTPI ( <i>uplo</i> , <i>diag</i> , <i>ap</i> , <i>n</i> )
C and C++	stri   dtri (uplo, diag, a, lda, n);
	stpi   dtpi ( <i>uplo</i> , <i>diag</i> , <i>ap</i> , <i>n</i> );
PL/I	CALL STRI   DTRI (uplo, diag, a, lda, n);
	CALL STPI   DTPI (uplo, diag, ap, n);

On Entry

uplo

indicates whether matrix **A** is an upper or lower triangular matrix, where:

If uplo = 'U', **A** is an upper triangular matrix.

If uplo = 'L', **A** is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

diag

indicates the characteristics of the diagonal of matrix **A**, where:

If diag = 'U', **A** is a unit triangular matrix.

If diag = 'N', **A** is not a unit triangular matrix.

Specified as: a single character. It must be 'U' or 'N'.

а

is the upper or lower triangular matrix  $\mathbf{A}$  of order n, stored in upper- or lower-triangular storage mode, respectively. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 101.

lda

is the leading dimension of the arrays specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

ар

is the upper or lower triangular matrix  $\mathbf{A}$  of order n, stored in upper- or lower-triangular-packed storage mode, respectively. Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 101.

n

is the order of matrix **A**. Specified as: a fullword integer;  $n \ge 0$ , where:

#### On Return

а

is the inverse of the upper or lower triangular matrix  $\mathbf{A}$  of order n, stored in upper- or lower-triangular storage mode, respectively. Returned as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 101 on page 540.

ap

is the inverse of the upper or lower triangular matrix  $\mathbf{A}$  of order n, stored in upper- or lower-triangular-packed storage mode, respectively. Returned as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 101 on page 540.

#### Notes

- 1. These subroutines accept lowercase letters for the *uplo* and *diag* arguments.
- 2. If matrix **A** is upper triangular (*uplo* = 'U'), these subroutines refer to only the upper triangular portion of the matrix. If matrix **A** is lower triangular, (*uplo* = 'L'), these subroutines refer to only the lower triangular portion of the matrix. The unreferenced elements are assumed to be zero.
- 3. The elements of the diagonal of a unit triangular matrix are always one, so you do not need to set these values.
- 4. For a description of triangular matrices and how they are stored in upper- and lower-triangular storage mode and in upper- and lower-triangular-packed storage mode, see "Triangular Matrix" on page 73.

**Function:** These subroutines find the inverse of triangular matrix A, where A is either upper or lower triangular:

$$A \leftarrow A^{-1}$$

where:

**A** is the triangular matrix of order *n*.

 $A^{-1}$  the inverse of the triangular matrix of order n.

If *n* is 0, no computation is performed. See references [8] and [36].

## **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: Matrix **A** is singular.

- One or more of the diagonal elements of matrix A are zero. The first column, i, of matrix A, in which a zero diagonal element is found, is identified in the computational error message.
- The return code is set to 1.

• i can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2145 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

## Input-Argument Errors

- 1. *uplo* ≠ 'U' or 'L'
- 2. *diag* ≠ 'U' or 'N'
- 3. n < 0
- $4. Ida \leq 0$
- 5. Ida < n

**Example 1:** This example shows how the inverse of matrix **A** is computed, where **A** is a 5 by 5 upper triangular matrix that is not unit triangular and is stored in upper-triangular storage mode. Matrix **A** is:

and where the following inverse matrix is computed. Matrix A-1 is:

## Call Statement and Input

$$A = \begin{bmatrix} 1.00 & 3.00 & 4.00 & 5.00 & 6.00 \\ . & 2.00 & 8.00 & 9.00 & 1.00 \\ . & . & 4.00 & 8.00 & 4.00 \\ . & . & . & -2.00 & 6.00 \\ . & . & . & . & -1.00 \end{bmatrix}$$

$$A = \begin{bmatrix} 1.00 & -1.50 & 2.00 & 3.75 & 35.00 \\ . & 0.50 & -1.00 & -1.75 & -14.00 \\ . & . & 0.25 & 1.00 & 7.00 \\ . & . & . & -0.50 & -3.00 \\ . & . & . & . & . & -1.00 \end{bmatrix}$$

Example 2: This example shows how the inverse of matrix A is computed, where A is a 5 by 5 lower triangular matrix that is unit triangular and is stored in lower-triangular storage mode. Matrix A is:

and where the following inverse matrix is computed. Matrix A-1 is:

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

$$A = \begin{bmatrix} . & . & . & . & . \\ 3.0 & . & . & . & . \\ 4.0 & 8.0 & . & . & . \\ 5.0 & 9.0 & 8.0 & . & . \\ 6.0 & 1.0 & 4.0 & 6.0 & . \end{bmatrix}$$

Output

$$A = \begin{bmatrix} . & . & . & . & . \\ -3.0 & . & . & . & . \\ 20.0 & -8.0 & . & . & . \\ -138.0 & 55.0 & -8.0 & . & . \\ 745.0 & -299.0 & 44.0 & -6.0 & . \end{bmatrix}$$

**Example 3:** This example shows how the inverse of matrix **A** is computed, where A is the same matrix shown in Example 1 and is stored in upper-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in Example 1 and is stored in upper-triangular-packed storage mode.

Call Statement and Input

**Example 4:** This example shows how the inverse of matrix **A** is computed, where **A** is the same matrix shown in Example 2 and is stored in lower-triangular-packed storage mode. The inverse matrix computed here is the same as the inverse matrix shown in Example 2 and is stored in lower-triangular-packed storage mode.

**Note:** Because matrix **A** is unit triangular, the diagonal elements are not referenced. ESSL assumes a value of 1.0 for the diagonal elements.

Call Statement and Input

## **Banded Linear Algebraic Equation Subroutines**

This section contains the banded linear algebraic equation subroutine descriptions.

## SGBF and DGBF—General Band Matrix Factorization

These subroutines factor general band matrix **A**, stored in general-band storage mode, using Gaussian elimination. To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGBS or DGBS, respectively.

Table 102. Data Types	
Α	Subroutine
Short-precision real	SGBF
Long-precision real	DGBF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SGBS and DGBS, respectively.

## Syntax

Fortran	CALL SGBF   DGBF (agb, lda, n, ml, mu, ipvt)
C and C++	sgbf   dgbf (agb, lda, n, ml, mu, ipvt);
PL/I	CALL SGBF   DGBF (agb, lda, n, ml, mu, ipvt);

## On Entry

agb

is the general band matrix A of order n, stored in general-band storage mode, to be factored. It has an upper band width mu and a lower band width ml. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 102, where  $lda \ge 2ml+mu+16$ .

lda

is the leading dimension of the array specified for agb. Specified as: a fullword integer; Ida > 0 and  $Ida \ge 2mI+mu+16$ .

is the order of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer; n > ml and n > mu.

ml

is the lower band width ml of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer;  $0 \le ml < n$ .

mu

is the upper band width mu of the matrix **A**. Specified as: a fullword integer;  $0 \le mu < n$ .

ipvt

See "On Return."

#### On Return

agb

is the transformed matrix  $\mathbf{A}$  of order n, containing the results of the factorization. See "Function" on page 547. Returned as: an lda by (at least) n array, containing numbers of the data type indicated in Table 102.

ipvt

is the integer vector ipvt of length n, containing the pivot information necessary to construct matrix L from the information contained in the output array agb.

Returned as: a one-dimensional array of (at least) length *n*, containing fullword integers.

#### **Notes**

- 1. *ipvt* is not a permutation vector in the strict sense. It is used to record column interchanges in *L* due to partial pivoting and to improve performance.
- 2. The entire *Ida* by *n* array specified for *agb* must remain unchanged between calls to the factorization and solve subroutines.
- 3. This subroutine can be used for tridiagonal matrices (ml = mu = 1); however, the tridiagonal subroutines SGTF/DGTF and SGTS/DGTS are faster.
- 4. For a description of how a general band matrix is stored in general-band storage mode in an array, see "General Band Matrix" on page 76.

**Function:** The general band matrix **A**, stored in general-band storage mode, is factored using Gaussian elimination with partial pivoting to compute the **LU** factorization of **A**, where:

*ipvt* is a vector containing the pivoting information.

L is a unit lower triangular band matrix.

*U* is an upper triangular band matrix.

The transformed matrix  $\mathbf{A}$  contains  $\mathbf{U}$  in packed format, along with the multipliers necessary to construct, with the help of  $\mathbf{ipvt}$ , a matrix  $\mathbf{L}$ , such that  $\mathbf{A} = \mathbf{LU}$ . This factorization can then be used by SGBS or DGBS, respectively, to solve the system of equations. See reference [38].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: Matrix A is singular.

- One or more columns of L and the corresponding diagonal of U contain all zeros (all columns of L are checked). The last column, i, of L with a corresponding U = 0 diagonal element is identified in the computational error message.
- The return code is set to 1.
- *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2103 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

### Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. ml < 0
- 3.  $ml \ge n$
- 4. mu < 0
- 5.  $mu \ge n$
- 6. Ida < 2mI + mu + 16

**Example:** This example shows a factorization of a general band matrix **A** of order 9, with a lower band width of 2 and an upper band width of 3. On input matrix **A** is:

```
1.0
     1.0
           1.0
                 1.0
                       0.0
                             0.0
                                    0.0
                                           0.0
                                                  0.0
                                           0.0
                                                  0.0
1.0
     1.0
           1.0
                 1.0
                       1.0
                             0.0
                                    0.0
4.0
     1.0
           1.0
                 1.0
                       1.0
                             1.0
                                    0.0
                                           0.0
                                                 0.0
     5.0
           1.0
                                          0.0
0.0
                 1.0
                       1.0
                             1.0
                                    1.0
                                                  0.0
0.0
     0.0
           6.0
                 1.0
                       1.0
                             1.0
                                    1.0
                                           1.0
                                                  0.0
0.0
     0.0
           0.0
                 7.0
                       1.0
                             1.0
                                    1.0
                                           1.0
                                                  1.0
0.0
     0.0
           0.0
                 0.0
                       8.0
                            1.0
                                    1.0
                                           1.0
                                                  1.0
0.0
     0.0
           0.0
                 0.0
                            9.0
                                    1.0
                                          1.0
                                                 1.0
                       0.0
0.0
     0.0
           0.0
                 0.0
                       0.0
                            0.0
                                  10.0
                                         11.0
                                                12.0
```

Matrix  $\bf A$  is stored in general-band storage mode in the two-dimensional array AGB of size LDA by N, where LDA = 2ml+mu+16 = 23. The array AGB is declared as AGB(1:23,1:9).

**Note:** Matrix **A** is the same matrix used in the examples in subroutines SGEF and DGEF (see "Example 1" on page 467) and SGEFCD and DGEFCD (see "Example" on page 490).

Call Statement and Input

```
0.0000
                   0.0000
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                                                                0.0000
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                                                                1.0000
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                                                                                    1.0000
           0.0000
                   0.0000
                            1.0000
                                     1.0000
                                              1.0000
                                                      1.0000
                                                                1.0000
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           0.0000
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                            1.0000
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                                                      1.0000
                                                                1.0000
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                                                                                    1.0000
           1.0000
                   1.0000
                            1.0000
                                     1.0000
                                              1.0000
                                                      1.0000
                                                                1.0000
                                                                          1.0000
                                                                                   12.0000
                   1.0000
                            1.0000
                                     1.0000
                                              1.0000
                                                      1.0000
                                                                         11.0000
           1.0000
                                                                1.0000
                                                                                    0.0000
           4.0000
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                                                               10.0000
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```

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                                                                                    12.0000
          0.0000
                   1.0000
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                                                                  1.0000
                                                                           11.0000
                                                                                     0.3111
                                    1.0000
          0.2500
                   0.2000
                            0.1600
                                    0.1400
                                              0.1250
                                                        0.1100
                                                                  0.1000
                                                                            5.5380
                                                                                    -325.00
          0.0000
                   0.1500
                            0.0000
                                    0.0714
                                              0.0000
                                                       -0.0556
                                                                 -0.0306
                                                                            0.9385
                                                                                     0.0000
          0.2500
                   0.1500
                            0.1000
                                    0.0714
                                             -0.0714
                                                       -0.0694
                                                                 -0.0194
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                            0.1000
          0.2500
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                                    0.0000
                                              0.0536
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          0.0000
                   0.0000
                            0.0000
                                    0.0000
                                              0.0000
                                                        0.0000
                                                                  0.0000
                                                                                      0.0000
```

IPVT = (2, -65534, -131070, -196606, -262142, -327678, -327678, -327680, -327680)

## SGBS and DGBS—General Band Matrix Solve

These subroutines solve the system Ax = b for x, where A is a general band matrix, and x and b are vectors. They use the results of the factorization of matrix A, produced by a preceding call to SGBF or DGBF, respectively.

Table 103. Data Types	
A, b, x	Subroutine
Short-precision real	SGBS
Long-precision real	DGBS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGBF and DGBF, respectively.

## **Syntax**

Fortran	CALL SGBS   DGBS (agb, Ida, n, ml, mu, ipvt, bx)
C and C++	sgbs   dgbs (agb, lda, n, ml, mu, ipvt, bx);
PL/I	CALL SGBS   DGBS (agb, lda, n, ml, mu, ipvt, bx);

On Entry

agb

is the factorization of general band matrix A, produced by a preceding call to SGBF or DGBF. Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 103, where  $Ida \ge 2mI + mu + 16$ .

lda

is the leading dimension of the array specified for *agb*. Specified as: a fullword integer; Ida > 0 and  $Ida \ge 2mI + mu + 16$ .

n

is the order of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer; n > ml and n > mu.

ml

is the lower band width ml of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer;  $0 \le ml < n$ .

mu

is the upper band width mu of the matrix **A**. Specified as: a fullword integer;  $0 \le mu < n$ .

ipvt

is the integer vector *ipvt* of length *n*, produced by a preceding call to SGBF or DGBF. It contains the pivot information necessary to construct matrix *L* from the information contained in the array specified for *agb*.

Specified as: a one-dimensional array of (at least) length n, containing fullword integers.

bx

is the vector  $\mathbf{b}$  of length n, containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 103.

On Return

hх

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 103.

#### Notes

- 1. The scalar data specified for input arguments *Ida*, *n*, *mI*, and *mu* for these subroutines must be the same as that specified for SGBF and DGBF, respectively.
- 2. The array data specified for input arguments *agb* and *ipvt* for these subroutines must be the same as the corresponding output arguments for SGBF and DGBF, respectively.
- 3. The entire *Ida* by *n* array specified for *agb* must remain unchanged between calls to the factorization and solve subroutines.
- 4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 5. This subroutine can be used for tridiagonal matrices (ml = mu = 1); however, the tridiagonal subroutines, SGTF/DGTF and SGTS/DGTS, are faster.
- 6. For a description of how a general band matrix is stored in general-band storage mode in an array, see "General Band Matrix" on page 76.

**Function:** The real system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  is solved for  $\mathbf{x}$ , where  $\mathbf{A}$  is a real general band matrix, stored in general-band storage mode, and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. These subroutines use the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to SGBF or DGBF, respectively. The transformed matrix  $\mathbf{A}$ , used by this computation, consists of the upper triangular matrix  $\mathbf{U}$  and the multipliers necessary to construct  $\mathbf{L}$  using  $\mathbf{i}\mathbf{p}\mathbf{v}\mathbf{t}$ , as defined in "Function" on page 547. See reference [38].

### **Error Conditions**

## Computational Errors

**Note:** If the factorization performed by SGBF or DGBF failed due to a singular matrix argument, the results returned by this subroutine are unpredictable, and there may be a divide-by-zero program exception message.

### Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. mI < 0
- 3.  $ml \ge n$
- 4. mu < 0
- 5.  $mu \ge n$
- 6. Ida < 2mI + mu + 16

**Example:** This example shows how to solve the system Ax = b, where general band matrix A is the same matrix factored in "Example" on page 548 for SGBF and DGBF. The input for AGB and IPVT in this example is the same as the output for that example.

Call Statement and Input

AGB LDA N ML MU IPVT ВХ CALL SGBS ( AGB , 23 , 9 , 2 , 3 , IPVT , BX )  ${\tt IPVT}$ = (2, -65534, -131070, -196606, -262142, -327678, -327678, -327680, -327680) ВХ = (4.0000, 5.0000, 9.0000, 10.0000, 11.0000, 12.0000, 12.0000, 12.0000, 33.0000) AGB = (same as output AGB in "Example" on page 548) Output ВХ = (1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 1.0000, 0.9999, 1.0001)

# SPBF, DPBF, SPBCHF, and DPBCHF—Positive Definite Symmetric Band Matrix Factorization

These subroutines factor positive definite symmetric band matrix **A**, stored in lower-band-packed storage mode, using:

- · Gaussian elimination for SPBF and DPBF
- · Cholesky factorization for SPBCHF and DPBCHF

To solve the system of equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPBS, DPBS, SPBCHS, or DPBCHS, respectively.

Table 104. Data Types	
Α	Subroutine
Short-precision real	SPBF and SPBCHF
Long-precision real	DPBF and DPBCHF

#### Notes:

- 1. The output from these factorization subroutines should be used only as input to the solve subroutines SPBS, DPBS, SPBCHS, and DPBCHS, respectively.
- 2. For optimal performance:
  - For wide band widths, use \_PBCHF.
  - For narrow band widths, use either \_PBF or \_PBCHF.
  - · For very narrow band widths:
    - Use either SPBF or SPBCHF.
    - Use DPBF.

## Syntax

Fortran	CALL SPBF   DPBF   SPBCHF   DPBCHF (apb, Ida, n, m)
C and C++	spbf   dpbf   spbchf   dpbchf (apb, lda, n, m);
PL/I	CALL SPBF   DPBF   SPBCHF   DPBCHF (apb, Ida, n, m);

On Entry

apb

is the positive definite symmetric band matrix **A** of order *n*, stored in lower-band-packed storage mode, to be factored. It has a half band width of *m*. Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 104. See "Notes" on page 554.

lda

n

m

is the leading dimension of the array specified for *apb*. Specified as: a fullword integer; Ida > 0 and Ida > m.

is the order n of matrix **A**. Specified as: a fullword integer; n > m.

is the half band width of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer;  $0 \le m < n$ .

On Return

apb

is the transformed matrix **A** of order *n*, containing the results of the factorization. See "Function" on page 554. Returned as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 104. For further details, see "Notes" on page 554.

#### **Notes**

- 1. These subroutines can be used for tridiagonal matrices (m = 1); however, the tridiagonal subroutines, SPTF/DPTF and SPTS/DPTS, are faster.
- 2. For SPBF and DPBF when m > 0, location APB(2,n) is sometimes set to 0.
- 3. For a description of how a positive definite symmetric band matrix is stored in lower-band-packed storage mode in an array, see "Positive Definite Symmetric Band Matrix" on page 85.

**Function:** The positive definite symmetric band matrix **A**, stored in lower-band-packed storage mode, is factored using Gaussian elimination in SPBF and DPBF and Cholesky factorization in SPBCHF and DPBCHF. The transformed matrix **A** contains the results of the factorization in packed format. This factorization can then be used by SPBS, DPBS, SPBCHS, and DPBCHS, respectively, to solve the system of equations.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DPBF works properly, when processing narrow band widths; therefore, you may want to scale your problem.

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

#### Computational Errors

- 1. Matrix **A** is not positive definite (for SPBF and DPBF).
  - One or more elements of *D* contain values less than or equal to 0; all elements of *D* are checked. The index *i* of the last nonpositive element encountered is identified in the computational error message.
  - The return code is set to 1.
  - i can be determined at run time by use of the ESSL error-handling facilities.
    To obtain this information, you must use ERRSET to change the number of
    allowable errors for error code 2104 in the ESSL error option table;
    otherwise, the default value causes your program to terminate when this
    error occurs. For details, see Chapter 4 on page 111.
- 2. Matrix **A** is not positive definite (for SPBCHF and DPBCHF).
  - The leading minor of order *i* has a nonpositive determinant. The order *i* is identified in the computational error message.
  - The return code is set to 1.
  - *i* can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to be terminate when this error occurs. For details, see Chapter 4 on page 111.

Input-Argument Errors

- 1. Ida ≤ 0
- 2. m < 0
- $3.\ m \ge n$
- 4. *m* ≥ *lda*

**Example 1:** This example shows a factorization of a real positive definite symmetric band matrix **A** of order 9, using Gaussian elimination, where on input, matrix **A** is:

and on output, matrix A is:

where array location APB(2,9) is set to 0.0.

Call Statement and Input

Example 2: This example shows a Cholesky factorization of the same matrix used in Example 1.

Call Statement and Input

# SPBS, DPBS, SPBCHS, and DPBCHS—Positive Definite Symmetric Band Matrix Solve

These subroutines solve the system Ax = b for x, where A is a positive definite symmetric band matrix, and x and b are vectors. They use the results of the factorization of matrix A, produced by a preceding call to SPBF, DPBF, SPBCHF, and DPBCHF, respectively, where:

- · Gaussian elimination was used by SPBF and DPBF.
- Cholesky factorization was used by SPBCHF and DPBCHF.

Table 105. Data Types	
A, b, x	Subroutine
Short-precision real	SPBS and SPBCHS
Long-precision real	DPBS and DPBCHS

### Notes:

- 1. The input to these solve subroutines must be the output from the factorization subroutines SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
- 2. For performance tradeoffs, see "SPBF, DPBF, SPBCHF, and DPBCHF—Positive Definite Symmetric Band Matrix Factorization" on page 553.

## Syntax

Fortran	CALL SPBS   DPBS   SPBCHS   DPBCHS (apb, Ida, n, m, bx)	
C and C++	spbs   dpbs   spbchs   dpbchs (apb, Ida, n, m, bx);	
PL/I	CALL SPBS   DPBS   SPBCHS   DPBCHS (apb, Ida, n, m, bx);	

## On Entry

apb

is the factorization of matrix A, produced by a preceding call to SPBF or DPBF. Specified as: an *Ida* by (at least) n array, containing numbers of the data type indicated in Table 105. See "Notes" on page 558.

lda

is the leading dimension of the array specified for apb. Specified as: a fullword integer; Ida > 0 and Ida > m.

*n* is the order *n* of matrix **A**. Specified as: a fullword integer; n > m.

m

is the half band width of the matrix  $\boldsymbol{A}$ . Specified as: a fullword integer;  $0 \le m < n$ .

bx

is the vector  $\boldsymbol{b}$  of length n, containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 105.

## On Return

bх

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 105.

#### **Notes**

- 1. The scalar data specified for input arguments *Ida*, *n*, and *m* for these subroutines must be the same as that specified for SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
- The array data specified for input argument apb for these subroutines must be the same as the corresponding output argument for SPBF, DPBF, SPBCHF, and DPBCHF, respectively.
- 3. These subroutines can be used for tridiagonal matrices (m = 1); however, the tridiagonal subroutines, SPTF/DPTF and SPTS/DPTS, are faster.
- 4. The vectors and matrices used in this computation must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- For a description of how a positive definite symmetric band matrix is stored in lower-band-packed storage mode in an array, see "Positive Definite Symmetric Band Matrix" on page 85.

**Function:** The system Ax = b is solved for x, where A is a positive definite symmetric band matrix, stored in lower-band-packed storage mode, and x and b are vectors. These subroutines use the results of the factorization of matrix A, produced by a preceding call to SPBF, DPBF, SPBCHF, or DPBCHF, respectively.

## **Error Conditions**

Computational Errors: None

**Note:** If the factorization subroutine resulted in a nonpositive definite matrix, error 2104 for SPBF and DPBF or error 2115 for SPBCHF and DPBCHF, results of these subroutines may be unpredictable.

Input-Argument Errors

- 1.  $Ida \leq 0$
- 2. m < 0
- 3.  $m \ge n$
- 4. *m* ≥ *lda*

**Example 1:** This example shows how to solve the system Ax = b, where matrix A is the same matrix factored in the "Example 1" on page 555 for SPBF and DPBF, using Gaussian elimination.

Call Statement and Input

This example shows how to solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ , where matrix  $\mathbf{A}$  is the same matrix factored in the "Example 2" on page 556 for SPBCHF and DPBCHF, using Cholesky factorization.

## Call Statement and Input

## SGTF and DGTF—General Tridiagonal Matrix Factorization

These subroutines compute the standard Gaussian factorization with partial pivoting for tridiagonal matrix **A**, stored in tridiagonal storage mode. To solve a tridiagonal system with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGTS or DGTS, respectively.

Table 106. Data Types	
c, d, e, f	Subroutine
Short-precision real	SGTF
Long-precision real	DGTF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SGTS and DGTS, respectively.

## Syntax

Fortran	CALL SGTF   DGTF (n, c, d, e, f, ipvt)
C and C++	sgtf   dgtf (n, c, d, e, f, ipvt);
PL/I	CALL SGTF   DGTF (n, c, d, e, f, ipvt);

## On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

c is the vector **c**, containing the lower subdiagonal of matrix **A** in positions 2 through *n* in an array, referred to as C. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 106.

is the vector **d**, containing the main diagonal of matrix **A**, in positions 1 through *n* in an array, referred to as D. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 106.

is the vector e, containing the upper subdiagonal of matrix A, in positions 1 through n-1 in an array, referred to as E. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 106.

f
See "On Return."
ipvt
See "On Return."

#### On Return

С

is the vector  $\mathbf{c}$ , containing part of the factorization of matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as  $\mathbf{c}$ . Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 106.

d

is the vector  $\mathbf{d}$ , containing part of the factorization of matrix  $\mathbf{A}$  in an array, referred to as D. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 106.

e

is the vector  $\mathbf{e}$ , containing part of the factorization of the matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as E. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 106 on page 560.

f

is the vector  $\mathbf{f}$ , containing part of the factorization of matrix  $\mathbf{A}$  in the first n positions in an array, referred to as F. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 106 on page 560.

ipvt

is the integer vector ipvt of length n, containing the pivot information. Returned as: a one-dimensional array of (at least) length n, containing fullword integers.

#### **Notes**

- 1. For a description of how tridiagonal matrices are stored, see "General Tridiagonal Matrix" on page 90.
- 2. *ipvt* is not a permutation vector in the strict sense. It is used to record column interchanges in the tridiagonal matrix due to partial pivoting.
- 3. The factorization matrix **A** is stored in nonstandard format.

**Function:** The standard Gaussian elimination with partial pivoting of tridiagonal matrix  $\boldsymbol{A}$  is computed. The factorization is returned by overwriting input arrays C, D, and E, and by writing into output array F, along with pivot information in vector *ipvt*. This factorization can then be used by SGTS or DGTS, respectively, to solve tridiagonal systems of linear equations. See references [43], [51], [52], and [84]. If n is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: Matrix A is singular or nearly singular.

- A pivot element has a value that cannot be reciprocated or is equal to 0. The index *i* of the element is identified in the computational error message.
- The return code is set to 1.
- *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2105 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

Input-Argument Errors: n < 0

**Example:** This example shows how to factor the following tridiagonal matrix **A** of order 4:

## Call Statement and Input

```
= ( . , 1.0, 1.0, 1.0)
       = (2.0, 3.0, 3.0, 3.0)
Ε
       = (2.0, 2.0, 2.0, .)
Output
С
       = (., -0.5, -0.5, -0.5)
       = (-0.5, -0.5, -0.5, -0.5)
       = (2.0, 2.0, 2.0, .)
Ε
IPVT
       = (X'00', X'00', X'00', X'00')
```

#### Notes

- 1. F is stored in an internal format and is passed unchanged to the solve subroutine.
- 2. A "." means you do not have to store a value in that position in the array. However, these storage positions are required and may be overwritten during the computation.

## SGTS and DGTS—General Tridiagonal Matrix Solve

These subroutines solve a tridiagonal system of linear equations using the factorization of tridiagonal matrix *A*, stored in tridiagonal storage mode, produced by SGTF or DGTF, respectively.

Table 107. Data Types	
c, d, e, f, b, x	Subroutine
Short-precision real	SGTS
Long-precision real	DGTS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGTF and DGTF, respectively.

## Syntax

Fortran	CALL SGTS   DGTS (n, c, d, e, f, ipvt, bx)
C and C++	sgts   dgts (n, c, d, e, f, ipvt, bx);
PL/I	CALL SGTS   DGTS (n, c, d, e, f, ipvt, bx);

## On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

С

is the vector  $\mathbf{c}$ , containing part of the factorization of matrix  $\mathbf{A}$  from SGTF or DGTF, respectively, in an array, referred to as  $\mathbb{C}$ . Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 107.

d

is the vector  $\mathbf{d}$ , containing part of the factorization of matrix  $\mathbf{A}$  from SGTF or DGTF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 107.

е

is the vector  $\mathbf{e}$ , containing part of the factorization of matrix  $\mathbf{A}$  from SGTF or DGTF, respectively, in an array, referred to as E. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 107.

f

is the vector  $\mathbf{f}$ , containing part of the factorization of matrix  $\mathbf{A}$  from SGTF or DGTF, respectively, in an array, referred to as F. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 107.

ipvt

is the integer vector *ipvt* of length *n*, containing the pivot information, produced by a preceding call to SGTF and DGTF, respectively. Specified as: a one-dimensional array of (at least) length *n*, containing fullword integers.

bx

is the vector  $\mathbf{b}$  of length n, containing the right-hand side of the system in the first n positions in an array, referred to as BX. Specified as: a one-dimensional

array of (at least) length n+1, containing numbers of the data type indicated in Table 107. For details on specifying the length, see "Notes" on page 564.

## On Return

bx

is the solution vector  $\mathbf{x}$  (at least) of length n, containing the solution of the tridiagonal system in the first n positions in an array, referred to as BX. Returned as: a one-dimensional array, of (at least) length (n+1), containing numbers of the data type indicated in Table 107 on page 563. For details about the length, see "Notes."

#### **Notes**

- 1. For a description of how tridiagonal matrices are stored, see "General Tridiagonal Matrix" on page 90.
- 2. Array BX can have a length of n if memory location BX(n+1) is addressable—that is, not in read-protected storage. If it is in read-protected storage, array BX must have a length of n+1. In both cases, the vector b (on input) and vector x (on output) reside in positions 1 through n in array BX. Array location BX(n+1) is not altered by these subroutines.

**Function:** Given the factorization produced by SGTF or DGTF, respectively, these subroutines use the standard forward elimination and back substitution to solve the tridiagonal system Ax = b, where A is a general tridiagonal matrix. See references [43], [51], [52], and [84].

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example:** This example solves the tridiagonal system Ax = b, where matrix A is the same matrix factored in "Example" on page 561 for SGTF and DGTF, and where:

$$b = (4.0, 6.0, 6.0, 4.0)$$
  
 $x = (1.0, 1.0, 1.0, 1.0)$ 

Call Statement and Input

```
N C D E F IPVT BX
| | | | | | | | | |
CALL DGTS(4, C, D, E, F, IPVT, BX)
```

```
C = (same as output C in "Example" on page 561)
D = (same as output D in "Example" on page 561)
E = (same as output E in "Example" on page 561)
F = (same as output F in "Example" on page 561)
IPVT = (same as output IPVT in "Example" on page 561)
BX = (4.0, 6.0, 6.0, 4.0, .)
```

```
BX = (1.0, 1.0, 1.0, 1.0, .)
```

# SGTNP, DGTNP, CGTNP, and ZGTNP—General Tridiagonal Matrix Combined Factorization and Solve with No Pivoting

These subroutines solve the tridiagonal system Ax = b using Gaussian elimination, where tridiagonal matrix A is stored in tridiagonal storage mode.

Table 108. Data Types	
c, d, e, b, x	Subroutine
Short-precision real	SGTNP
Long-precision real	DGTNP
Short-precision complex	CGTNP
Long-precision complex	ZGTNP

**Note:** In general, these subroutines provide better performance than the \_GTNPF and \_GTNPS subroutines; however, in the following instances, you get better performance by using \_GTNPF and \_GTNPS:

- For small n
- When performing a single factorization followed by multiple solves

## Syntax

Fortran	CALL SGTNP   DGTNP   CGTNP   ZGTNP (n, c, d, e, bx)
C and C++	sgtnp   dgtnp   cgtnp   zgtnp (n, c, d, e, bx);
PL/I	CALL SGTNP   DGTNP   CGTNP   ZGTNP (n, c, d, e, bx);

## On Entry

n

is the order n of tridiagonal matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

С

is the vector  $\mathbf{c}$ , containing the lower subdiagonal of matrix  $\mathbf{A}$  in positions 2 through n in an array, referred to as C. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 108. On output, C is overwritten; that is, the original input is not preserved.

d

is the vector  $\mathbf{d}$ , containing the main diagonal of matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as D. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 108. On output, D is overwritten; that is, the original input is not preserved.

e

is the vector  $\mathbf{e}$ , containing the upper subdiagonal of matrix  $\mathbf{A}$  in positions 1 through n-1 in an array, referred to as E. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 108. On output, E is overwritten; that is, the original input is not preserved.

bx

is the vector  $\mathbf{b}$ , containing the right-hand side of the system in the first n positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 108.

On Return

bx

is the solution vector  $\mathbf{x}$  of length n, containing the solution of the tridiagonal system in the first n positions in an array, referred to as BX. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 108 on page 565.

**Note:** For a description of how tridiagonal matrices are stored, see "General Tridiagonal Matrix" on page 90.

**Function:** The solution of the tridiagonal system Ax = b is computed by Gaussian elimination.

No pivoting is done. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small main diagonal elements are generated. Underflow or accuracy loss may occur if large main diagonal elements are generated.

For performance reasons, complex divides are done without scaling. Computing the inverse in this way restricts the range of numbers for which the ZGTNP subroutine works properly.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DGTNP and ZGTNP work properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DGTNP and (1.0, 0.0) for ZGTNP.

## **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a factorization of the real tridiagonal matrix **A**, of order 4:

It then finds the solution of the tridiagonal system Ax = b, where b is:

and x is:

On output, arrays C, D, and E are overwritten.

Call Statement and Input

**Example 2:** This example shows a factorization of the complex tridiagonal matrix **A**, of order 4:

It then finds the solution of the tridiagonal system Ax = b, where b is:

$$((-11.0,19.0), (-14.0,50.0), (-17.0,93.0), (-13.0,85.0))$$

and x is:

$$((1.0,-1.0), (2.0,-2.0), (3.0,-3.0), (4.0,-4.0))$$

On output, arrays C, D, and E are overwritten.

Call Statement and Input

# SGTNPF, DGTNPF, CGTNPF, and ZGTNPF—General Tridiagonal Matrix Factorization with No Pivoting

These subroutines factor tridiagonal matrix **A**, stored in tridiagonal storage mode, using Gaussian elimination. To solve a tridiagonal system of linear equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SGTNPS, DGTNPS, CGTNPS, or ZGTNPS, respectively.

Table 109. Data Types	
c, d, e	Subroutine
Short-precision real	SGTNPF
Long-precision real	DGTNPF
Short-precision complex	CGTNPF
Long-precision complex	ZGTNPF

#### Notes:

- The output from these factorization subroutines should be used only as input to the solve subroutines SGTNPS, DGTNPS, CGTNPS, and ZGTNPS, respectively.
- 2. In general, the \_GTNP subroutines provide better performance than the \_GTNPF and \_GTNPS subroutines; however, in the following instances, you get better performance by using \_GTNPF and \_GTNPS:
  - For small n
  - When performing a single factorization followed by multiple solves

#### Syntax

Fortran	CALL SGTNPF   DGTNPF   CGTNPF   ZGTNPF (n, c, d, e, iopt)
C and C++	sgtnpf   dgtnpf   cgtnpf   zgtnpf (n, c, d, e, iopt);
PL/I	CALL SGTNPF   DGTNPF   CGTNPF   ZGTNPF (n, c, d, e, iopt);

#### On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

c is the vector **c**, containing the lower subdiagonal of matrix **A** in positions 2 through *n* in an array, referred to as C. Specified as: a one-dimensional array, of (at least) length n, containing numbers of the data type indicated in Table 109.

a i

is the vector  $\mathbf{d}$ , containing the main diagonal of matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as D. Specified as: a one-dimensional array, of (at least) length n, containing numbers of the data type indicated in Table 109.

е

is the vector  $\mathbf{e}$ , containing the upper subdiagonal of matrix  $\mathbf{A}$  in positions 1 through n-1 in an array, referred to as E. Specified as: a one-dimensional array, of (at least) length n, containing numbers of the data type indicated in Table 109.

iopt

indicates the type of computation to be performed, where:

If iopt = 0 or 1, Gaussian elimination is used to factor the matrix.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

С

is the vector  $\mathbf{c}$ , containing part of the factorization of matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as C. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 109 on page 568.

d

is the vector  $\mathbf{d}$ , containing part of the factorization of matrix  $\mathbf{A}$  in an array, referred to as D. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 109 on page 568.

е

is the vector  $\mathbf{e}$ , containing part of the factorization of matrix  $\mathbf{A}$  in positions 1 through n in an array, referred to as  $\mathbf{E}$ . Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 109 on page 568. It has the same length as  $\mathbf{E}$  on entry.

**Note:** For a description of how tridiagonal matrices are stored, see "General Tridiagonal Matrix" on page 90.

**Function:** The factorization of a diagonally-dominant tridiagonal matrix **A** is computed using Gaussian elimination, This factorization can then be used by SGTNPS, DGTNPS, CGTNPS, or ZGTNPS respectively, to solve the tridiagonal systems of linear equations. See reference [71].

No pivoting is done by these subroutines. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small main diagonal elements are generated. Underflow or accuracy loss may occur if large main diagonal elements are generated.

For performance reasons, complex divides are done without scaling. Computing the inverse in this way restricts the range of numbers for which ZGTNPF works properly.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DGTNPF and ZGTNPF work properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DGTNPF and (1.0, 0.0) for ZGTNPF.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. n < 0

2.  $iopt \neq 0 \text{ or } 1$ 

**Example 1:** This example shows a factorization of the tridiagonal matrix **A**, of order 4:

## Call Statement and Input

```
= ( . , 1.0, 1.0, 1.0)
       = (1.0, 2.0, 3.0, 1.0)
       = (1.0, 1.0, 1.0, .)
Output
С
       = ( . , -1.0, -1.0, 1.0)
       = (-1.0, -1.0, -1.0, -1.0)
       = (1.0, 1.0, -1.0, .)
```

## **Example 2:** This example shows a factorization of the tridiagonal matrix **A**, of order 4:

### Call Statement and Input

```
= (., (1.0, 1.0), (2.0, 2.0), (3.0, 3.0))
        = ((7.0, 7.0), (8.0, 8.0), (9.0, 9.0), (10.0, 10.0))
        = ((4.0, 4.0), (5.0, 5.0), (6.0, 6.0), .)
Output
C
        = (., (-0.142, 0.0), (-0.269, 0.0), (3.0, 3.0))
        = ((-0.0714, 0.0714), (-0.0673, 0.0673), (-0.0854, 0.0854),
           (-0.05, 0.05))
Ε
        = ((4.0, 4.0), (5.0, 5.0), (-0.6, 0.0), .)
```

#### Notes

1. A "." means you do not have to store a value in that position in the array. However, these storage positions are required and may be overwritten during the computation.

# SGTNPS, DGTNPS, CGTNPS, and ZGTNPS—General Tridiagonal Matrix Solve with No Pivoting

These subroutines solve a tridiagonal system of equations using the factorization of matrix  $\boldsymbol{A}$ , stored in tridiagonal storage mode, produced by SGTNPF, DGTNPF, CGTNPF, or ZGTNPF, respectively.

Table 110. Data Types	
c, d, e, b, x	Subroutine
Short-precision real	SGTNPS
Long-precision real	DGTNPS
Short-precision complex	CGTNPS
Long-precision complex	ZGTNPS

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively.

## Syntax

Fortran	CALL SGTNPS   DGTNPS   CGTNPS   ZGTNPS (n, c, d, e, bx)
C and C++	sgtnps   dgtnps   cgtnps   zgtnps (n, c, d, e, bx);
PL/I	CALL SGTNPS   DGTNPS   CGTNPS   ZGTNPS (n, c, d, e, bx);

## On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

С

is the vector c, containing part of the factorization of matrix A from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as c. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 110.

d

is the vector d, containing part of the factorization of matrix A from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 110.

e

is the vector  $\mathbf{e}$ , containing part of the factorization of matrix  $\mathbf{A}$  from SGTNPF, DGTNPF, CGTNPF, and ZGTNPF, respectively, in an array, referred to as E. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 110.

bx

is the vector  $\mathbf{b}$ , containing the right-hand side of the system in the first n positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 110.

## On Return

bх

is the solution vector  $\mathbf{x}$  of length  $\mathbf{n}$ , containing the solution of the tridiagonal system in the first *n* positions in an array, referred to as BX. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 110.

**Note:** For a description of how tridiagonal matrices are stored, see "General Tridiagonal Matrix" on page 90.

**Function:** The solution of tridiagonal system Ax = b is computed using the factorization produced by SGTNPF, DGTNPF, CGTNPF, or ZGTNPF, respectively. The factorization is based on Gaussian elimination. See reference [71].

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example finds the solution of tridiagonal system Ax = b, where matrix A is the same matrix factored in "Example 1" on page 570 for SGTNPF and DGTNPF. **b** is:

and x is:

Call Statement and Input

- = (same as output C in "Example 1" on page 570) D = (same as output D in "Example 1" on page 570) Ε = (same as output E in "Example 1" on page 570)
- ВХ (2.0, 4.0, 5.0, 2.0)

Output

BX = 
$$(1.0, 1.0, 1.0, 1.0)$$

**Example 2:** This example finds the solution of tridiagonal system Ax = b, where matrix A is the same matrix factored in "Example 2" on page 570 for CGTNPF and ZGTNPF. b is:

$$((-11.0,19.0), (-14.0,50.0), (-17.0,93.0), (-13.0,85.0))$$

and x is:

$$((0.0,1.0), (1.0,2.0), (2.0,3.0), (3.0,4.0))$$

Call Statement and Input

## SGTNPS, DGTNPS, CGTNPS, and ZGTNPS

```
\mathsf{N} \mathsf{C} \mathsf{D} \mathsf{E} \mathsf{BX}
С
         = (same as output C in "Example 2" on page 570)
D
         = (same as output D in "Example 2" on page 570)
         = (same as output E in "Example 2" on page 570)
Ε
            ((-11.0, 19.0), (-14.0, 50.0), (-17.0, 93.0), (-13.0, 8))
Output
ВХ
         = ((0.0, 1.0), (1.0, 2.0), (2.0, 3.0), (3.0, 4.0))
```

# SPTF and DPTF—Positive Definite Symmetric Tridiagonal Matrix Factorization

These subroutines factor symmetric tridiagonal matrix *A*, stored in symmetric-tridiagonal storage mode, using Gaussian elimination. To solve a tridiagonal system of linear equations with one or more right-hand sides, follow the call to these subroutines with one or more calls to SPTS or DPTS, respectively.

Table 111. Data Types	
c, d	Subroutine
Short-precision real	SPTF
Long-precision real	DPTF

**Note:** The output from these factorization subroutines should be used only as input to the solve subroutines SPTS and DPTS, respectively.

## Syntax

Fortran	CALL SPTF   DPTF (n, c, d, iopt)
C and C++	sptf   dptf (n, c, d, iopt);
PL/I	CALL SPTF   DPTF (n, c, d, iopt);

## On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

С

is the vector c, containing the off-diagonal of matrix c in positions 2 through c in an array, referred to as c. Specified as: a one-dimensional array, of (at least) length c, containing numbers of the data type indicated in Table 111.

d

is the vector  $\mathbf{d}$ , containing the main diagonal of matrix  $\mathbf{A}$  in positions 1 through n in an array referred to as D. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 111.

iopt

indicates the type of computation to be performed, where:

If iopt = 0 or 1, Gaussian elimination is used to factor the matrix.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

C

is the vector c, containing part of the factorization of matrix A in an array, referred to as c. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 111.

d

is the vector d, containing part of the factorization of matrix A in positions 1 through n in an array, referred to as D. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 111. It has the same length as D on entry.

**Note:** For a description of how positive definite symmetric tridiagonal matrices are stored, see "Positive Definite Symmetric Tridiagonal Matrix" on page 92.

**Function:** The factorization of positive definite symmetric tridiagonal matrix **A** is computed using Gaussian elimination. This factorization can then be used by SPTS or DPTS, respectively, to solve the tridiagonal systems of linear equations. See reference [71].

No pivoting is done. Therefore, these subroutines should not be used when pivoting is necessary to maintain the numerical accuracy of the solution. Overflow may occur if small pivots are generated.

For performance reasons, divides are done in a way that reduces the effective exponent range for which DPTF works properly; therefore, you may want to scale your problem, such that the diagonal elements are close to 1.0 for DPTF.

#### **Error Conditions**

Computational Errors: None

**Note:** There is no test for positive definiteness in these subroutines.

Input-Argument Errors

1. 
$$n < 0$$
  
2.  $iopt \neq 0 \text{ or } 1$ 

**Example:** This example shows a factorization of the tridiagonal matrix **A**, of order 4:

Call Statement and Input

#### Notes

A "." means you do not have to store a value in that position in the array.
 However, these storage positions are required and may be overwritten during the computation.

## SPTS and DPTS—Positive Definite Symmetric Tridiagonal Matrix Solve

These subroutines solve a positive definite symmetric tridiagonal system of equations using the factorization of matrix **A**, stored in symmetric-tridiagonal storage mode, produced by SPTF and DPTF, respectively.

Table 112. Data Types		
c, d, b, x Subroutine		
Short-precision real	SPTS	
Long-precision real	DPTS	

**Note:** The input to these solve subroutines must be the output from the factorization subroutines SPTF and DPTF, respectively.

#### **Syntax**

Fortran	CALL SPTS   DPTS (n, c, d, bx)	
C and C++	spts   dpts (n, c, d, bx);	
PL/I	CALL SPTS   DPTS (n, c, d, bx);	

#### On Entry

n

is the order n of tridiagonal matrix A. Specified as: a fullword integer;  $n \ge 0$ .

c is the vector **c**, containing part of the factorization of matrix **A** from SPTF or DPTF, respectively, in an array, referred to as C. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 112.

is the vector **d**, containing part of the factorization of matrix **A** from SPTF or DPTF, respectively, in an array, referred to as D. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 112.

bx

is the vector **b**, containing the right-hand side of the system in the first *n* positions in an array, referred to as BX. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 112.

#### On Return

bx

is the solution vector  $\mathbf{x}$  of length n, containing the solution of the tridiagonal system in the first n positions in an array, referred to as BX. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 112.

**Note:** For a description of how tridiagonal matrices are stored, see "Positive Definite or Negative Definite Symmetric Matrix" on page 69.

**Function:** The solution of positive definite symmetric tridiagonal system Ax = b is computed using the factorization produced by SPTF or DPTF, respectively. The factorization is based on Gaussian elimination. See reference [71].

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 0

**Example:** This example finds the solution of tridiagonal system Ax = b, where matrix A is the same matrix factored in "Example" on page 575 for SPTF and DPTF. **b** is:

and x is:

Call Statement and Input

BX = 
$$(1.0, 1.0, 1.0, 1.0)$$

### STBSV, DTBSV, CTBSV, and ZTBSV—Triangular Band Equation Solve

STBSV and DTBSV solve one of the following triangular banded systems of equations with a single right-hand side, using the vector  $\mathbf{x}$  and triangular band matrix  $\mathbf{A}$  or its transpose:

Solution	Equation	
1. $\mathbf{x} \leftarrow \mathbf{A}^{-1}\mathbf{x}$	Ax = b	
2. $\mathbf{x} \leftarrow \mathbf{A}^{-T}\mathbf{x}$	$A^{T}x = b$	

CTBSV and ZTBSV solve one of the following triangular banded systems of equations with a single right-hand side, using the vector  $\mathbf{x}$  and triangular band matrix  $\mathbf{A}$ , its transpose, or its conjugate transpose:

Solution	Equation	
1. $\mathbf{x} \leftarrow \mathbf{A}^{-1}\mathbf{x}$	Ax = b	
2. $\mathbf{x} \leftarrow \mathbf{A}^{-T}\mathbf{x}$	$A^{T}x = b$	
3. $\mathbf{x} \leftarrow \mathbf{A} - H\mathbf{x}$	$A^H x = b$	

Matrix **A** can be either upper or lower triangular and is stored in upper- or lower-triangular-band-packed storage mode, respectively.

Table 113. Data Types		
A, x	Subprogram	
Short-precision real	STBSV	
Long-precision real	DTBSV	
Short-precision complex	CTBSV	
Long-precision complex	ZTBSV	

#### Syntax

Fortran	CALL STBSV   DTBSV   CTBSV   ZTBSV (uplo, trans, diag, n, k, a, lda, x, incx)
C and C++	stbsv   dtbsv   ctbsv   ztbsv (uplo, trans, diag, n, k, a, lda, x, incx);
PL/I	CALL STBSV   DTBSV   CTBSV   ZTBSV (uplo, trans, diag, n, k, a, lda, x, incx);

On Entry

uplo

indicates whether matrix **A** is an upper or lower triangular band matrix, where:

If uplo = 'U', **A** is an upper triangular matrix.

If uplo = 'L', **A** is a lower triangular matrix.

Specified as: a single character. It must be 'U' or 'L'.

trans

indicates the form of matrix **A** used in the system of equations, where:

If trans = 'N', **A** is used, resulting in solution 1.

If trans = 'T',  $A^T$  is used, resulting in solution 2.

If  $trans = {}^{\shortmid}C^{\shortmid}$ ,  $A^{H}$  is used, resulting in solution 3.

Specified as: a single character. It must be 'N', 'T', or 'C'. diag

indicates the characteristics of the diagonal of matrix A, where:

If diag = 'U', **A** is a unit triangular matrix.

If diag = 'N', **A** is not a unit triangular matrix.

Specified as: a single character. It must be 'U' or 'N'.

is the order of triangular band matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

k is the upper or lower band width k of the matrix A. Specified as: a fullword integer;  $k \ge 0$ .

is the upper or lower triangular band matrix **A** of order *n*, stored in upper- or lower-triangular-band-packed storage mode, respectively. Specified as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 113 on page 578.

lda

n

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge k+1$ .

is the vector  $\mathbf{x}$  of length n, containing the right-hand side of the triangular system to be solved. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 113 on page 578.

incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0 or incx < 0.

#### On Return

Χ

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 113 on page 578.

#### **Notes**

- 1. These subroutines accept lowercase letters for the *uplo*, *trans*, and *diag* arguments.
- 2. For STBSV and DTBSV, if you specify 'C' for the *trans* argument, it is interpreted as though you specified 'T'.
- 3. Matrix **A** and vector **x** must have no common elements; otherwise, results are unpredictable.
- 4. For unit triangular matrices, the elements of the diagonal are assumed to be 1.0 for real matrices and (1.0, 0.0) for complex matrices, and you do not need to set these values in the array.
- 5. For both upper and lower triangular band matrices, if you specify  $k \ge n$ , ESSL assumes, **for purposes of the computation only**, that the upper or lower band width of matrix A is n-1; that is, it processes matrix A of order n, as though it is a (nonbanded) triangular matrix. However, ESSL uses the original value for k for the purposes of finding the locations of element  $a_{11}$  and all other elements in the array specified for A, as described in "Triangular Band"

Matrix" on page 86. For an illustration of this technique, see "Example 3" on page 582.

- 6. For a description of triangular band matrices and how they are stored in upperand lower-triangular-band-packed storage mode, see "Triangular Band Matrix" on page 86.
- 7. If you are using a lower triangular band matrix, it may save your program some time if you use this alternate approach instead of using lower-triangular-band-packed storage mode. Leave matrix *A* in full-matrix storage mode when you pass it to ESSL and specify the *Ida* argument to be *Ida*+1, which is the leading dimension of matrix *A* plus 1. ESSL then processes the matrix elements in the same way as though you had set them up in lower-triangular-band-packed storage mode.

**Function:** These subroutines solve a triangular banded system of equations with a single right-hand side. The solution, x, may be any of the following, where triangular band matrix A, its transpose, or its conjugate transpose is used, and where A can be either upper- or lower-triangular:

```
1. \mathbf{x} \leftarrow \mathbf{A}^{-1}\mathbf{x}
```

2.  $\mathbf{X} \leftarrow \mathbf{A}^{-\mathsf{T}}\mathbf{X}$ 

3.  $x \leftarrow A^{-H}x$  (for CTBSV and ZTBSV only)

where:

x is a vector of length n.

**A** is an upper or lower triangular band matrix of order *n*, stored in upper- or lower-triangular-band-packed storage mode, respectively.

See references [34], [46], and [38]. If *n* is 0, no computation is performed.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

```
1. n < 0
```

2. k < 0

 $3. Ida \leq 0$ 

4. Ida < k+1

5. incx = 0

6. *uplo* ≠ 'L' or 'U'

7. *trans* ≠ 'T', 'N', or 'C'

8. *diag* ≠ 'N' or 'U'

**Example 1:** This example shows the solution  $x \leftarrow A^{-1}x$ . Matrix A is a real 9 by 9 upper triangular band matrix with an upper band width of 2 that is not unit triangular, stored in upper-triangular-band-packed storage mode. Vector x is a vector of length 9, where matrix A is:

#### Call Statement and Input

**Example 2:** This example shows the solution  $x \leftarrow A^{-T}x$ , solving the same system as in Example 1. Matrix A is a real 9 by 9 lower triangular band matrix with a lower band width of 2 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector x is a vector of length 9 where matrix A is:

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 2.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 3.0 & 1.0 & 4.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 1.0 & 3.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & 3.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0$$

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 4.0 & 4.0 & 4.0 & 3.0 & 3.0 & 3.0 & 2.0 & 1.0 \\ 1.0 & 2.0 & 1.0 & 2.0 & 1.0 & 2.0 & 0.0 & . & . \\ 1.0 & 3.0 & 1.0 & 2.0 & 1.0 & 2.0 & 0.0 & . & . \end{bmatrix}$$

X = (same as input X in Example 1)

Output

**Example 3:** This example shows the solution  $x \leftarrow A^{-T}x$ , where k > n. Matrix **A** is a real 4 by 4 upper triangular band matrix with an upper band width of 3, even though *k* is specified as 5. It is not unit triangular and is stored in upper-triangular-band-packed storage mode. Vector x is a vector of length 4 where matrix A is:

Call Statement and Input

$$X = (5.0, 18.0, 32.0, 41.0)$$

Output

$$X = (5.0, 4.0, 3.0, 2.0)$$

**Example 4:** This example shows the solution  $x \leftarrow A^{-T}x$ . Matrix A is a complex 7 by 7 lower triangular band matrix with a lower band width of 3 that is not unit triangular, stored in lower-triangular-band-packed storage mode. Vector x is a vector of length 7. Matrix A is:

Call Statement and Input

```
A = \begin{bmatrix} (1.0, 0.0) & (2.0, 1.0) & (3.0, 1.0) & (4.0, 1.0) & (2.0, 1.0) & (3.0, 1.0) & (2.0, 1.0) \\ (1.0, 2.0) & (2.0, 2.0) & (3.0, 3.0) & (4.0, 2.0) & (5.0, 1.0) & (6.0, 1.0) \\ (1.0, 3.0) & (2.0, 3.0) & (3.0, 3.0) & (4.0, 3.0) & (5.0, 2.0) & & & & \\ (1.0, 4.0) & (2.0, 4.0) & (3.0, 3.0) & (4.0, 4.0) & & & & & \\ X = & ((2.0, 2.0), & (7.0, 1.0), & (1.0, 1.0), & (8.0, 1.0), \\ & & & & (2.0, 0.0), & (8.0, 1.0), & (1.0, 2.0)) & & & \\ Output \\ X = & ((-12.048, -13.136), & (6.304, -1.472), & (-1.880, 1.040), \\ & & & & (2.600, -1.800), & (-2.160, 1.880), & (0.800, -1.400), \\ & & & & & (0.800, 0.600) & & \\ \end{bmatrix}
```

### **Sparse Linear Algebraic Equation Subroutines**

This section contains the sparse linear algebraic equation subroutine descriptions.

## DGSF—General Sparse Matrix Factorization Using Storage by Indices, Rows, or Columns

This subroutine factors sparse matrix **A** by Gaussian elimination, using a modified Markowitz count with threshold pivoting. The sparse matrix can be stored by indices, rows, or columns. To solve the system of equations, follow the call to this subroutine with a call to DGSS.

#### Syntax

Fortran	CALL DGSF (iopt, n, nz, a, ia, ja, lna, iparm, rparm, oparm, aux, naux)
C and C++	dgsf (iopt, n, nz, a, ia, ja, lna, iparm, rparm, oparm, aux, naux);
PL/I	CALL DGSF (iopt, n, nz, a, ia, ja, Ina, iparm, rparm, oparm, aux, naux);

#### On Entry

iopt

indicates the storage technique used for sparse matrix A, where:

If iopt = 0, it is stored by indices.

If iopt = 1, it is stored by rows.

If iopt = 2, it is stored by columns.

Specified as: a fullword integer; iopt = 0, 1, or 2.

n

is the order n of sparse matrix A. Specified as: a fullword integer;  $n \ge 0$ .

nz

is the number of elements in sparse matrix A, stored in an array, referred to as A. Specified as: a fullword integer; nz > 0.

а

is the sparse matrix A, to be factored, stored in an array, referred to as A. Specified as: an array of length lna, containing long-precision real numbers.

ia

is the array, referred to as IA, where:

If iopt = 0, it contains the row numbers that correspond to the elements in array A.

If iopt = 1, it contains the row pointers.

If iopt = 2, it contains the row numbers that correspond to the elements in array A.

Specified as: an array of length lna, containing fullword integers; IA(i)  $\geq$  1. See "Sparse Matrix" on page 92 for more information on storage techniques.

ja

is the array, referred to as JA, where:

If iopt = 0, it contains the column numbers that correspond to the elements in array A.

If iopt = 1, it contains the column numbers that correspond to the elements in array A.

If iopt = 2, it contains the column pointers.

Specified as: an array of length Ina, containing fullword integers;  $JA(i) \ge 1$ . See "Sparse Matrix" on page 92 for more information on storage techniques.

Ina

is the length of the arrays specified for *a*, *ia*, and *ja*. Specified as: a fullword integer; *lna* > 2*nz*. If you do not specify a sufficient amount, it results in an error. See "Error Conditions" on page 588.

The size of *lna* depends on the structure of the input matrix. The requirement that *lna* > 2*nz* does not guarantee a successful run of the program. If the input matrix is expected to have many fill-ins, *lna* should be set larger. Larger *lna* may result in a performance improvement.

For details on how *Ina* relates to storage compressions, see "Performance and Accuracy Considerations" on page 461.

iparm

is an array of parameters, IPARM(i), where:

 IPARM(1) determines whether the default values for iparm and rparm are used by this subroutine.

If IPARM(1) = 0, the following default values are used:

```
IPARM(2) = 10

IPARM(3) = 1

IPARM(4) = 0

RPARM(1) = 10^{-12}

RPARM(2) = 0.1
```

If IPARM(1) = 1, the default values are not used.

- IPARM(2) determines the number of minimal Markowitz counts that are examined to determine a pivot. (See reference [95].)
- IPARM(3) has the following meaning, where:

```
If IPARM(3) = 0, this subroutine checks the values in arrays IA and JA.
```

If IPARM(3) = 1, this subroutine assumes that the input values are correct in arrays IA and JA.

IPARM(4) has the following meaning, where:

```
If IPARM(4) = 0, this computation is not performed.
```

If IPARM(4) = 1, this subroutine computes:

The absolute value of the smallest pivot element The absolute value of the largest element in  $\boldsymbol{U}$ .

These values are stored in OPARM(2) and OPARM(3), respectively.

• IPARM(5) is reserved.

Specified as: an array of (at least) length 5, containing fullword integers, where the *iparm* values must be:

```
IPARM(1) = 0 or 1

IPARM(2) \geq 1

IPARM(3) = 0 or 1

IPARM(4) = 0 or 1
```

is an array of parameters, RPARM(i), where:

• RPARM(1) contains the lower bound of the absolute value of all elements in

rparm

the matrix. If a pivot element is less than this number, the matrix is reported as singular. Any computed element whose absolute value is less than this number is set to 0.

- RPARM(2) is the threshold pivot tolerance used to control the choice of pivots.
- RPARM(3) is reserved.
- RPARM(4) is reserved.
- RPARM(5) is reserved.

Specified as: a one-dimensional array of (at least) length 5, containing long-precision real numbers, where the *rparm* values must be:

```
RPARM(1) \ge 0.0
0.0 \le RPARM(2) \le 1.0
```

For additional information about *rparm*, see "Performance and Accuracy Considerations" on page 461.

#### oparm

See "On Return."

aux

is the storage work area used by this subroutine. Its size is specified by *naux*. Specified as: an area of storage, containing long-precision real numbers.

#### naux

is the size of the work area specified by aux—that is, the number of elements in aux. Specified as: a fullword integer;  $naux \ge 10n+100$ .

#### On Return

а

is the transformed array, referred to as A, containing the factored matrix  $\boldsymbol{A}$ , required as input to DGSS. Returned as: a one-dimensional array of length lna, containing long-precision real numbers.

ia

is the transformed array, referred to as IA, required as input to DGSS. Returned as: a one-dimensional array of length *lna*, containing fullword integers.

ja

is the transformed array, referred to as JA, required as input to DGSS. Returned as: a one-dimensional array of length *lna*, containing fullword integers.

#### oparm

is an array of parameters, OPARM(i), where:

- OPARM(1) is the amount of fill-ins for the sparse processing portion of the algorithm.
- OPARM(2) contains the absolute value of the smallest pivot element of the matrix. This value is computed and set only if IPARM(4) = 1.
- OPARM(3) contains the absolute value of the largest element encountered in
   *U* after the factorization. This value is computed and set only if
   IPARM(4) = 1.
- OPARM(4) is reserved.
- OPARM(5) is reserved.

Returned as: a one-dimensional array of length 5, containing long-precision real numbers.

aux

is the storage work area used by this subroutine. It contains the information required as input for DGSS. Specified as: an area of storage, containing long-precision real numbers.

#### Notes

- 1. For a description of the three storage techniques used by this subroutine for sparse matrices, see "Sparse Matrix" on page 92.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The matrix **A** is factored by Gaussian elimination, using a modified Markowitz count with threshold pivoting to compute the sparse LU factorization of **A**:

LU = PAQ

where:

 $\boldsymbol{A}$  is a general sparse matrix of order n, stored by indices, columns, or rows in arrays A, IA, and JA.

L is a unit lower triangular matrix.

**U** is an upper triangular matrix.

**P** is a permutation matrix.

**Q** is a permutation matrix.

To solve the system of equations, follow the call to this subroutine with a call to DGSS. If n is 0, no computation is performed. See references [10], [47], and [87].

#### **Error Conditions**

#### Computational Errors

- 1. If this subroutine has to perform storage compressions, an attention message is issued. When this occurs, the performance of this subroutine is affected. The performance can be improved by increasing the value specified for *Ina*.
- 2. The following errors with their corresponding return codes can occur in this subroutine. Where a value of *i* is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.
  - For error 2117, return code 2 indicates that the pivot element in a column, *i*, is smaller than the value specified in RPARM(1).
  - For error 2118, return code 3 indicates that pivot element in a row, *i*, is smaller than the value specified in RPARM(1).
  - For error 2120, return code 4 indicates that a row, *i*, is found empty on factorization. The matrix is singular.
  - For error 2121, return code 5 indicates that a column is found empty on factorization. The matrix is singular.

- For error 2119, return code 6 indicates that the storage space indicated by *lna* is insufficient.
- For error 2122, return code 7 indicates that no pivot element was found in the active submatrix.

#### Input-Argument Errors

```
1. iopt \neq 0, 1, \text{ or } 2

2. n < 0

3. nz \leq 0

4. lna \leq 2nz

5. IPARM(1) \neq 0 \text{ or } 1

6. IPARM(2) \leq 0

7. IPARM(3) \neq 0 \text{ or } 1

8. IPARM(4) \neq 0 \text{ or } 1

9. RPARM(1) < 0.0

10. RPARM(2) < 0.0 \text{ or } RPARM(2) > 1.0

11. iopt = 1 \text{ and } ia(i) \geq ia(i+1), i = 1, n

12. iopt = 2 \text{ and } ja(i) \geq ja(i+1), i = 1, n

13. iopt = 0 \text{ or } 1 \text{ and } ja(i) < 1 \text{ or } ja(i) > n, i = 1, nz

14. iopt = 0 \text{ or } 1 \text{ and } ja(i) < 1 \text{ or } ja(i) > n, i = 1, nz
```

- 15. There are duplicate indices in a row or column of the input matrix.
- 16. The matrix is singular if a row or column of the input matrix is empty.
- 17. *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example factors 5 by 5 sparse matrix  $\mathbf{A}$ , which is stored by indices in arrays A, IA, and JA. The three storage techniques are shown in this example, and the output is the same regardless of the storage technique used. The matrix is factored using Gaussian elimination with threshold pivoting. Matrix  $\mathbf{A}$  is:

**Note:** In this example, only nonzero elements are used as input to the matrix.

Call Statement and Input (Storage-By-Indices)

```
IOPT N NZ A IA JA LNA IPARM RPARM OPARM AUX NAUX
                    CALL DGSF( 0 , 5, 13, A, IA, JA, 27 , IPARM, RPARM, OPARM, AUX, 150 )
       = (2.0, 1.0, 1.0, 3.0, 4.0, 1.0, 5.0, 2.0, 2.0, 1.0, 1.0,
Α
          . , . )
IΑ
         (1, 2, 2, 3, 3, 4, 4, 4, 4, 5, 5, 1, 2, ..., ..., ...,
          . , . , . , . , . , . , . , . )
JA
         (1, 1, 2, 3, 4, 4, 5, 1, 2, 3, 4, 3, 5, ., ., ., ., .,
         (1, 3, 1, 1)
IPARM
RPARM
       = (1.D-12, 0.1D0)
```

Call Statement and Input (Storage-By-Rows)

```
IOPT N NZ A IA JA LNA IPARM RPARM OPARM AUX NAUX
CALL DGSF( 1 , 5, 13, A, IA, JA, 27 , IPARM, RPARM, OPARM, AUX, 150 )
      = (2.0, 4.0, 1.0, 1.0, 3.0, 3.0, 4.0, 2.0, 2.0, 1.0, 5.0,
Α
         . , . )
IΑ
         JA
         (1, 3, 1, 2, 5, 3, 4, 1, 2, 4, 5, 3, 4, ., ., ., ., .,
                   , . , . , . , . , . , . )
      = (1, 3, 1, 1)
IPARM
RPARM
      = (1.D-12, 0.1D0)
Call Statement and Input (Storage-By-Columns)
       IOPT N NZ A IA JA LNA IPARM RPARM OPARM AUX NAUX
        CALL DGSF(2, 5, 13, A, IA, JA, 27, IPARM, RPARM, OPARM, AUX, 150)
      = (2.0, 1.0, 2.0, 1.0, 2.0, 4.0, 3.0, 1.0, 4.0, 1.0, 1.0,
         . , . )
IΑ
         (1, 2, 4, 2, 4, 1, 3, 5, 3, 4, 5, 2, 4, ., ., ., ., .,
                 , . , . , . , . , . , . )
         JA
         . , . , . , . , . )
         (1, 3, 0, 1)
IPARM
RPARM
         (1.D-12, 0.1D0)
Output
         (0.5, ., 0.3, 1.0, ., 1.0, ., 3.0, ., ., ., 1.0,
         1.0, ., ., ., ., ., ., ., -1.7, -0.5, -1.0, -1.0,
         4.0, -3.0, -4.0
IΑ
         (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, ., ., ., ., .,
         .,.,.,2,1,1,3,3,5,5
         (1, 0, 5, 2, 0, 4, 0, 2, 0, 0, 0, 3, 4, ., ., ., .,
JA
         .,.,4,2,4,4,1,3,1)
OPARM
         (1.000000, 0.333333, 3.000000)
```

### DGSS—General Sparse Matrix or Its Transpose Solve Using Storage by Indices, Rows, or Columns

This subroutine solves either of the following systems:

$$Ax = b$$
  
 $A^{\mathsf{T}}x = b$ 

where  $\mathbf{A}$  is a sparse matrix,  $\mathbf{A}^T$  is the transpose of sparse matrix  $\mathbf{A}$ , and  $\mathbf{x}$  and  $\mathbf{b}$  are vectors. DGSS uses the results of the factorization of matrix  $\mathbf{A}$ , produced by a preceding call to DGSF.

**Note:** The input to this solve subroutine must be the output from the factorization subroutine, DGSF.

#### Syntax

Fortran	CALL DGSS (jopt, n, a, ia, ja, lna, bx, aux, naux)
C and C++	dgss (jopt, n, a, ia, ja, lna, bx, aux, naux);
PL/I	CALL DGSS (jopt, n, a, ia, ja, lna, bx, aux, naux);

#### On Entry

jopt

indicates the type of computation to be performed, where:

If jopt = 0, Ax = b is solved, where the right-hand side is not sparse.

If jopt = 1,  $A^Tx = b$  is solved, where the right-hand side is not sparse.

If jopt = 10, Ax = b is solved, where the right-hand side is sparse.

If jopt = 11,  $A^Tx = b$  is solved, where the right-hand side is sparse.

Specified as: a fullword integer; jopt = 0, 1, 10, or 11.

n

is the order n of sparse matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

a is the factorization of sparse matrix A, stored in array A, produced by a preceding call to DGSF. Specified as: an array of length Ina, containing long-precision real numbers.

ia

is the array, referred to as IA, produced by a preceding call to DGSF. Specified as: an array of length *lna*, containing fullword integers.

ja

is the array, referred to as JA, produced by a preceding call to DGSF. Specified as: an array of length *lna*, containing fullword integers.

Ina

is the length of the arrays A, IA, and JA. In DGSS, lna must be identical to the value specified in DGSF; otherwise, results are unpredictable. Specified as: a fullword integer; lna > 0.

b>

is the vector  $\mathbf{b}$  of length n, containing the right-hand side of the system. Specified as: a one-dimensional array of (at least) length n, containing long-precision real numbers.

aux

is the storage work area passed to this subroutine by a preceding call to DGSF. Its size is specified by naux. Specified as: an area of storage, containing long-precision real numbers.

naux

is the size of the work area specified by aux—that is, the number of elements in aux. Specified as: a fullword integer;  $naux \ge 10n+100$ .

#### On Return

ia

is the transformed array, referred to as IA, which can be used as input in subsequent calls to this subroutine. This may result in a performance increase. Specified as: an array of length *lna*, containing fullword integers.

bx

is the solution vector  $\mathbf{x}$  of length n, containing the results of the computation. Specified as: a one-dimensional array, containing long-precision real numbers.

#### **Notes**

- 1. The input arguments n, Ina, and naux, must be the same as those specified for DGSF. Whereas, the input arguments a, ia, ja, and aux must be those produced on output by DGSF. Otherwise, results are unpredictable.
- 2. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The system Ax = b is solved for x, where A is a sparse matrix and xand **b** are vectors. Depending on the value specified for the *jopt* argument, DGSS can also solve the system  $A^Tx = b$ , where  $A^T$  is the transpose of sparse matrix A.

If the value specified for the jopt argument is 0 or 10, the following equation is solved:

$$Ax = b$$

If the value specified for the jopt argument is 1 or 11, the following equation is solved:

$$A^Tx = b$$

DGSS uses the results of the factorization of matrix A, produced by a preceding call to DGSF. The transformed matrix **A** consists of the upper triangular matrix **U** and the lower triangular matrix L.

See references [10], [47], and [87].

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $jopt \neq 0, 1, 10, or 11$
- 2. n < 0
- 3.  $lna \leq 0$

4. *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to solve the system Ax = b, where matrix A is a 5 by 5 sparse matrix. The right-hand side is not sparse.

**Note:** The input for this subroutine is the same as the output from DGSF, except for BX.

Matrix A is:

Call Statement and Input

**Example 2:** This example shows how to solve the system  $A^Tx = b$ , using the same matrix A used in Example 1. The input is also the same as in Example 1, except for the *jopt* argument. The right-hand side is not sparse.

Call Statement and Input

**Example 3:** This example shows how to solve the system Ax = b, using the same matrix A as in Examples 1 and 2. The input is also the same as in Examples 1 and 2, except for the *jopt* and bx arguments. The right-hand side is sparse.

#### Call Statement and Input

ВХ = (0.0, 0.0, 0.0, 1.0, 0.0)

#### Output

**Example 4:** This example shows how to solve the system  $A^Tx = b$ , using the same matrix A as in Examples 1, 2, and 3. The input is also the same as in Examples 1, 2, and 3, except for the *jopt* argument. The right-hand side is sparse.

#### Call Statement and Input

ВХ = (0.0, 0.0, 0.0, 1.0, 0.0)

#### Output

# DGKFS—General Sparse Matrix or Its Transpose Factorization, Determinant, and Solve Using Skyline Storage Mode

This subroutine can perform either or both of the following functions for general sparse matrix  $\mathbf{A}$ , stored in skyline storage mode, and for vectors  $\mathbf{x}$  and  $\mathbf{b}$ :

- Factor **A** and, optionally, compute the determinant of **A**.
- Solve the system Ax = b or A<sup>T</sup>x = b using the results of the factorization of matrix A, produced on this call or a preceding call to this subroutine.

You also have the choice of using profile-in or diagonal-out skyline storage mode for  $\boldsymbol{A}$  on input or output.

**Note:** The input to the solve performed by this subroutine must be the output from the factorization performed by this subroutine.

#### Syntax

Fortran	CALL DGKFS (n, au, nu, idu, al, nl, idl, iparm, rparm, aux, naux, bx, ldbx, mbx)
C and C++	dgkfs (n, au, nu, idu, al, nl, idl, iparm, rparm, aux, naux, bx, ldbx, mbx);
PL/I	CALL DGKFS (n, au, nu, idu, al, nl, idl, iparm, rparm, aux, naux, bx, ldbx, mbx);

#### On Entry

n

au

is the order of general sparse matrix A. Specified as: a fullword integer;  $n \ge 0$ .

is the array, referred to as AU, containing one of three forms of the upper triangular part of general sparse matrix  $\boldsymbol{A}$ , depending on the type of computation performed, where:

- If you are doing a **factor and solve** or a **factor only**, and if IPARM(3) = 0, then AU contains the unfactored upper triangle of general sparse matrix A.
- If you are doing a **factor only**, and if IPARM(3) > 0, then AU contains the partially factored upper triangle of general sparse matrix **A**. The first IPARM(3) columns in the upper triangle of **A** are already factored. The remaining columns are factored in this computation.
- If you are doing a **solve only**, then AU contains the factored upper triangle of general sparse matrix **A**, produced by a preceding call to this subroutine.

#### In each case:

If IPARM(4) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(4) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

Specified as: a one-dimensional array of (at least) length *nu*, containing long-precision real numbers.

nu

is the length of array AU. Specified as: a fullword integer;  $nu \ge 0$  and  $nu \ge (IDU(n+1)-1)$ .

idu

is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix  $\bf{A}$  (in one of its three forms) in array AU. Specified as: a one-dimensional array of (at least) length n+1, containing fullword integers.

al

is the array, referred to as AL, containing one of three forms of the lower triangular part of general sparse matrix **A**, depending on the type of computation performed, where:

- If you are doing a factor and solve or a factor only, and if IPARM(3) = 0, then AL contains the unfactored lower triangle of general sparse matrix A.
- If you are doing a factor only, and if IPARM(3) > 0, then AL contains the
  partially factored lower triangle of general sparse matrix A. The first
  IPARM(3) rows in the lower triangle of A are already factored. The
  remaining rows are factored in this computation.
- If you are doing a solve only, then AL contains the factored lower triangle
  of general sparse matrix A, produced by a preceding call to this subroutine.

**Note:** In all these cases, entries in AL for diagonal elements of **A** are not assumed to have meaningful values.

In each case:

If IPARM(4) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(4) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

Specified as: a one-dimensional array of (at least) length *nl*, containing long-precision real numbers.

nl

is the length of array AL. Specified as: a fullword integer;  $nl \ge 0$  and  $nl \ge (IDL(n+1)-1)$ .

idl

is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix **A** (in one of its three forms) in array AL. Specified as: a one-dimensional array of (at least) length *n*+1, containing fullword integers. *iparm* 

is an array of parameters, IPARM(i), where:

• IPARM(1) indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:

If IPARM(1) = 0, the following default values are used. For restrictions, see "Notes" on page 602.

```
IPARM(2) = 0

IPARM(3) = 0

IPARM(4) = 0

IPARM(5) = 0

IPARM(10) = 0

IPARM(11) = -1

IPARM(12) = -1

IPARM(13) = -1

IPARM(14) = -1

IPARM(15) = 0

RPARM(10) = 10^{-12}
```

If IPARM(1) = 1, the default values are not used.

• IPARM(2) indicates the type of computation performed by this subroutine. The following table gives the IPARM(2) values for each variation:

Type of Computation	Ax = b	Ax = b and Determinant(A)	$A^{T}x = b$	$A^{T}x = b$ and Determinant(A)
Factor and Solve	0	10	100	110
Factor Only	1	11	N/A	N/A
Solve Only	2	N/A	102	N/A

• IPARM(3) indicates whether a full or partial factorization is performed on matrix **A**, where:

If IPARM(3) = 0, and:

If you are doing a **factor and solve** or a **factor only**, then a full factorization is performed for matrix  $\boldsymbol{A}$  on rows and columns 1 through n.

If you are doing a **solve only**, this argument has no effect on the computation, but must be set to 0.

If IPARM(3) > 0, and you are doing a **factor only**, then a partial factorization is performed on matrix  $\boldsymbol{A}$ . Rows 1 through IPARM(3) of columns 1 through IPARM(3) in matrix  $\boldsymbol{A}$  must be in factored form from a preceding call to this subroutine. The factorization is performed on rows IPARM(3)+1 through  $\boldsymbol{n}$  and columns IPARM(3)+1 through  $\boldsymbol{n}$ . For an illustration, see "Notes" on page 602.

• IPARM(4) indicates the input storage mode used for matrix **A**. This determines the arrangement of data in arrays AU, IDU, AL, and IDL on input, where:

If IPARM(4) = 0, diagonal-out skyline storage mode is used.

If IPARM(4) = 1, profile-in skyline storage mode is used.

IPARM(5) indicates the output storage mode used for matrix A. This
determines the arrangement of data in arrays AU, IDU, AL, and IDL on
output, where:

If IPARM(5) = 0, diagonal-out skyline storage mode is used.

If IPARM(5) = 1, profile-in skyline storage mode is used.

- IPARM(6) through IPARM(9) are reserved.
- IPARM(10) has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, then IPARM(10) indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:

If IPARM(10) = 0, the following default values are used. For restrictions, see "Notes" on page 602.

IPARM(11) = -1

IPARM(12) = -1

IPARM(13) = -1

IPARM(14) = -1

IPARM(15) = 0

 $RPARM(10) = 10^{-12}$ 

If IPARM(10) = 1, the default values are not used.

If you are doing a **solve only**, this argument is not used.

• IPARM(11) through IPARM(15) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, then IPARM(11) through IPARM(15) control the type of processing to apply to pivot elements occurring in regions 1 through 5, respectively. The pivot elements are  $u_{kk}$  for k=1, n when doing a full factorization, and they are k=IPARM(3)+1, n when doing a partial factorization. The region in which a pivot element falls depends on the sign and magnitude of the pivot element. The regions are determined by RPARM(10). For a description of the regions and associated pivot values, see "Notes" on page 602. For each region i for i=1,5, where the pivot occurs in region i, the processing applied to the pivot element is determined by IPARM(10+i), where:

If IPARM(10+i) = -1, the pivot element is trapped and computational error 2126 is generated. See "Error Conditions" on page 604. If IPARM(10+i) = 0, for i = 1, 2, 4, and 5, processing continues normally.

**Note:** A value of 0 is not permitted for region 3, because if processing continues, a divide-by-zero exception occurs.

If IPARM(10+i) = 1, the pivot element is replaced with the value in RPARM(10+i), and processing continues normally.

If you are doing a **solve only**, these arguments are not used.

IPARM(16) through IPARM(25), see "On Return" on page 600.

Specified as: a one-dimensional array of (at least) length 25, containing fullword integers, where:

```
IPARM(1) = 0 or 1

IPARM(2) = 0, 1, 2, 10, 11, 100, 102, or 110

If IPARM(2) = 0, 2, 10, 100, 102, or 110, then IPARM(3) = 0

If IPARM(2) = 1 or 11, then 0 \le IPARM(3) \le n

IPARM(4), IPARM(5) = 0 or 1

If IPARM(2) = 0, 1, 10, 11, 100, or 110, then:

IPARM(10) = 0 or 1

IPARM(11), IPARM(12) = -1, 0, or 1

IPARM(13) = -1 or 1

IPARM(14), IPARM(15) = -1, 0, or 1
```

rparm

is an array of parameters, RPARM(i), where:

- RPARM(1) through RPARM(9) are reserved.
- RPARM(10) has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, RPARM(10) is the tolerance value for small pivots. This sets the bounds for the pivot regions, where pivots are processed according to the options you specify for the five regions in IPARM(11) through IPARM(15), respectively. The suggested value is  $10^{-15} \le IPARM(10) \le 1$ .

If you are doing a solve only, this argument is not used.

RPARM(11) through RPARM(15) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, RPARM(11) through RPARM(15) are the fix-up values to use for the pivots in regions 1 through 5, respectively. For each RPARM(10+i) for i = 1,5, where the pivot occurs in region i:

If IPARM(10+i) = 1, the pivot is replaced with RPARM(10+i), where |RPARM(10+i)| should be a sufficiently large nonzero value to avoid overflow when calculating the reciprocal of the pivot. The suggested value is  $10^{-15} \le |\text{RPARM}(10+i)| \le 1$ .

If IPARM(10+i)  $\neq$  1, RPARM(10+i) is not used.

If you are doing a solve only, these arguments are not used.

• RPARM(16) through RPARM(25), see "On Return" on page 600.

Specified as: a one-dimensional array of (at least) length 25, containing long-precision real numbers, where if IPARM(2) = 0, 1, 10, 11, 100, or 110, then:

```
RPARM(10) \geq 0.0
RPARM(11) through RPARM(15) \neq 0.0
```

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing long-precision real numbers. naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DGKFS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,

If you are doing a **factor only**, use  $naux \ge 5n$ .

If you are doing a **factor and solve** or a **solve only**, use  $naux \ge 5n+4mbx$ .

bx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, bx is the array, containing the mbx right-hand side vectors b of the system Ax = b or  $A^Tx = b$ . Each vector b is length b and is stored in the corresponding column of the array.

If you are doing a factor only, this argument is not used in the computation.

Specified as: an *Idbx* by (at least) *mbx* array, containing long-precision real numbers.

ldbx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *ldbx* is the leading dimension of the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $ldbx \ge n$  and:

If  $mbx \neq 0$ , then ldbx > 0.

If mbx = 0, then  $ldbx \ge 0$ .

#### mbx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *mbx* is the number of right-hand side vectors, **b**, in the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $mbx \ge 0$ .

#### On Return

au

is the array, referred to as AU, containing the upper triangular part of the LU factored form of general sparse matrix A, where:

If IPARM(5) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(5) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

(If mbx = 0 and you are doing a solve only, then au is unchanged on output.) Returned as: a one-dimensional array of (at least) length nu, containing long-precision real numbers.

idu

is the array, referred to as IDU, containing the relative positions of the diagonal elements of the factored output matrix  $\bf{A}$  in array AU. (If mbx = 0 and you are doing a solve only, then idu is unchanged on output.) Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

al

is the array, referred to as AL, containing the lower triangular part of the LU factored form of general sparse matrix A, where:

If IPARM(5) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(5) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

**Note:** You should assume that entries in AL for diagonal elements of **A** do not have meaningful values.

(If mbx = 0 and you are doing a solve only, then *al* is unchanged on output.) Returned as: a one-dimensional array of (at least) length *nl*, containing long-precision real numbers.

idl

is the array, referred to as IDL, containing the relative positions of the diagonal elements of the factored output matrix  $\bf A$  in array AL. (If mbx = 0 and you are doing a solve only, then idl is unchanged on output.) Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

iparm

is an array of parameters, IPARM(i), where:

- IPARM(1) through IPARM(15) are unchanged.
- IPARM(16) has the following meaning, where:

If you are doing a factor and solve or a factor only, and:

If IPARM(16) = -1, your factorization did not complete successfully, resulting in computational error 2126.

If IPARM(16) > 0, it is the row number k, in which the maximum absolute value of the ratio  $a_{kk}/u_{kk}$  occurred, where:

If IPARM(3) = 0, k can be any of the rows, 1 through n, in the full factorization.

If IPARM(3) > 0, k can be any of the rows, IPARM(3)+1 through n, in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- IPARM(17) through IPARM(20) are reserved.
- IPARM(21) through IPARM(25) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, IPARM(21) through IPARM(25) have the following meanings for each region i for i = 1,5, respectively:

If IPARM(20+i) = -1, your factorization did not complete successfully, resulting in computational error 2126.

If IPARM(20+i)  $\geq$  0, it is the number of pivots in region i for the columns that were factored in matrix A, where:

If IPARM(3) = 0, columns 1 through n were factored in the full factorization.

If IPARM(3) > 0, columns IPARM(3)+1 through n were factored in the partial factorization.

If you are doing a **solve only**, these arguments are not used in the computation and are unchanged.

Returned as: a one-dimensional array of (at least) length 25, containing fullword integers.

#### rparm

is an array of parameters, RPARM(i), where:

- RPARM(1) through RPARM(15) are unchanged.
- RPARM(16) has the following meaning, where:

If you are doing a factor and solve or a factor only, and:

If RPARM(16) = 0.0, your factorization did not complete successfully, resulting in computational error 2126.

If |RPARM(16)| > 0.0, it is the ratio for row k,  $a_{kk}/u_{kk}$ , having the maximum absolute value. Row k is indicated in IPARM(16), and:

If IPARM(3) = 0, the ratio corresponds to one of the rows, 1 through n, in the full factorization.

If IPARM(3) > 0, the ratio corresponds to one of the rows, IPARM(3)+1 through n, in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

• RPARM(17) and RPARM(18) have the following meaning, where:

If you are **computing the determinant** of matrix **A**, then RPARM(17) is the mantissa, *detbas*, and RPARM(18) is the power of 10, *detpwr*, used to

express the value of the determinant: detbas(10<sup>detpwr</sup>), where 1 ≤ *detbas* < 10. Also:

If IPARM(3) = 0, the determinant is computed for columns 1 through nin the full factorization.

If IPARM(3) > 0, the determinant is computed for columns IPARM(3)+1 through *n* in the partial factorization.

If you are **not computing the determinant** of matrix **A**, these arguments are not used in the computation and are unchanged.

RPARM(19) through RPARM(25) are reserved.

Returned as: a one-dimensional array of (at least) length 25, containing long-precision real numbers.

bx

has the following meaning, where:

If you are doing a factor and solve or a solve only, bx is the array, containing the *mbx* solution vectors **x** of the system Ax = b or  $A^Tx = b$ . Each vector **x** is length n and is stored in the corresponding column of the array. (If mbx = 0, then bx is unchanged on output.)

If you are doing a factor only, this argument is not used in the computation and is unchanged.

Returned as: an *ldbx* by (at least) *mbx* array, containing long-precision real numbers.

#### Notes

- 1. If you set either IPARM(1) = 0 or IPARM(10) = 0, indicating you want to use the default values for IPARM(11) through IPARM(15) and RPARM(10), then:
  - Matrix A must be positive definite.
  - No pivots are fixed, using RPARM(11) through RPARM(15) values.
  - · No small pivots are tolerated; that is, the value should be |pivot| > RPARM(10).
- 2. Many of the input and output parameters for iparm and rparm are defined for the five pivot regions handled by this subroutine. The limits of the regions are based on RPARM(10), as shown in Figure 11. The pivot values in each region are:

```
Region 1: pivot < -RPARM(10)
Region 2: -RPARM(10) \le pivot < 0
Region 3: pivot = 0
Region 4: 0 < pivot \le RPARM(10)
Region 5: pivot > RPARM(10)
```

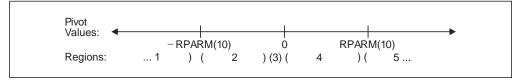


Figure 11. Five Pivot Regions

- 3. The IPARM(4) and IPARM(5) arguments allow you to specify the same or different skyline storage modes for your input and output arrays for matrix A. This allows you to change storage modes as needed. However, if you are concerned with performance, you should use diagonal-out skyline storage mode for both input and output, if possible, because there is less overhead.
  - For a description of how sparse matrices are stored in skyline storage mode, see "Profile-In Skyline Storage Mode" on page 103 and "Diagonal-Out Skyline Storage Mode" on page 101.
- 4. Following is an illustration of the portion of matrix  $\mathbf{A}$  factored in the partial factorization when IPARM(3) > 0. In this case, the subroutine assumes that rows and columns 1 through IPARM(3) are already factored and that rows and columns IPARM(3)+1 through n are to be factored in this computation.

You use the partial factorization function when, for design or storage reasons, you must factor the matrix  $\boldsymbol{A}$  in stages. When doing a partial factorization, you must use the same skyline storage mode for all parts of the matrix as it is progressively factored.

- 5. Your various arrays must have no common elements; otherwise, results are unpredictable.
- 6. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** This subroutine can factor, compute the determinant of, and solve general sparse matrix **A**, stored in skyline storage mode. For all computations, input matrix **A** can be stored in either diagonal-out or profile-in skyline storage mode. Output matrix **A** can also be stored in either of these modes and can be different from the mode used for input.

Matrix **A** is factored into the following form using specified pivot processing:

$$A = LU$$

where:

U is an upper triangular matrix.L is a lower triangular matrix.

The transformed matrix **A**, factored into its **LU** form, is stored in packed format in arrays AU and AL. The inverse of the diagonal of matrix  $\boldsymbol{U}$  is stored in the corresponding elements of array AU. The off-diagonal elements of the upper triangular matrix **U** are stored in the corresponding off-diagonal elements of array AU. The off-diagonal elements of the lower triangular matrix L are stored in the corresponding off-diagonal elements of array AL. (The diagonal elements stored in array AL do not have meaningful values.)

The partial factorization of matrix **A**, which you can do when you specify the factor-only option, assumes that the first IPARM(3) rows and columns are already factored in the input matrix. It factors the remaining n-IPARM(3) rows and columns in matrix A. (See "Notes" on page 602 for an illustration.) It updates only the elements in arrays AU and AL corresponding to the part of matrix **A** that is factored.

The determinant can be computed with any of the factorization computations. With a full factorization, you get the determinant for the whole matrix. With a partial factorization, you get the determinant for only that part of the matrix factored in this computation.

The system Ax = b or  $A^Tx = b$ , having multiple right-hand sides, is solved for x, using the transformed matrix A produced by this call or a subsequent call to this subroutine.

See references [9], [12], [25], [47], and [65]. If *n* is 0, no computation is performed. If mbx is 0, no solve is performed.

#### **Error Conditions**

#### Resource Errors

- Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.
- Unable to allocate internal work area.

#### Computational Errors

- 1. If a pivot occurs in region i for i = 1,5 and IPARM(10+i) = 1, the pivot value is replaced with RPARM(10+i), an attention message is issued, and processing continues.
- 2. Unacceptable pivot values occurred in the factorization of matrix A.
  - One or more diagonal elements of **U** contains unacceptable pivots and no valid fixup is applicable. The row number i of the first unacceptable pivot element is identified in the computational error message.
  - The return code is set to 2.
  - i can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2126 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

- 1. n < 0
- 2. nu < 0
- 3. IDU(n+1) > nu+1
- 4.  $IDU(i+1) \leq IDU(i)$  for i = 1, n

```
5. IDU(i+1) > IDU(i)+i and IPARM(4) = 0 for i = 1, n
 6. IDU(i) > IDU(i-1)+i and IPARM(4) = 1 for i = 2, n
 7. nI < 0
 8. IDL(n+1) > nl+1
 9. IDL(i+1) \leq IDL(i) for i = 1, n
10. IDL(i+1) > IDL(i)+i and IPARM(4) = 0 for i = 1, n
11. IDL(i) > IDL(i-1)+i and IPARM(4) = 1 for i = 2, n
12. IPARM(1) \neq 0 or 1
13. IPARM(2) \neq 0, 1, 2, 10, 11, 100, 102, or 110
14. IPARM(3) < 0
15. IPARM(3) > n
16. IPARM(3) > 0 and IPARM(2) \neq 1 or 11
17. IPARM(4), IPARM(5) \neq 0 or 1
18. IPARM(2) = 0, 1, 10, 11, 100, or 110 and:
        IPARM(10) \neq 0 \text{ or } 1
        IPARM(11), IPARM(12) \neq -1, 0, or 1
        IPARM(13) \neq -1 \text{ or } 1
        IPARM(14), IPARM(15) \neq -1, 0, or 1
        RPARM(10) < 0.0
        RPARM(10+i) = 0.0 and IPARM(10+i) = 1 for i = 1.5
19. IPARM(2) = 0, 2, 10, 100, 102, or 110 and:
        Idbx \le 0 and mbx \ne 0 and n \ne 0
        ldbx < 0 and mbx = 0
        ldbx < n \text{ and } mbx \neq 0
        mbx < 0
```

20. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to factor a 9 by 9 general sparse matrix  $\boldsymbol{A}$  and solve the system  $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$  with three right-hand sides. The default values are used for IPARM and RPARM. Input matrix  $\boldsymbol{A}$ , shown here, is stored in diagonal-out skyline storage mode. Matrix  $\boldsymbol{A}$  is:

```
2.0 2.0 2.0 0.0 0.0 0.0 0.0 0.0
                                  0.0
2.0 4.0 4.0 2.0 2.0 0.0 0.0 0.0
                                  2.0
2.0 4.0 6.0 4.0 4.0 0.0 2.0 0.0
                                  4.0
2.0 4.0 6.0 6.0 6.0 2.0 4.0 0.0
                                  6.0
0.0 0.0 0.0 2.0 4.0 4.0 4.0 2.0
                                  4.0
0.0 2.0 4.0 6.0 8.0 6.0 8.0 4.0 10.0
0.0 0.0 0.0 2.0 4.0 6.0
                        8.0 6.0
                                 8.0
0.0 0.0 0.0 2.0 4.0 6.0
                        8.0 8.0 10.0
2.0 4.0 6.0 6.0 8.0 6.0 10.0 8.0 16.0
```

Output matrix A, shown here, is in LU factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix B is:

```
0.5 2.0
          2.0
                                     0.0
               0.0
                     0.0
                          0.0
                               0.0
1.0
     0.5
          2.0
                2.0
                     2.0
                          0.0
                               0.0
                                     0.0
                                          2.0
     1.0
          0.5
                2.0
                     2.0
                          0.0
                               2.0
1.0
     1.0
          1.0
                0.5
                     2.0
                          2.0
                               2.0
                                     0.0
0.0
          0.0
                     0.5
                          2.0
                               2.0
                                     2.0
                                          2.0
     0.0
                1.0
                     1.0
                          0.5
                               2.0
0.0
     1.0
          1.0
                1.0
                                     2.0
                                          2.0
0.0
     0.0
          0.0
                1.0
                     1.0
                          1.0
                               0.5
                                    2.0
                                          2.0
0.0
     0.0
          0.0
                1.0
                    1.0
                          1.0
                               1.0
                                    0.5
                                          2.0
1.0
     1.0
          1.0
               1.0 1.0 1.0 1.0 1.0
                                          0.5
```

#### Call Statement and Input

```
NU IDU AL NL IDL IPARM
                                             RPARM AUX
                                                       NAUX BX
CALL DGKFS( 9 , AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57 , BX , 12 , 3 )
                   ΑU
                           = (2.0, 4.0, 2.0, 6.0, 4.0, 2.0, 6.0, 4.0, 2.0, 4.0, 6.0,
                               4.0, 2.0, 6.0, 4.0, 2.0, 8.0, 8.0, 4.0, 4.0, 2.0, 8.0,
                               6.0, 4.0, 2.0, 16.0, 10.0, 8.0, 10.0, 4.0, 6.0, 4.0, 2.0)
                   IDU
                           = (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
                              (0.0, 0.0, 2.0, 0.0, 4.0, 2.0, 0.0, 6.0, 4.0, 2.0, 0.0,
                   ΑL
                              2.0, 0.0, 8.0, 6.0, 4.0, 2.0, 0.0, 6.0, 4.0, 2.0, 0.0,
                              8.0, 6.0, 4.0, 2.0, 0.0, 8.0, 10.0, 6.0, 8.0, 6.0, 6.0,
                              4.0, 2.0)
                   IDL
                              (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
                   IPARM
                              . , . , . , . , . , . , . , . , . )
```

#### RPARM =(not relevant)

```
18.00
           6.00
                   12.00
                   32.00
                            48.00
          16.00
                   52.00
          26.00
                            78.00
          36.00
                   72.00
                           108.00
          20.00
                   40.00
                            60.00
ВХ
          48.00
                   96.00
                           144.00
          34.00
                   68.00
                           102.00
          38.00
                   76.00
                           114.00
          66.00
                  132.00
                          198.00
```

#### Output

```
IDL
       =(same as input)
TPARM
       = (0, . , . , . , . , .
           ., 9, ., ., ., 0, 0, 0, 0, 9)
RPARM
           .,8.0,.,.,.,.,.,.,.,.)
                  3.00
        1.00
             2.00
        1.00 2.00
                  3.00
        1.00 2.00 3.00
        1.00 2.00
                  3.00
        1.00 2.00
                  3.00
        1.00 2.00
                  3.00
        1.00 2.00
                  3.00
        1.00 2.00 3.00
        1.00 2.00 3.00
```

**Example 2:** This example shows how to factor the 9 by 9 general sparse matrix  $\boldsymbol{A}$  from Example 1, solve the system  $\boldsymbol{A}^T\boldsymbol{x} = \boldsymbol{b}$  with three right-hand sides, and compute the determinant of  $\boldsymbol{A}$ . The default values for pivot processing are used for IPARM. Input matrix  $\boldsymbol{A}$  is stored in profile-in skyline storage mode. Output matrix  $\boldsymbol{A}$  is in  $\boldsymbol{L}\boldsymbol{U}$  factored form with  $\boldsymbol{U}^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. It is the same as output matrix  $\boldsymbol{A}$  in Example 1.

Call Statement and Input

```
N AU NU IDU AL NL IDL IPARM RPARM AUX NAUX BX LDBX MBX
                                                               &darrow
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57, BX, 12, 3)
                  ΑU
                          = (2.0, 2.0, 4.0, 2.0, 4.0, 6.0, 2.0, 4.0, 6.0, 2.0, 4.0,
                              6.0, 4.0, 2.0, 4.0, 6.0, 2.0, 4.0, 4.0, 8.0, 8.0, 2.0,
                              4.0, 6.0, 8.0, 2.0, 4.0, 6.0, 4.0, 10.0, 8.0, 10.0, 16.0)
                  IDU
                             (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)
                            (0.0, 2.0, 0.0, 2.0, 4.0, 0.0, 2.0, 4.0, 6.0, 0.0, 2.0,
                  ΑL
                              0.0, 2.0, 4.0, 6.0, 8.0, 0.0, 2.0, 4.0, 6.0, 0.0, 2.0,
                              4.0, 6.0, 8.0, 0.0, 2.0, 4.0, 6.0, 6.0, 8.0, 6.0, 10.0,
                              8.0, 0.0
                  IDL
                             (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)
                  IPARM
                             . , . , . , . , . , . , . , . )
                  RPARM
                          =(not relevant)
```

```
30.00
          10.00
                  20.00
          20.00
                  40.00
                          60.00
          28.00
                  56.00
                          84.00
          30.00
                  60.00
                          90.00
          40.00
                  80.00
                         120.00
ВХ
          30.00
                  60.00
                          90.00
          44.00
                  88.00 132.00
          28.00
                  56.00
                          84.00
          60.00 120.00 180.00
```

#### Output

```
ΑU
       =(same as output AU in Example 1)
IDU
       =(same as output IDU in Example 1)
ΑL
       =(same as output AL in Example 1)
IDL
       =(same as output IDL in Example 1)
          (1, 110, 0, 1, 0, . , . , . , . , 0, . , . , . ,
IPARM
           9, . , . , . , 0, 0, 0, 0, 9)
RPARM
          ., 8.0, 5.12, 2.0, ., ., ., ., ., .)
BX
       =(same as output BX in Example 1)
```

**Example 3:** This example shows how to factor a 9 by 9 negative-definite general sparse matrix  $\mathbf{A}$ , solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  with three right-hand sides, and compute the determinant of  $\mathbf{A}$ . (Default values for pivot processing are not used for IPARM because  $\mathbf{A}$  is negative-definite.) Input matrix  $\mathbf{A}$ , shown here, is stored in diagonal-out skyline storage mode:

```
0.0
     -2.0
           -2.0
                        0.0
                             0.0
                                    0.0
                                          0.0
                  0.0
                 -2.0
                                    0.0
-2.0 -4.0
          -4.0
                       -2.0
                                          0.0
                             0.0
                                                -2.0
-2.0 -4.0
          -6.0
                -4.0
                       -4.0
                             0.0
                                   -2.0
                                          0.0
                                                -4.0
-2.0 -4.0
          -6.0
                -6.0
                      -6.0
                            -2.0
                                   -4.0
                                          0.0
                                                -6.0
0.0
      0.0
           0.0
                -2.0
                      -4.0 -4.0
                                   -4.0
                                         -2.0
                                                -4.0
           -4.0 -6.0 -8.0 -6.0
0.0
     -2.0
                                   -8.0
                                         -4.0
                                               -10.0
            0.0 -2.0 -4.0 -6.0
0.0
      0.0
                                   -8.0 -6.0
                                               -8.0
            0.0 -2.0 -4.0 -6.0
0.0
      0.0
                                   -8.0 -8.0
                                              -10.0
-2.0
           -6.0 -6.0 -8.0 -6.0 -10.0 -8.0 -16.0
```

Output matrix A, shown here, is in LU factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix A is:

```
0.0
-0.5 -2.0
            -2.0
                    0.0
                                        0.0
                                              0.0
                          0.0
                                 0.0
            -2.0
1.0
      -0.5
                   -2.0
                         -2.0
                                 0.0
                                        0.0
                                              0.0
                                                   -2.0
                   -2.0
1.0
       1.0
            -0.5
                         -2.0
                                 0.0
                                       -2.0
                                              0.0
                                                   -2.0
1.0
       1.0
             1.0
                   -0.5
                         -2.0
                                -2.0
                                       -2.0
                                              0.0
                                                   -2.0
0.0
       0.0
                    1.0
                         -0.5
                                -2.0
                                       -2.0
                                             -2.0
                                                   -2.0
             0.0
0.0
       1.0
                          1.0
                                -0.5
                                       -2.0
                                             -2.0
                                                   -2.0
             1.0
                    1.0
0.0
       0.0
             0.0
                    1.0
                          1.0
                                 1.0
                                       -0.5
                                             -2.0
                                                   -2.0
0.0
       0.0
             0.0
                    1.0
                          1.0
                                 1.0
                                        1.0
                                             -0.5
                                                  -2.0
1.0
       1.0
             1.0
                    1.0
                          1.0
                                 1.0
                                              1.0 -0.5
                                        1.0
```

#### Call Statement and Input

```
N AU NU IDU AL NL IDL IPARM RPARM AUX NAUX BX
                                                        LDBX MBX
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 57, BX, 12, 3)
                ΑU
                        = (-2.0, -4.0, -2.0, -6.0, -4.0, -2.0, -6.0, -4.0, -2.0,
                           -4.0, -6.0, -4.0, -2.0, -6.0, -4.0, -2.0, -8.0, -8.0,
                           -4.0, -4.0, -2.0, -8.0, -6.0, -4.0, -2.0, -16.0, -10.0,
                           -8.0, -10.0, -4.0, -6.0, -4.0, -2.0)
                IDU
                        = (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
                ΑL
                         (0.0, 0.0, -2.0, 0.0, -4.0, -2.0, 0.0, -6.0, -4.0, -2.0,
                           0.0, -2.0, 0.0, -8.0, -6.0, -4.0, -2.0, 0.0, -6.0, -4.0,
                           -2.0, 0.0, -8.0, -6.0, -4.0, -2.0, 0.0, -8.0, -10.0,
                           -6.0, -8.0, -6.0, -6.0, -4.0, -2.0
                IDL
                        = (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
                 IPARM
                         (1, 10, 0, 0, 0, ., ., ., ., 1, 0, -1, -1, -1, -1, .,
                           . , . , . , . , . , . , . , . )
                          (.,.,.,.,.,.,.,.,.,.,.,10^{-15},.,.,.,
                RPARM
                                       , . , . , . , . , . , . , . , . )
                BX
                        =(same as input BX in Example 1)
                 Output
                ΑU
                        = (-0.5, -0.5, -2.0, -0.5, -2.0, -2.0, -0.5, -2.0, -2.0,
                           -0.5, -2.0, -2.0, -2.0, -0.5, -2.0, -2.0, -0.5, -2.0,
                           -2.0, -2.0, -2.0, -0.5, -2.0, -2.0, -2.0, -0.5, -2.0,
                           -2.0, -2.0, -2.0, -2.0, -2.0, -2.0)
                IDU
                        =(same as input)
                ΑL
                        1.0, 1.0)
                 IDL
                        =(same as input)
                          (1, 10, 0, 0, 0, ., ., ., ., 1, 0, -1, -1, -1, -1, 9,
                 IPARM
                           .,.,.,.,9,0,0,0,0
                RPARM
                          .,.,.,8.0, -5.12, 2.0, .,.,.,.,.,.)
```

**Example 4:** This example shows how to factor the first six rows and columns, referred to as matrix **A1**, of the 9 by 9 general sparse matrix **A** from Example 1 and compute the determinant of **A1**. Input matrix **A1**, shown here, is stored in diagonal-out skyline storage mode. Input matrix **A1** is:

Output matrix A1, shown here, is in LU factored form with  $U^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Output matrix A1 is:

```
    0.5
    2.0
    2.0
    0.0
    0.0
    0.0

    1.0
    0.5
    2.0
    2.0
    2.0
    0.0

    1.0
    1.0
    0.5
    2.0
    2.0
    0.0

    1.0
    1.0
    1.0
    0.5
    2.0
    2.0

    0.0
    0.0
    0.0
    1.0
    0.5
    2.0

    0.0
    1.0
    1.0
    1.0
    1.0
    0.5
```

#### Call Statement and Input

```
AU NU IDU AL NL IDL IPARM
                                               RPARM AUX NAUX
                                                                       LDBX
                                                                              MBX
CALL DGKFS( 6, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 45, BX, LDBX, MBX)
ΑU
         =(same as input AU in Example 1)
IDU
         = (1, 2, 4, 7, 10, 14, 17)
ΑL
         =(same as input AL in Example 1)
IDL
           (1, 2, 4, 7, 11, 13, 18)
           (1, 11, 0, 0, 0, ., ., ., 0, ., ., ., ., ., .,
IPARM
RPARM
         =(not relevant)
ВХ
         =(not relevant)
LDBX
         =(not relevant)
MBX
         =(not relevant)
```

# Output

```
ΑU
                                                        = (0.5, 0.5, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0,
                                                                                 2.0, 2.0, 0.5, 2.0, 2.0, 8.0, 8.0, 4.0, 4.0, 2.0, 8.0,
                                                                                 6.0, 4.0, 2.0, 16.0, 10.0, 8.0, 10.0, 4.0, 6.0, 4.0, 2.0)
IDU
                                                        =(same as input)
                                                                          ΑL
                                                                                 1.0, 0.0, 1.0, 1.0, 1.0, 0.0, 6.0, 4.0, 2.0, 0.0,
                                                                                8.0, 6.0, 4.0, 2.0, 0.0, 8.0, 10.0, 6.0, 8.0, 6.0, 6.0,
                                                                                 4.0, 2.0
 IDL
                                                        =(same as input)
 IPARM
                                                                          (1, 11, 0, 0, 0, \dots, \dots, 0, \dots, 3, \dots,
                                                                                   .,.,.,0,0,0,6)
RPARM
                                                                          ., 3.0, 6.4, 1.0, ., ., .,
ВХ
                                                        =(same as input)
LDBX
                                                        =(same as input)
MBX
                                                         =(same as input)
```

**Example 5:** This example shows how to do a partial factorization of the 9 by 9 general sparse matrix **A** from Example 1, where the first six rows and columns were factored in Example 4. It factors the remaining three rows and columns and computes the determinant of that part of the matrix. The input matrix, referred to as **A2**, shown here, is made up of the output factored matrix **A1** plus the three remaining unfactored rows and columns of matrix **A**. Matrix **A2** is:

```
0.5 2.0
         2.0
                              0.0 0.0
                                         0.0
              0.0
                   0.0
                        0.0
1.0 0.5
         2.0
              2.0
                   2.0
                              0.0
                                   0.0
                                         2.0
                        0.0
1.0
    1.0
         0.5
              2.0
                   2.0
                        0.0
                              2.0
                                   0.0
                                         4.0
    1.0
         1.0
              0.5
                   2.0
                        2.0
                              4.0
                                   0.0
                                         6.0
0.0
    0.0
         0.0
              1.0
                   0.5
                        2.0
                              4.0
                                   2.0
                                         4.0
                        0.5
                                   4.0
                                        10.0
0.0
    1.0
         1.0
              1.0
                   1.0
                              8.0
0.0
    0.0
         0.0
              2.0
                   4.0
                        6.0
                              8.0
                                   6.0
                                         8.0
                   4.0
0.0
         0.0 2.0
                                        10.0
    0.0
                        6.0
                              8.0 8.0
2.0
    4.0
         6.0
              6.0
                   8.0
                        6.0
                             10.0 8.0
                                        16.0
```

Both parts of input matrix **A2** are stored in diagonal-out skyline storage mode.

Output matrix **A2** is the same as output matrix **A** in Example 1 and is stored in diagonal-out skyline storage mode.

# Call Statement and Input

```
N AU NU IDU AL NL IDL
                                  IPARM
                                         RPARM AUX
                                                   NAUX
                                                            LDBX
                                                                  MBX
                                               CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 45, BX, LDBX, MBX)
ΑU
       =(same as output AU in Example 4)
IDU
       =(same as input IDU in Example 1)
ΑL
       =(same as output AL in Example 4)
IDL
       =(same as input IDL in Example 1)
IPARM
          . , . , . , . , . , . , . , . , . )
RPARM
       =(not relevant)
```

ВХ

```
=(not relevant)
LDBX
      =(not relevant)
MBX
      =(not relevant)
Output
ΑU
      =(same as output AU in Example 1)
IDU
      =(same as output IDU in Example 1)
ΑL
      =(same as output AL in Example 1)
IDL
      =(same as output IDL in Example 1)
      IPARM
         .,.,.,.,0,0,0,0,3)
RPARM
         ., 8.0, 8.0, 0.0, ., ., ., ., ., .)
ВХ
      =(same as input)
LDBX
      =(same as input)
MBX
      =(same as input)
```

**Example 6:** This example shows how to solve the system Ax = b with one right-hand side for a general sparse matrix A. Input matrix A, used here, is the same as factored output matrix A from Example 1, stored in profile-in skyline storage mode. Here, output matrix A is unchanged on output and is stored in profile-in skyline storage mode.

# Call Statement and Input

```
N AU NU IDU AL NL IDL IPARM
                                    RPARM AUX NAUX BX LDBX MBX
CALL DGKFS( 9, AU, 33, IDU, AL, 35, IDL, IPARM, RPARM, AUX, 49, BX, 9, 1)
               ΑU
                       (0.5, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0,
                         2.0, 0.5, 2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 0.5, 2.0,
                         2.0, 2.0, 0.5, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 0.5)
               IDU
                      = (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)
               ΑL
                      1.0, 0.0
               IDL
                        (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)
                       IPARM
                         . , . , . , . , . , . , . , . )
               RPARM
                      =(not relevant)
               ВХ
                        (12.0, 58.0, 114.0, 176.0, 132.0, 294.0, 240.0, 274.0,
                         406.0)
               Output
               ΑU
                      =(same as input)
               IDU
                      =(same as input)
               ΑL
                      =(same as input)
               IDL
                      =(same as input)
                      =(same as input)
               IPARM
               RPARM
                      =(not relevant)
               BX
                      = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)
```

# DSKFS—Symmetric Sparse Matrix Factorization, Determinant, and Solve Using Skyline Storage Mode

This subroutine can perform either or both of the following functions for symmetric sparse matrix  $\mathbf{A}$ , stored in skyline storage mode, and for vectors  $\mathbf{x}$  and  $\mathbf{b}$ :

- Factor **A** and, optionally, compute the determinant of **A**.
- Solve the system Ax = b using the results of the factorization of matrix A, produced on this call or a preceding call to this subroutine.

You have the choice of using either Gaussian elimination or Cholesky decomposition. You also have the choice of using profile-in or diagonal-out skyline storage mode for **A** on input or output.

**Note:** The input to the solve performed by this subroutine must be the output from the factorization performed by this subroutine.

# Syntax

Fortran	CALL DSKFS (n, a, na, idiag, iparm, rparm, aux, naux, bx, ldbx, mbx)	
C and C++	dskfs (n, a, na, idiag, iparm, rparm, aux, naux, bx, ldbx, mbx);	
PL/I	CALL DSKFS (n, a, na, idiag, iparm, rparm, aux, naux, bx, ldbx, mbx);	

# On Entry

n

is the order of symmetric sparse matrix  $\mathbf{A}$ . Specified as: a fullword integer;  $n \ge 0$ .

а

is the array, referred to as A, containing one of three forms of the upper triangular part of symmetric sparse matrix A, depending on the type of computation performed, where:

- If you are doing a **factor and solve** or a **factor only**, and if IPARM(3) = 0, then A contains the unfactored upper triangle of symmetric sparse matrix  $\mathbf{A}$ .
- If you are doing a **factor only**, and if IPARM(3) > 0, then A contains the partially factored upper triangle of symmetric sparse matrix **A**. The first IPARM(3) columns in the upper triangle of **A** are already factored. The remaining columns are factored in this computation.
- If you are doing a solve only, then A contains the factored upper triangle of sparse matrix A, produced by a preceding call to this subroutine.

#### In each case:

If IPARM(4) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(4) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

Specified as: a one-dimensional array of (at least) length *na*, containing long-precision real numbers.

na

is the length of array A. Specified as: a fullword integer;  $na \ge 0$  and  $na \ge (IDIAG(n+1)-1)$ .

idiag

is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix A (in one of its three forms) in array A. Specified as: a one-dimensional array of (at least) length n+1, containing fullword integers.

iparm

is an array of parameters, IPARM(i), where:

 IPARM(1) indicates whether certain default values for iparm and rparm are used by this subroutine, where:

If IPARM(1) = 0, the following default values are used. For restrictions, see "Notes" on page 620.

IPARM(2) = 0IPARM(3) = 0IPARM(4) = 0IPARM(5) = 0IPARM(10) = 0IPARM(11) = -1IPARM(12) = -1IPARM(13) = -1IPARM(14) = -1IPARM(15) = 0 $RPARM(10) = 10^{-12}$ 

If IPARM(1) = 1, the default values are not used.

• IPARM(2) indicates the type of computation performed by this subroutine. The following table gives the IPARM(2) values for each variation:

Type of Computation	Gaussian Elimination Ax = b	Gaussian Elimination Ax = b and Determinant(A)	Cholesky Decomposition $Ax = b$	Cholesky Decomposition $Ax = b$ and Determinant(A)
Factor and Solve	0	10	100	110
Factor Only	1	11	101	111
Solve Only	2	N/A	102	N/A

• IPARM(3) indicates whether a full or partial factorization is performed on matrix A, where:

If IPARM(3) = 0, and:

If you are doing a factor and solve or a factor only, then a full factorization is performed for matrix A on rows and columns 1 through

If you are doing a **solve only**, this argument has no effect on the computation, but must be set to 0.

If IPARM(3) > 0, and you are doing a **factor only**, then a partial factorization is performed on matrix  $\mathbf{A}$ . Rows 1 through IPARM(3) of columns 1 through IPARM(3) in matrix A must be in factored form from a preceding call to this subroutine. The factorization is performed on rows

IPARM(3)+1 through n and columns IPARM(3)+1 through n. For an illustration, see "Notes" on page 620.

• IPARM(4) indicates the input storage mode used for matrix **A**. This determines the arrangement of data in arrays A and IDIAG on input, where:

```
If IPARM(4) = 0, diagonal-out skyline storage mode is used.
```

```
If IPARM(4) = 1, profile-in skyline storage mode is used.
```

IPARM(5) indicates the output storage mode used for matrix A. This
determines the arrangement of data in arrays A and IDAIG on output,
where:

```
If IPARM(5) = 0, diagonal-out skyline storage mode is used.
```

If IPARM(5) = 1, profile-in skyline storage mode is used.

- IPARM(6) through IPARM(9) are reserved.
- IPARM(10) has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, then IPARM(10) indicates whether certain default values for *iparm* and *rparm* are used by this subroutine, where:

If IPARM(10) = 0, the following default values are used. For restrictions, see "Notes" on page 620.

```
See Notes on page 620.

IPARM(11) = -1

IPARM(12) = -1

IPARM(13) = -1

IPARM(14) = -1

IPARM(15) = 0

RPARM(10) = 10^{-12}

If IPARM(10) = 1, the default values are not used.
```

If you are doing a solve only, this argument is not used.

• IPARM(11) through IPARM(15) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, then IPARM(11) through IPARM(15) control the type of processing to apply to pivot elements occurring in regions 1 through 5, respectively. The pivot elements are  $d_{kk}$  for Gaussian elimination and  $r_{kk}$  for Cholesky decomposition for k=1, n when doing a full factorization, and they are k= IPARM(3)+1, n when doing a partial factorization. The region in which a pivot element falls depends on the sign and magnitude of the pivot element. The regions are determined by RPARM(10). For a description of the regions and associated pivot values, see "Notes" on page 620. For each region i for i=1,5, where the pivot occurs in region i, the processing applied to the pivot element is determined by IPARM(10+i), where:

If IPARM(10+i) = -1, the pivot element is trapped and computational error 2126 is generated. See "Error Conditions" on page 622. If IPARM(10+i) = 0, processing continues normally.

**Note:** A value of 0 is not permitted for region 3, because if processing continues, a divide-by-zero exception occurs. In addition, if you are doing a Cholesky decomposition, a value of 0 is not permitted in regions 1 and 2, because a square root exception occurs.

If IPARM(10+i) = 1, the pivot element is replaced with the value in RPARM(10+i), and processing continues normally.

If you are doing a **solve only**, these arguments are not used.

IPARM(16) through IPARM(25), see "On Return" on page 618.

Specified as: a one-dimensional array of (at least) length 25, containing fullword integers, where:

```
IPARM(1) = 0 or 1

IPARM(2) = 0, 1, 2, 10, 11, 100, 101, 102, 110, or 111

If IPARM(2) = 0, 2, 10, 100, 102, or 110, then IPARM(3) = 0

If IPARM(2) = 1, 11, 101, or 111, then 0 \le IPARM(3) \le n

IPARM(4), IPARM(5) = 0 or 1

If IPARM(2) = 0, 1, 10, or 11, then:

IPARM(10) = 0 or 1

IPARM(11), IPARM(12) = -1, 0, or 1

IPARM(13) = -1 or 1

IPARM(14), IPARM(15) = -1, 0, or 1

IPARM(10) = 0 or 1

IPARM(11), IPARM(12), IPARM(13) = -1 or 1

IPARM(14), IPARM(15) = -1, 0, or 1
```

is an array of parameters, RPARM(i), where:

- RPARM(1) through RPARM(9) are reserved.
- RPARM(10) has the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, RPARM(10) is the tolerance value for small pivots. This sets the bounds for the pivot regions, where pivots are processed according to the options you specify for the five regions in IPARM(11) through IPARM(15), respectively. The suggested value is  $10^{-15} \le \text{IPARM}(10) \le 1$ .

If you are doing a **solve only**, this argument is not used.

• RPARM(11) through RPARM(15) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, RPARM(11) through RPARM(15) are the fix-up values to use for the pivots in regions 1 through 5, respectively. For each RPARM(10+i) for i = 1,5, where the pivot occurs in region i:

If IPARM(10+i) = 1, the pivot is replaced with RPARM(10+i), where |RPARM(10+i)| should be a sufficiently large nonzero value to avoid overflow when calculating the reciprocal of the pivot. For Gaussian elimination, the suggested value is  $10^{-15} \le |\text{RPARM}(10+i)| \le 1$ . For Cholesky decomposition, the value must be RPARM(10+i) > 0. If IPARM(10+i)  $\ne$  1, RPARM(10+i) is not used.

If you are doing a solve only, these arguments are not used.

• RPARM(16) through RPARM(25), see "On Return" on page 618.

Specified as: a one-dimensional array of (at least) length 25, containing long-precision real numbers, where if IPARM(2) = 0, 1, 10, 11, 100, 101, 110, or 111, then:

```
RPARM(10) \ge 0.0
If IPARM(2) = 0, 1, 10, or 11, then RPARM(11) through RPARM(15) \ne 0.0
If IPARM(2) = 100, 101, 110, or 111, then RPARM(11) through
RPARM(15) > 0.0
```

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing long-precision real numbers. naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DSKFS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, If you are doing a **factor only**, you can use  $naux \ge n$ ; however, for optimal performance, use  $naux \ge 3n$ .

If you are doing a factor and solve or a solve only, use  $naux \ge 3n+4mbx$ .

For further details on error handling and the special factor-only case, see "Notes" on page 620.

bx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, bx is the array, containing the mbx right-hand side vectors b of the system Ax = b. Each vector b is length n and is stored in the corresponding column of the array.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: an *Idbx* by (at least) *mbx* array, containing long-precision real numbers.

ldbx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *ldbx* is the leading dimension of the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $ldbx \ge n$  and:

```
If mbx \neq 0, then ldbx > 0.

If mbx = 0, then ldbx \geq 0.

mbx
```

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, *mbx* is the number of right-hand side vectors, **b**, in the array specified for *bx*.

If you are doing a **factor only**, this argument is not used in the computation.

Specified as: a fullword integer;  $mbx \ge 0$ .

#### On Return

а

is the array, referred to as A, containing the upper triangular part of symmetric sparse matrix  $\mathbf{A}$  in  $\mathbf{LDL}^{\mathsf{T}}$  or  $\mathbf{R}^{\mathsf{T}}\mathbf{R}$  factored form, where:

If IPARM(5) = 0, diagonal-out skyline storage mode is used for  $\mathbf{A}$ .

If IPARM(5) = 1, profile-in skyline storage mode is used for  $\mathbf{A}$ .

(If mbx = 0 and you are doing a solve only, then a is unchanged on output.) Returned as: a one-dimensional array of (at least) length na, containing long-precision real numbers.

# idiag

is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of the factored output matrix  $\mathbf{A}$  in array A. (If mbx = 0 and you are doing a solve only, then idiag is unchanged on output.)

Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

#### iparm

is an array of parameters, IPARM(i), where:

- IPARM(1) through IPARM(15) are unchanged.
- IPARM(16) has the following meaning, where:

If you are doing a factor and solve or a factor only, and:

If IPARM(16) = -1, your factorization did not complete successfully, resulting in computational error 2126.

If IPARM(16) > 0, it is the row number k, in which the maximum absolute value of the ratio  $a_{kk}/d_{kk}$  for Gaussian elimination and  $a_{kk}/r_{kk}$  for Cholesky decomposition occurred, where:

If IPARM(3) = 0, k can be any of the rows, 1 through n, in the full factorization.

If IPARM(3) > 0, k can be any of the rows, IPARM(3)+1 through n, in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

- IPARM(17) through IPARM(20) are reserved.
- IPARM(21) through IPARM(25) have the following meaning, where:

If you are doing a **factor and solve** or a **factor only**, IPARM(21) through IPARM(25) have the following meanings for each region i for i = 1,5, respectively:

If IPARM(20+i) = -1, your factorization did not complete successfully, resulting in computational error 2126.

If IPARM(20+i)  $\geq$  0, it is the number of pivots in region i for the columns that were factored in matrix A, where:

If IPARM(3) = 0, columns 1 through n were factored in the full factorization.

If IPARM(3) > 0, columns IPARM(3)+1 through n were factored in the partial factorization.

If you are doing a **solve only**, these arguments are not used in the computation and are unchanged.

Returned as: a one-dimensional array of (at least) length 25, containing fullword integers.

#### rparm

is an array of parameters, RPARM(i), where:

- RPARM(1) through RPARM(15) are unchanged.
- RPARM(16) has the following meaning, where:

If you are doing a factor and solve or a factor only, and:

If RPARM(16) = 0.0, your factorization did not complete successfully, resulting in computational error 2126.

If |RPARM(16)| > 0.0, it is the ratio for row k,  $a_{kk}/d_{kk}$  for Gaussian elimination and  $a_{kk}/r_{kk}$  for Cholesky decomposition, having the maximum absolute value. Row k is indicated in IPARM(16), and:

If IPARM(3) = 0, the ratio corresponds to one of the rows, 1 through n, in the full factorization.

If IPARM(3) > 0, the ratio corresponds to one of the rows, IPARM(3)+1 through n, in the partial factorization.

If you are doing a **solve only**, this argument is not used in the computation and is unchanged.

• RPARM(17) and RPARM(18) have the following meaning, where:

If you are **computing the determinant** of matrix A, then RPARM(17) is the mantissa, *detbas*, and RPARM(18) is the power of 10, *detpwr*, used to express the value of the determinant:  $detbas(10^{detpwr})$ , where  $1 \le detbas < 10$ . Also:

If IPARM(3) = 0, the determinant is computed for columns 1 through n in the full factorization.

If IPARM(3) > 0, the determinant is computed for columns IPARM(3)+1 through n in the partial factorization.

If you are **not computing the determinant** of matrix **A**, these arguments are not used in the computation and are unchanged.

RPARM(19) through RPARM(25) are reserved.

Returned as: a one-dimensional array of (at least) length 25, containing long-precision real numbers.

bx

has the following meaning, where:

If you are doing a **factor and solve** or a **solve only**, bx is the array, containing the mbx solution vectors x of the system Ax = b. Each vector x is length n and is stored in the corresponding column of the array. (If mbx = 0, then bx is unchanged on output.)

If you are doing a **factor only**, this argument is not used in the computation and is unchanged.

Returned as: an *ldbx* by (at least) *mbx* array, containing long-precision real numbers.

#### Notes

- 1. When doing a **solve only**, you should specify the same factorization method in IPARM(2), Gaussian elimination or Cholesky decomposition, that you specified for your factorization on a previous call to this subroutine.
- 2. If you set either IPARM(1) = 0 or IPARM(10) = 0, indicating you want to use the default values for IPARM(11) through IPARM(15) and RPARM(10), then:
  - Matrix **A** must be positive definite.
  - No pivots are fixed, using RPARM(11) through RPARM(15) values.
  - No small pivots are tolerated; that is, the value should be |pivot| > RPARM(10).
- 3. Many of the input and output parameters for *iparm* and *rparm* are defined for the five pivot regions handled by this subroutine. The limits of the regions are based on RPARM(10), as shown in Figure 12. The pivot values in each region are:

```
Region 1: pivot < -RPARM(10)
Region 2: -RPARM(10) \le pivot < 0
```

Region 3: pivot = 0

Region 4:  $0 < pivot \le RPARM(10)$ Region 5: pivot > RPARM(10)

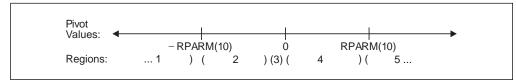


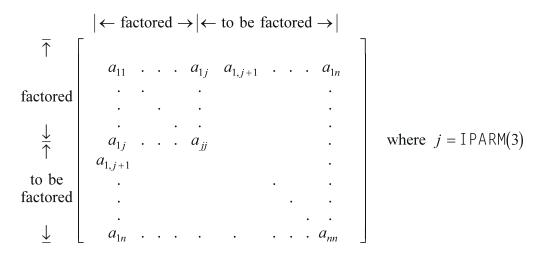
Figure 12. Five Pivot Regions

4. The IPARM(4) and IPARM(5) arguments allow you to specify the same or different skyline storage modes for your input and output arrays for matrix A. This allows you to change storage modes as needed. However, if you are concerned with performance, you should use diagonal-out skyline storage mode for both input and output, if possible, because there is less overhead.

For a description of how sparse matrices are stored in skyline storage mode, see "Profile-In Skyline Storage Mode" on page 103 and "Diagonal-Out Skyline Storage Mode" on page 101. Those descriptions use different array and variable names from the ones used here. To relate the two sets, use the following table:

Name Here	Name in the Storage Description
A	AU
na	nu
IDIAG	IDU

5. Following is an illustration of the portion of matrix  $\mathbf{A}$  factored in the partial factorization when IPARM(3) > 0. In this case, the subroutine assumes that rows and columns 1 through IPARM(3) are already factored and that rows and columns IPARM(3)+1 through n are to be factored in this computation.



You use the partial factorization function when, for design or storage reasons, you must factor the matrix  $\boldsymbol{A}$  in stages. When doing a partial factorization, you must use the same skyline storage mode for all parts of the matrix as it is progressively factored.

- 6. Your various arrays must have no common elements; otherwise, results are unpredictable.
- 7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** This subroutine can factor, compute the determinant of, and solve symmetric sparse matrix **A**, stored in skyline storage mode. It can use either Gaussian elimination or Cholesky decomposition. For all computations, input matrix **A** can be stored in either diagonal-out or profile-in skyline storage mode. Output matrix **A** can also be stored in either of these modes and can be different from the mode used for input.

For Gaussian elimination, matrix **A** is factored into the following form using specified pivot processing:

$$A = LDL^{T}$$

where:

**D** is a diagonal matrix.

L is a lower triangular matrix.

The transformed matrix  $\mathbf{A}$ , factored into its  $\mathbf{LDL}^{\mathsf{T}}$  form, is stored in packed format in array A, such that the inverse of the diagonal matrix  $\mathbf{D}$  is stored in the corresponding elements of array A. The off-diagonal elements of the unit upper triangular matrix  $\mathbf{L}^{\mathsf{T}}$  are stored in the corresponding off-diagonal elements of array A.

For Cholesky decomposition, matrix **A** is factored into the following form using specified pivot processing:

 $A = R^T R$ 

where *R* is an upper triangular matrix

The transformed matrix A, factored into its  $R^TR$  form, is stored in packed format in array A, such that the inverse of the diagonal elements of the upper triangular matrix **R** is stored in the corresponding elements of array A. The off-diagonal elements of matrix **R** are stored in the corresponding off-diagonal elements of array

The partial factorization of matrix A, which you can do when you specify the factor-only option, assumes that the first IPARM(3) rows and columns are already factored in the input matrix. It factors the remaining n-IPARM(3) rows and columns in matrix A. (See "Notes" on page 620 for an illustration.) It updates only the elements in array A corresponding to the part of matrix **A** that is factored.

The determinant can be computed with any of the factorization computations. With a full factorization, you get the determinant for the whole matrix. With a partial factorization, you get the determinant for only that part of the matrix factored in this computation.

The system Ax = b, having multiple right-hand sides, is solved for x using the transformed matrix **A** produced by this call or a subsequent call to this subroutine.

See references [9], [12], [25], [47], [65]. If n is 0, no computation is performed. If mbx is 0, no solve is performed.

#### **Error Conditions**

# Resource Errors

- Error 2015 is unrecoverable. naux = 0, and unable to allocate work area.
- · Unable to allocate internal work area.

# Computational Errors

- 1. If a pivot occurs in region i for i = 1,5 and IPARM(10+i) = 1, the pivot value is replaced with RPARM(10+i), an attention message is issued, and processing continues.
- 2. Unacceptable pivot values occurred in the factorization of matrix **A**.
  - One or more diagonal elements of D or R contains unacceptable pivots and no valid fixup is applicable. The row number *i* of the first unacceptable pivot element is identified in the computational error message.
  - The return code is set to 2.
  - i can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2126 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

# Input-Argument Errors

```
1. n < 0
 2. na < 0
 3. IDIAG(n+1) > na+1
 4. IDIAG(i+1) \leq IDIAG(i) for i = 1, n
 5. IDIAG(i+1) > IDIAG(i)+i and IPARM(4) = 0 for i = 1, n
 6. IDIAG(i) > IDIAG(i-1)+i and IPARM(4) = 1 for i = 2, n
 7. IPARM(1) \neq 0 or 1
 8. IPARM(2) \neq 0, 1, 2, 10, 11, 100, 101, 102, 110, or 111
 9. IPARM(3) < 0
10. IPARM(3) > n
11. IPARM(3) > 0 and IPARM(2) \neq 1, 11, 101, or 111
12. IPARM(4), IPARM(5) \neq 0 or 1
13. IPARM(2) = 0, 1, 10, or 11 and:
        IPARM(10) \neq 0 \text{ or } 1
        IPARM(11), IPARM(12) \neq -1, 0, or 1
        IPARM(13) \neq -1 or 1
        IPARM(14), IPARM(15) \neq -1, 0, or 1
        RPARM(10) < 0.0
        RPARM(10+i) = 0.0 and IPARM(10+i) = 1 for i = 1,5
14. IPARM(2) = 100, 101, 110, or 111 and:
        IPARM(10) \neq 0 \text{ or } 1
        IPARM(11), IPARM(12), IPARM(13) \neq -1 or 1
        IPARM(14), IPARM(15) \neq -1, 0, or 1
        RPARM(10) < 0.0
        RPARM(10+i) \le 0.0 and IPARM(10+i) = 1 for i = 1,5
15. IPARM(2) = 0, 2, 10, 100, 102, or 110 and:
        Idbx \le 0 and mbx \ne 0 and n \ne 0
        ldbx < 0 and mbx = 0
        ldbx < n \text{ and } mbx \neq 0
        mbx < 0
```

16. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to factor a 9 by 9 symmetric sparse matrix  $\mathbf{A}$  and solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  with three right-hand sides. It uses Gaussian elimination. The default values are used for IPARM and RPARM. Input matrix  $\mathbf{A}$ , shown here, is stored in diagonal-out skyline storage mode. Matrix  $\mathbf{A}$  is:

```
      1.0
      1.0
      1.0
      1.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0.0
      0
```

Output matrix A, shown here, is in  $LDL^{T}$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix A is:

```
1.0 1.0
                              0.0
                                   0.0
          1.0 1.0
                    0.0
                         0.0
1.0 1.0
          1.0
               1.0
                    1.0
                         1.0
                              0.0
                                   1.0
                                         0.0
1.0
    1.0
          1.0
               1.0
                    1.0
                         1.0
                              0.0
1.0
     1.0
          1.0
               1.0
                    1.0
                         1.0
                              0.0
                                         0.0
0.0
     1.0
               1.0
                    1.0
                         1.0
                                   1.0
          1.0
                              1.0
                                         0.0
0.0
     1.0
               1.0
                    1.0
                         1.0
                              1.0
          1.0
                                   1.0
                                         1.0
0.0
     0.0
          0.0
               0.0
                    1.0
                         1.0
                              1.0
                                   1.0
                                        1.0
0.0
    1.0
          1.0
               1.0
                    1.0
                         1.0
                              1.0
                                   1.0
                                        1.0
0.0
    0.0
          0.0
               0.0
                    0.0 1.0 1.0 1.0
                                        1.0
```

# Call Statement and Input

# RPARM =(not relevant)

```
4.00
                  8.00
                         12.00
          10.00
                 20.00
                         30.00
          15.00
                 30.00
                         45.00
          19.00
                 38.00
                         57.00
          19.00
                 38.00
                         57.00
ВХ
          23.00
                 46.00
                         69.00
          11.00
                 22.00
                         33.00
          28.00
                 56.00
                         84.00
          10.00
                 20.00
                         30.00
```

#### Output

**Example 2:** This example shows how to factor the 9 by 9 symmetric sparse matrix  $\bf{A}$  from Example 1, solve the system  $\bf{A} \bf{x} = \bf{b}$  with three right-hand sides, and compute the determinant of  $\bf{A}$ . It uses Gaussian elimination. The default values for pivot processing are used for IPARM. Input matrix  $\bf{A}$  is stored in profile-in skyline storage mode. Output matrix  $\bf{A}$  is in  $\bf{L} \bf{D} \bf{L}^T$  factored form with  $\bf{D}^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. It is the same as output matrix  $\bf{A}$  in Example 1.

Call Statement and Input

```
A NA IDIAG IPARM RPARM AUX NAUX BX LDBX MBX
CALL DSKFS( 9, A, 33, IDIAG, IPARM, RPARM, AUX, 39, BX, 12, 3)
Α
         = (1.0, 1.0, 2.0, 1.0, 2.0, 3.0, 1.0, 2.0, 3.0, 4.0, 1.0,
            2.0, 3.0, 4.0, 1.0, 2.0, 3.0, 4.0, 5.0, 1.0, 2.0, 3.0,
            1.0, 2.0, 3.0, 4.0, 5.0, 3.0, 7.0, 1.0, 2.0, 3.0, 4.0)
IDIAG
            (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)
IPARM
          (1, 10, 0, 1, 0, ., ., ., ., 0, ., ., ., ., ., .,
RPARM
         =(not relevant)
           4.00
                  8.00
                       12.00
          10.00
                20.00
                        30.00
          15.00
                30.00
                        45.00
          19.00
                38.00
                        57.00
          19.00
                38.00
                        57.00
ВХ
          23.00
                46.00
                        69.00
          11.00
                22.00
                        33.00
          28.00
                56.00
                        84.00
          10.00
                20.00
                        30.00
```

# Output

**Example 3:** This example shows how to factor a 9 by 9 negative-definite symmetric sparse matrix  $\mathbf{A}$ , solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  with three right-hand sides, and compute the determinant of  $\mathbf{A}$ . It uses Gaussian elimination. (Default values for pivot processing are not used for IPARM because  $\mathbf{A}$  is negative-definite.) Input matrix  $\mathbf{A}$ , shown here, is stored in diagonal-out skyline storage mode. Matrix  $\mathbf{A}$  is:

```
-1.0 -1.0 -1.0 -1.0
                       0.0
                             0.0
                                  0.0
                                        0.0
                                              0.0
     -2.0
          -2.0 -2.0
                      -1.0 -1.0
                                  0.0
                                       -1.0
                                              0.0
-1.0 -2.0 -3.0 -3.0
                      -2.0 -2.0
                                  0.0
                                      -2.0
                                              0.0
     -2.0 -3.0 -4.0
                      -3.0 -3.0
-1.0
                                  0.0
                                       -3.0
                                              0.0
0.0 -1.0 -2.0 -3.0
                      -4.0 -4.0 -1.0
                                       -4.0
                                              0.0
    -1.0 -2.0 -3.0
                      -4.0 -5.0 -2.0
0.0
                                      -5.0
                                            -1.0
0.0
                      -1.0 -2.0 -3.0 -3.0
      0.0
            0.0
                 0.0
                                            -2.0
0.0
                      -4.0 -5.0 -3.0
     -1.0
           -2.0
                -3.0
                                      -7.0
                                             -3.0
            0.0
                 0.0
                       0.0 - 1.0 - 2.0 - 3.0
                                            -4.0
```

Output matrix A, shown here, is in  $LDL^{T}$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Matrix A is:

```
0.0
-1.0
       1.0
                    1.0
                          0.0
                                 0.0
                                       0.0
                                             0.0
1.0
     -1.0
             1.0
                   1.0
                          1.0
                                1.0
                                       0.0
                                             1.0
                                                    0.0
1.0
       1.0
                                                    0.0
            -1.0
                   1.0
                          1.0
                                1.0
                                       0.0
                                             1.0
1.0
       1.0
             1.0 -1.0
                          1.0
                                1.0
                                       0.0
                                             1.0
                                                    0.0
0.0
       1.0
             1.0
                   1.0 -1.0
                                1.0
                                       1.0
                                             1.0
                                                    0.0
0.0
       1.0
             1.0
                   1.0
                          1.0 -1.0
                                             1.0
                                                    1.0
                                       1.0
0.0
       0.0
             0.0
                   0.0
                          1.0
                                1.0
                                      -1.0
                                             1.0
                                                    1.0
0.0
       1.0
             1.0
                   1.0
                          1.0
                                1.0
                                       1.0
                                            -1.0
                                                    1.0
0.0
             0.0
                   0.0
                                1.0
                                                  -1.0
       0.0
                          0.0
                                       1.0
                                             1.0
```

Call Statement and Input

```
N A NA IDIAG
                          IPARM
                                 RPARM
                                        AUX NAUX BX LDBX MBX
CALL DSKFS(9, A, 33, IDIAG, IPARM, RPARM, AUX, 39, BX, 12, 3)
        = (-1.0, -2.0, -1.0, -3.0, -2.0, -1.0, -4.0, -3.0, -2.0,
Α
            -1.0, -4.0, -3.0, -2.0, -1.0, -5.0, -4.0, -3.0, -2.0,
            -1.0, -3.0, -2.0, -1.0, -7.0, -3.0, -5.0, -4.0, -3.0,
            -2.0, -1.0, -4.0, -3.0, -2.0, -1.0
IDIAG
          (1, 2, 4, 7, 11, 15, 20, 23, 30, 34)
IPARM
           (1, 10, 0, 0, 0, ., ., ., ., 1, 0, -1, -1, -1, -1, .,
            . , . , . , . , . , . , . , . )
        = ( . , . , . , . , . , . , . , . , . , 10<sup>-15</sup>, . , . ,
RPARM
             . , . , . , . , . , . , . , . , . , . )
ВХ
        =(same as input BX in Example 1)
```

Output:

```
Α
        = (-1.0, -1.0, 1.0, -1.0, 1.0, -1.0, 1.0, 1.0, 1.0,
           -1.0, 1.0, 1.0, 1.0, -1.0, 1.0, 1.0, 1.0, 1.0, -1.0, 1.0,
            1.0, -1.0 \ 1.0, \ 1.0, \ 1.0, \ 1.0, \ 1.0, \ 1.0, \ -1.0, \ 1.0, \ 1.0,
            1.0)
IDIAG
        =(same as input)
IPARM
        = (1, 10, 0, 0, 0, . , . , . , . , 1, 0, -1, -1, -1, -1, 8,
            .,.,.,9,0,0,0,0)
RPARM
           (.,.,.,.,.,.,.,.,.,.,.,10^{-15},.,.,.,
             .,.,.,7.0, -1.0, 0.0, .,.,.,.,.,.)
                      -3.00
         -1.00 -2.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
         -1.00 -2.00 -3.00
```

**Example 4:** This example shows how to factor the first six rows and columns, referred to as matrix **A1**, of the 9 by 9 symmetric sparse matrix **A** from Example 1 and compute the determinant of **A1**. It uses Gaussian elimination. Input matrix **A1**, shown here, is stored in diagonal-out skyline storage mode. Input matrix **A1** is:

Output matrix A1, shown here, is in  $LDL^{T}$  factored form with  $D^{-1}$  on the diagonal, and is stored in diagonal-out skyline storage mode. Output matrix A1 is:

Call Statement and Input

```
Α
      =(same as input A in Example 1)
IDIAG
      = (1, 2, 4, 7, 11, 15, 20)
IPARM
       (1, 11, 0, 0, 0, ., ., ., 0, ., ., ., ., ., .,
RPARM
      =(not relevant)
BX
      =(not relevant)
LDBX
      =(not relevant)
MBX
      =(not relevant)
Output
Α
      7.0, 3.0, 5.0, 4.0, 3.0, 2.0, 1.0, 4.0, 3.0, 2.0, 1.0
IDIAG
      =(same as input)
IPARM
        (1, 11, 0, 0, 0, ., ., ., 0, ., ., ., ., 6,
         .,.,.,.,0,0,0,0,6
RPARM
        ., 5.0, 1.0, 0.0, ., ., ., ., ., .)
ВХ
      =(same as input)
LDBX
      =(same as input)
MBX
      =(same as input)
```

**Example 5:** This example shows how to do a partial factorization of the 9 by 9 symmetric sparse matrix **A** from Example 1, where the first six rows and columns were factored in Example 4. It factors the remaining three rows and columns and computes the determinant of that part of the matrix. It uses Gaussian elimination. The input matrix, referred to as **A2**, shown here, is made up of the output factored matrix **A1** plus the three remaining unfactored rows and columns of matrix **A** Matrix **A2** is:

```
1.0 1.0 1.0 1.0 0.0 0.0 0.0 0.0
1.0 1.0
       1.0 1.0
                 1.0
                      1.0
                          0.0
                               1.0
1.0 1.0 1.0 1.0 1.0
                      1.0
                          0.0
                                   0.0
1.0
    1.0
        1.0
             1.0
                 1.0
                      1.0
                          0.0
0.0 1.0 1.0 1.0 1.0 1.0 1.0
                              4.0 0.0
0.0
   1.0
        1.0
            1.0 1.0
                     1.0
                         2.0
0.0
    0.0 \quad 0.0
             0.0 1.0
                      2.0
                          3.0
                               3.0
                                   2.0
0.0 1.0
        2.0
             3.0 4.0
                      5.0
                          3.0
                              7.0
                                   3.0
0.0 0.0
        0.0
             0.0 0.0 1.0 2.0 3.0 4.0
```

Both parts of input matrix *A2* are stored in diagonal-out skyline storage mode.

Output matrix **A2** is the same as output matrix **A** in Example 1 and is stored in diagonal-out skyline storage mode.

```
Call Statement and Input
```

```
IPARM
      . , . , . , . , . , . , . , . , . )
RPARM
      =(not relevant)
      =(not relevant)
BX
LDBX
      =(not relevant)
MBX
      =(not relevant)
Output
Α
      =(same as output A in Example 1)
IDIAG
      =(same as output IDIAG in Example 1)
IPARM
      = (1, 11, 6, 0, 0, ..., ..., 0, ..., ..., 8,
         .,.,.,0,0,0,0,3)
      RPARM
         ., 7.0, 1.0, 0.0, ., ., ., ., ., .)
ВХ
      =(same as input)
I DBX
      =(same as input)
MBX
      =(same as input)
```

**Example 6:** This example shows how to solve the system Ax = b with one right-hand side for a symmetric sparse matrix A. Input matrix A, used here, is the same as factored output matrix A from Example 1, stored in profile-in skyline storage mode. It specifies Gaussian elimination, as used in Example 1. Here, output matrix A is unchanged on output and is stored in profile-in skyline storage mode.

Call Statement and Input

```
N A NA IDIAG IPARM RPARM AUX NAUX BX LDBX MBX
CALL DSKFS (9, A, 33, IDIAG, IPARM, RPARM, AUX, 31, BX, 9, 1)
Α
     IDIAG
     = (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)
     IPARM
        . , . , . , . , . , . , . , . , . )
RPARM
     =(not relevant)
ВХ
      = (10.0, 38.0, 64.0, 87.0, 103.0, 133.0, 80.0, 174.0, 80.0)
Output
     =(same as input)
IDIAG
     =(same as input)
IPARM
     =(same as input)
APARM
     =(same as input)
ВХ
     = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0)
```

**Example 7:** This example shows how to factor a 9 by 9 symmetric sparse matrix  $\mathbf{A}$  and solve the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  with four right-hand sides. It uses Cholesky decomposition. Input matrix  $\mathbf{A}$ , shown here, is stored in profile-in skyline storage mode Matrix  $\mathbf{A}$  is:

```
1.0
1.0
     1.0
            1.0
                   0.0
                          1.0
                                 0.0
                                        0.0
                                              0.0
1.0
     5.0
            3.0
                   0.0
                          3.0
                                 0.0
                                        0.0
                                              0.0
                                                     3.0
     3.0
1.0
           11.0
                   3.0
                          5.0
                                 3.0
                                        3.0
                                              0.0
                                                     5.0
0.0
     0.0
            3.0
                  17.0
                          5.0
                                 5.0
                                        5.0
                                              0.0
                                                     5.0
     3.0
            5.0
                   5.0
                         29.0
                                 7.0
                                        7.0
                                              0.0
                                                     9.0
1.0
0.0
     0.0
            3.0
                   5.0
                          7.0
                                39.0
                                        9.0
                                              6.0
                                                     9.0
                                9.0
0.0
     0.0
            3.0
                   5.0
                          7.0
                                      53.0
                                              8.0
                                                    11.0
0.0
     0.0
            0.0
                   0.0
                          0.0
                                 6.0
                                        8.0
                                             66.0
                                                    10.0
1.0
     3.0
            5.0
                   5.0
                          9.0
                                 9.0
                                             10.0
                                                    89.0
                                      11.0
```

Output matrix A, shown here, is in  $R^TR$  factored form with the inverse of the diagonal of R on the diagonal, and is stored in profile-in skyline storage mode. Matrix A is:

```
1.0
     1.0
                 0.0
                                     0.0
                                            0.0
                                                   1.0
            1.0
                       1.0
                              0.0
1.0
      .5
            1.0
                  0.0
                       1.0
                              0.0
                                     0.0
                                            0.0
                                                  1.0
1.0
     1.0
           .333
                  1.0
                       1.0
                              1.0
                                     1.0
                                            0.0
                                                  1.0
0.0
     0.0
            1.0
                  .25
                       1.0
                              1.0
                                     1.0
                                            0.0
                                                  1.0
1.0
     1.0
            1.0
                 1.0
                        .2
                              1.0
                                     1.0
                                                  1.0
                                            0.0
0.0
                                                  1.0
     0.0
            1.0
                  1.0
                       1.0
                             .167
                                     1.0
                                            1.0
0.0
     0.0
            1.0
                  1.0
                       1.0
                              1.0
                                    .143
                                            1.0
                                                  1.0
0.0
     0.0
            0.0
                 0.0
                       0.0
                              1.0
                                     1.0
                                           .125
                                                  1.0
1.0
     1.0
            1.0
                 1.0
                       1.0
                              1.0
                                            1.0
                                                 .111
                                     1.0
```

# Call Statement and Input

```
N A NA IDIAG
                            IPARM
                                    RPARM
                                           AUX NAUX
                                                     ВХ
                                                         LDBX MBX
CALL DSKFS( 9, A, 34, IDIAG, IPARM, RPARM, AUX, 43, BX, 10, 4)
Α
         = (1.0, 1.0, 5.0, 1.0, 3.0, 11.0, 3.0, 17.0, 1.0, 3.0, 5.0,
             5.0, 29.0, 3.0, 5.0, 7.0, 39.0, 3.0, 5.0, 7.0, 9.0, 53.0,
             6.0, 8.0, 66.0, 1.0, 3.0, 5.0, 5.0, 9.0, 9.0, 11.0, 10.0,
            89.0)
IDIAG
            (1, 3, 6, 8, 13, 17, 22, 25, 34, 35)
            (1, 110, 0, 1, 1, ., ., ., ., 0, .,
IPARM
RPARM
         =(not relevant)
                           15.00
                                   20.00
            5.00
                   10.00
           15.00
                   30.00
                           45.00
                                   60.00
           34.00
                   68.00
                          102.00
                                  136.00
           40.00
                   80.00
                          120.00
                                  160.00
ВХ
           66.00
                  132.00
                          198.00
                                  264.00
           78.00
                  156.00
                          234.00
                                  312.00
          96.00
                 192.00
                          288.00
                                  384.00
```

360.00

568.00

90.00

142.00

180.00

284.00

270.00

426.00

```
Output
```

```
Α
        = (1.0, 1.0, .5, 1.0, 1.0, .333, 1.0, .25, 1.0, 1.0, 1.0,
           1.0, .2, 1.0, 1.0, 1.0, .167, 1.0, 1.0, 1.0, 1.0, .143,
           1.0, 1.0, .125, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0,
            .111)
IDIAG
        =(same as input)
IPARM
        = (1, 110, 0, 1, 1, . , . , . , 0, . , . , . , . ,
           9, . , . , . , 0, 0, 0, 0, 9)
RPARM
            ., 9.89, 1.32, 11.0, ., ., ., ., ., .)
         1.00 2.00 3.00
                         4.00
                    3.00
         1.00 2.00
                         4.00
         1.00 2.00 3.00
                         4.00
         1.00 2.00
                    3.00
ВХ
        1.00 2.00
                    3.00
                         4.00
         1.00 2.00
                    3.00
                         4.00
         1.00 2.00
                    3.00
                         4.00
         1.00 2.00
                    3.00
                        4.00
         1.00 2.00 3.00 4.00
```

# DSRIS—Iterative Linear System Solver for a General or Symmetric Sparse Matrix Stored by Rows

This subroutine solves a general or symmetric sparse linear system of equations, using an iterative algorithm, with or without preconditioning. The methods include conjugate gradient (CG), conjugate gradient squared (CGS), generalized minimum residual (GMRES), more smoothly converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR). The preconditioners include an incomplete LU factorization, an incomplete Cholesky factorization (for positive definite symmetric matrices), diagonal scaling, or symmetric successive over-relaxation (SSOR) with two possible choices for the diagonal matrix: one uses the absolute values sum of the input matrix, and the other uses the diagonal obtained from the LU factorization. The sparse matrix is stored using storage-by-rows for general matrices and upper- or lower-storage-by-rows for symmetric matrices. Matrix  $\bf A$  and vectors  $\bf x$  and  $\bf b$  are used:

Ax = b

where **A**, **x**, and **b** contain long-precision real numbers.

# **Syntax**

Fortran	CALL DSRIS (stor, init, n, ar, ja, ia, b, x, iparm, rparm, aux1, naux1, aux2, naux2)
C and C++	dsris (stor, init, n, ar, ja, ia, b, x, iparm, rparm, aux1, naux1, aux2, naux2);
PL/I	CALL DSRIS (stor, init, n, ar, ja, ia, b, x, iparm, rparm, aux1, naux1, aux2, naux2);

On Entry

stor

indicates the form of sparse matrix **A** and the storage mode used, where:

If stor = 'G', A is a general sparse matrix, stored using storage-by-rows.

If stor = 'U', A is a symmetric sparse matrix, stored using upper-storage-by-rows.

If *stor* = 'L', **A** is a symmetric sparse matrix, stored using lower-storage-by-rows.

Specified as: a single character. It must be 'G', 'U', or 'L'. init

indicates the type of computation to be performed, where:

If *init* = 'I', the preconditioning matrix is computed, the internal representation of the sparse matrix is generated, and the iteration procedure is performed. The coefficient matrix and preconditioner in internal format are saved in *aux1*.

If init = 'S', the iteration procedure is performed using the coefficient matrix and the preconditioner in internal format, stored in aux1, created in a preceding call to this subroutine with init = 'I'. You use this option to solve the same matrix for different right-hand sides, b, optimizing your performance. As long as you do not change the coefficient matrix and preconditioner in aux1, any number of calls can be made with init = 'S'.

Specified as: a single character. It must be 'I' or 'S'.

*n* is the order of the linear system Ax = b and the number of rows and columns in sparse matrix A. Specified as: a fullword integer;  $n \ge 0$ .

ar

is the sparse matrix  $\mathbf{A}$  of order n, stored by rows in an array, referred to as AR. The *stor* argument indicates the storage variation used for storing matrix  $\mathbf{A}$ . Specified as: a one-dimensional array, containing long-precision real numbers. The number of elements in this array can be determined by subtracting 1 from the value in IA(n+1).

ja

is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix **A**. Specified as: a one-dimensional array, containing fullword integers;  $1 \le (JA \text{ elements}) \le n$ . The number of elements in this array can be determined by subtracting 1 from the value in IA(n+1).

ia

is the row pointer array, referred to as IA, containing the starting positions of each row of matrix  $\mathbf{A}$  in array AR and one position past the end of array AR. Specified as: a one-dimensional array of (at least) length n+1, containing fullword integers; IA(i+1)  $\geq$  IA(i) for i=1, n+1.

b

is the vector  $\boldsymbol{b}$  of length n, containing the right-hand side of the matrix problem. Specified as: a one-dimensional array of (at least) length n, containing long-precision real numbers.

Χ

is the vector  $\mathbf{x}$  of length n, containing your initial guess of the solution of the linear system. Specified as: a one-dimensional array of (at least) length n, containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

iparm

is an array of parameters, IPARM(i), where:

IPARM(1) controls the number of iterations.

If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.

If IPARM(1) = 0, the following default values are used:

IPARM(1) = 300

IPARM(2) = 4

IPARM(4) = 4

IPARM(5) = 1

 $RPARM(1) = 10^{-6}$ 

RPARM(2) = 1

 IPARM(2) is the flag used to select the iterative procedure used in this subroutine.

If IPARM(2) = 1, the conjugate gradient (CG) method is used. Note that this algorithm should only be used with positive definite symmetric matrices.

If IPARM(2) = 2, the conjugate gradient squared (CGS) method is used.

If IPARM(2) = 3, the generalized minimum residual (GMRES) method, restarted after k steps, is used.

If IPARM(2) = 4, the more smoothly converging variant of the CGS method (Bi-CGSTAB) is used.

If IPARM(2) = 5, the transpose-free quasi-minimal residual method (TFQMR) is used.

• IPARM(3) has the following meaning, where:

If IPARM(2)  $\neq$  3, then IPARM(3) is not used.

If IPARM(2) = 3, then IPARM(3) = k, where k is the number of steps after which the generalized minimum residual method is restarted. A value for k in the range of 5 to 10 is suitable for most problems.

• IPARM(4) is the flag that determines the type of preconditioning.

If IPARM(4) = 1, the system is not preconditioned.

If IPARM(4) = 2, the system is preconditioned by a diagonal matrix.

If IPARM(4) = 3, the system is preconditioned by SSOR splitting with the diagonal given by the absolute values sum of the input matrix.

If IPARM(4) = 4, the system is preconditioned by an incomplete LU factorization.

If IPARM(4) = 5, the system is preconditioned by SSOR splitting with the diagonal given by the incomplete LU factorization.

**Note:** The multithreaded version of DSRIS only runs on multiple threads when IPARM(4) = 1 or 2.

- IPARM(5) is the flag used to select the stopping criterion used in the computation, where the following items are used in the definitions of the stopping criteria below:
  - $\varepsilon$  is the desired relative accuracy and is stored in RPARM(1).
  - $-x_i$  is the solution found at the *j*-th iteration.
  - $r_j$  and  $r_0$  are the preconditioned residuals obtained at iterations j and 0, respectively. (The residual at iteration j is given by  $\mathbf{b} \mathbf{A} x_i$ .)

If IPARM(5) = 1, the iterative method is stopped when:

$$||r_i||_2 / ||x_i||_2 < \varepsilon$$

**Note:** IPARM(5) = 1 is the default value assumed by ESSL if you do not specify one of the values described here; therefore, if you do not update your program to set an IPARM(5) value, you, by default, use the above stopping criterion.

If IPARM(5) = 2, the iterative method is stopped when:

$$||r_i||_2 / ||r_0||_2 < \varepsilon$$

If IPARM(5) = 3, the iterative method is stopped when:

$$||x_i - x_{i-1}||_2 / ||x_i||_2 < \varepsilon$$

**Note:** Stopping criterion 3 performs poorly with the TFQMR method; therefore, if you specify TFQMR (IPARM(2) = 5), you should not specify stopping criterion 3.

• IPARM(6), see "On Return" on page 636.

Specified as: an array of (at least) length 6, containing fullword integers, where:  $IPARM(1) \ge 0$ 

```
IPARM(2) = 1, 2, 3, 4, \text{ or } 5
If IPARM(2) = 3, \text{ then } IPARM(3) > 0
IPARM(4) = 1, 2, 3, 4, \text{ or } 5
IPARM(5) = 1, 2, \text{ or } 3 \text{ (Other values default to stopping criterion } 1.)
IPARM(5) = 1, 2, \text{ or } 3 \text{ (Other values default to stopping criterion } 1.)
```

is an array of parameters, RPARM(i), where:

RPARM(1) is the relative accuracy  $\epsilon$  used in the stopping criterion. See "Notes" on page 637.

RPARM(2), see "On Return" on page 636.

RPARM(3) has the following meaning, where:

- If IPARM(4) ≠ 3, then RPARM(3) is not used.
- If IPARM(4) = 3, then RPARM(3) is the acceleration parameter used in SSOR. (A value in the range 0.5 to 2.0 is suitable for most problems.)

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers, where:

```
RPARM(1) \ge 0
If IPARM(4) = 3, RPARM(3) > 0
```

aux1

is working storage for this subroutine, where:

If init = 'I', the working storage is computed. It can contain any values.

If *init* = 'S', the working storage is used in solving the linear system. It contains the coefficient matrix and preconditioner in internal format, computed in an earlier call to this subroutine.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1.

Specified as: a fullword integer, where:

In these formulas *nw* has the following value:

```
If stor = 'G', then nw = IA(n+1)-1+n.

If stor = 'U' or 'L', then nw = 2(IA(n+1)-1).

If IPARM(4) = 1, use naux1 = (3/2)nw+(7/2)n+40.

If IPARM(4) = 2, use naux1 = (3/2)nw+(9/2)n+40.

If IPARM(4) = 3, 4, or 5, then:

If IPARM(2) \neq 1, use naux1 = 3nw+10n+60.

If IPARM(2) = 1, use naux1 = 3nw+(21/2)n+60.
```

**Note:** If you receive an attention message, you have not specified sufficient auxiliary storage to achieve optimal performance, but it is enough to perform the computation. To obtain optimal performance, you need to use the amount given by the attention message.

aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is working storage used by this subroutine that is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing naux2 long-precision real numbers.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, DSRIS dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

## Otherwise,

```
If IPARM(2) = 1, use naux2 \ge 4n.

If IPARM(2) = 2, use naux2 \ge 7n.

If IPARM(2) = 3, use naux2 \ge (k+2)n+k(k+4)+1, where k = IPARM(3).

If IPARM(2) = 4, use naux2 \ge 7n.

If IPARM(2) = 5, use naux2 \ge 9n.
```

#### On Return

ar

is the sparse matrix  $\mathbf{A}$  of order n, stored by rows in an array, referred to as AR. The *stor* argument indicates the storage variation used for storing matrix  $\mathbf{A}$ . The order of the elements in each row of  $\mathbf{A}$  in AR may be changed on output.

Returned as: a one-dimensional array, containing long-precision real numbers. The number of elements in this array can be determined by subtracting 1 from the value in IA(n+1).

ja

is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix **A**. These elements correspond to the arrangement of the contents of AR on output.

Returned as: a one-dimensional array, containing fullword integers;  $1 \le (JA \text{ elements}) \le n$ . The number of elements in this array can be determined by subtracting 1 from the value in IA(n+1).

Χ

is the vector  $\mathbf{x}$  of length n, containing the solution of the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . Returned as: a one-dimensional array of (at least) length n, containing long-precision real numbers.

# iparm

is an array of parameters, IPARM(i), where:

IPARM(1) through IPARM(5) are unchanged.

IPARM(6) contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 6, containing fullword integers. rparm

is an array of parameters, RPARM(i), where:

RPARM(1) is unchanged.

RPARM(2) contains the estimate of the error of the solution. If the process converged, RPARM(2)  $\leq \epsilon$ .

RPARM(3) is unchanged.

Returned as: a one-dimensional array of length 3, containing long-precision real numbers.

#### aux1

is working storage for this subroutine, containing the coefficient matrix and preconditioner in internal format, ready to be passed in a subsequent invocation

of this subroutine. Returned as: an area of storage, containing *naux1* long-precision real numbers.

#### Notes

1. If you want to solve the same sparse linear system of equations multiple times using a different algorithm with the same preconditioner and using a different right-hand side each time, you get the best performance by using the following technique. Call DSRIS the first time with init = 'I'. This solves the system, and then stores the coefficient matrix and preconditioner in internal format in aux1. On the subsequent invocations of DSRIS with different right-hand sides, specify init = 'S'. This indicates to DSRIS to use the contents of aux1, saving the time to convert your coefficient matrix and preconditioner to internal format. If you use this technique, you should not modify the contents of aux1 between calls to DSRIS.

In some cases, you can specify a different algorithm in IPARM(2) when making calls with init = 'S'. (See "Example 2" on page 640.) However, DSRIS sometimes needs different information in aux1 for different algorithms. When this occurs, DSRIS issues an attention message, continues processing the computation, and then resets the contents of aux1. Your performance is not improved in this case, which is functionally equivalent to calling DSRIS with init = 'I'.

- 2. If you use the CG method with *init* = 'I', you must use the CG method when you specify *init* = 'S'. However, if you use a different method with *init* = 'I', you can use any other method, except CG, when you specify *init* = 'S'.
- 3. These subroutines accept lowercase letters for the *stor* and *init* arguments.
- 4. Matrix **A**, vector **x**, and vector **b** must have no common elements; otherwise, results are unpredictable.
- 5. In this subroutine, a value of RPARM(1) = 0 is permitted to force the solver to evaluate exactly IPARM(1) iterations. The algorithm computes a sequence of approximate solution vectors  $\mathbf{x}$  that converge to the solution. The iterative procedure is stopped when the selected stopping criterion is satisfied or when more than the maximum number of iterations (in IPARM(1)) is reached.

For the stopping criteria specified in IPARM(5), the relative accuracy  $\epsilon$  (in RPARM(1)) must be specified reasonably (10<sup>-4</sup> to 10<sup>-8</sup>). If you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

- 6. For a description of how sparse matrices are stored by rows, see "Storage-by-Rows" on page 99.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

Function: The linear system:

Ax = b

is solved using one of the following methods: conjugate gradient (CG), conjugate gradient squared (CGS), generalized minimum residual (GMRES), more smoothly converging variant of the CGS method (Bi-CGSTAB), or transpose-free quasi-minimal residual method (TFQMR), where:

**A** is a sparse matrix of order *n*. The matrix is stored in arrays AR, IA, and JA. If it is general, it is stored by rows. If it is symmetric, it can be stored using upper-or lower-storage-by-rows.

**x** is a vector of length *n*.

 $\boldsymbol{b}$  is a vector of length n.

One of the following preconditioners is used:

- · an incomplete LU factorization
- an incomplete Cholesky factorization (for positive definite symmetric matrices)
- · diagonal scaling
- symmetric successive over-relaxation (SSOR) with two possible choices for the diagonal matrix:
  - the absolute values sum of the input matrix
  - the diagonal obtained from the LU factorization

See references [36], [53], [76], [80], [83], and [89].

When you call this subroutine to solve a system for the first time, you specify init = 'I'. After that, you can solve the same system any number of times by calling this subroutine each time with init = 'S'. These subsequent calls use the coefficient matrix and preconditioner, stored in internal format in aux1. You optimize performance by doing this, because certain portions of the computation have already been performed.

# **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see "What Can You Do about ESSL Computational Errors?" on page 48.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector **x** contains the approximate solution computed at the last iteration.
- For error 2130, return code 2 indicates that the incomplete LU factorization of A could not be completed, because one pivot was 0.
- For error 2124, the subroutine has been called with init = 'S', but the data contained in aux1 was computed for a different algorithm. An attention message is issued. Processing continues, and the contents of aux1 are reset correctly.
- For error 2134, return code 3 indicates that the data contained in aux1 is not consistent with the input sparse matrix. The subroutine has been called with init = 'S', and aux1 contains an incomplete factorization and internal data storage for the input matrix A that was computed by a previous call to the subroutine when init = 'I'. This error indicates that aux1 has been modified since the last call to the subroutine, or that the input matrix is not the same as

the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(4) = 1 or 4.

- For error 2131, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain zero.
- For error 2129, return code 5 indicates that the matrix is not positive definite.
- For error 2128, return code 8 indicates an internal ESSL error. Please contact your IBM Representative.

# Input-Argument Errors

```
1. n < 0

2. stor \neq 'G', 'U', or 'L'

3. init \neq 'l' or 'S'

4. IA(n+1) < 1

5. IA(i+1)-IA(i) < 0, for any i = 1, n = 1

6. IPARM(1) < 0

7. IPARM(2) \neq 1, 2, 3, 4, or 5

8. IPARM(3) \leq 0 and IPARM(2) = 3

9. IPARM(4) \neq 1, 2, 3, 4, or 5

10. IPARM(1) < 0

11. IPARM(3) \leq 0 and IPARM(4) = 3
```

- 12. *naux1* is too small—that is, less than the minimum required value. Return code 6 is returned if error 2015 is recoverable.
- 13. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 7 is returned for *naux2* if error 2015 is recoverable.

**Example 1:** This example finds the solution of the linear system Ax = b for the sparse matrix A, which is stored by rows in arrays AR, IA, and JA. The system is solved using the Bi-CGSTAB algorithm. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARM(1). The algorithm is allowed to perform 20 iterations. The process converges after 9 iterations. Matrix A is:

$$\begin{bmatrix} 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 \end{bmatrix}$$

# Call Statement and Input

```
AR
        = (2.0, 2.0, -1.0, 1.0, 2.0, 1.0, 2.0, -1.0, 1.0, 2.0, -1.0,
           1.0, 2.0, -1.0, 1.0, 2.0, -1.0, 1.0, 2.0, -1.0, 1.0, 2.0
JA
          (1, 2, 3, 2, 3, 1, 4, 5, 4, 5, 6, 5, 6, 7, 6, 7, 8, 7, 8,
           9, 8, 9)
IΑ
        = (1, 2, 4, 6, 9, 12, 15, 18, 21, 23)
В
          (2.0, 1.0, 3.0, 2.0, 2.0, 2.0, 2.0, 2.0, 3.0)
          Χ
IPARM(1) = 20
IPARM(2) =
IPARM(3) =
          0
IPARM(4) = 1
IPARM(5) = 10
RPARM(1) = 1.D-7
RPARM(3) = 1.0
Output
        = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 9
RPARM(2) = 0.29D-16
```

**Example 2:** This example finds the solution of the linear system  $\mathbf{A}\mathbf{x} = \mathbf{b}$  for the same sparse matrix  $\mathbf{A}$  used in Example 1. It also uses the same right-hand side in  $\mathbf{b}$  and the same initial guesses in  $\mathbf{x}$ . However, the system is solved using a different algorithm, conjugate gradient squared (CGS). Because INIT is 'S', the best performance is achieved. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARM(1). The algorithm is allowed to perform 20 iterations. The process converges after 9 iterations.

Call Statement and Input

```
JΑ
           STOR INIT
                           AR
                                   IA B
                                             Χ
                                                 IPARM
                                                         RPARM
                                                                 AUX1
                                                                        NAUX1
                                                                                AUX2
                                                                                      NAUX2
                     N
CALL DSRIS( ^{\prime}G^{\prime}, ^{\prime}S^{\prime}, 9 , AR , JA , IA , B , X , IPARM , RPARM , AUX1 ,
                                                                          98 , AUX2 ,
                                                                                        63)
                    AR
                             =(same as input AR in Example 1)
                    JA
                             =(same as input JA in Example 1)
                    IΑ
                             =(same as input IA in Example 1)
                    В
                             =(same as input B in Example 1)
                    Χ
                             =(same as input X in Example 1)
                    IPARM(1) = 20
                    IPARM(2) = 2
                    IPARM(3) =
                    IPARM(4) = 1
                    IPARM(5) = 10
                    RPARM(1) = 1.D-7
                    RPARM(3) = 1.0
                    Output
                             IPARM(6) = 9
                    RPARM(2) = 0.42D-19
```

**Example 3:** This example finds the solution of the linear system Ax = b for the sparse matrix A, which is stored by rows in arrays AR, IA, and JA. The system is solved using the two-term conjugate gradient method (CG), preconditioned by

incomplete LU factorization. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARM(1). The algorithm is allowed to perform 20 iterations. The process converges after 1 iteration. Matrix  $\boldsymbol{A}$  is:

```
0.0
 2.0
       0.0
             -1.0
                     0.0
                            0.0
                                   0.0
                                          0.0
                                                0.0
              0.0
0.0
       2.0
                    -1.0
                            0.0
                                   0.0
                                         0.0
                                                0.0
                                                       0.0
-1.0
       0.0
              2.0
                     0.0
                           -1.0
                                   0.0
                                         0.0
                                                0.0
                                                       0.0
      -1.0
                     2.0
                            0.0
0.0
              0.0
                                  -1.0
                                         0.0
                                                0.0
                                                       0.0
       0.0
                            2.0
                                   0.0
0.0
             -1.0
                     0.0
                                         -1.0
                                                0.0
                                                       0.0
 0.0
       0.0
              0.0
                    -1.0
                            0.0
                                   2.0
                                         0.0
                                               -1.0
                                                       0.0
              0.0
0.0
       0.0
                     0.0
                          -1.0
                                  0.0
                                         2.0
                                                0.0
                                                      -1.0
                                                       0.0
 0.0
       0.0
              0.0
                     0.0
                            0.0
                                 -1.0
                                         0.0
                                                2.0
 0.0
       0.0
              0.0
                     0.0
                            0.0
                                   0.0
                                                0.0
                                                       2.0
                                        -1.0
```

# Call Statement Input

```
STOR INIT
                       AR
                                TΑ
                                    В
                                        Χ
                                           TPARM
                                                  RPARM
                                                         AUX1
                                                               NAUX1
                                                                      AUX2
                                                                            NAUX2
                            JA
CALL DSRIS( ^{\prime}G^{\prime}, ^{\prime}I^{\prime}, 9 , AR , JA , IA , B , X , IPARM , RPARM , AUX1 ,
                                                               223
                                                                    , AUX2 ,
                                                                              36)
                         = (2.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0,
                            -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0, 2.0, -1.0, -1.0,
                            2.0, -1.0, 2.0
                 JA
                           (1, 3, 2, 4, 1, 3, 5, 2, 4, 6, 3, 5, 7, 4, 6, 8, 5, 7, 9,
                            6, 8, 7, 9)
                 IΑ
                           (1, 3, 5, 8, 11, 14, 17, 20, 22, 24)
                 В
                           Χ
                            IPARM(1) =
                           20
                 IPARM(2) =
                           1
                 IPARM(3) =
                 IPARM(4) =
                 IPARM(5) =
                           1
                 RPARM(1) = 1.D-7
                 RPARM(3) = 1.0
                 Output
                          IPARM(6) =
                          1
                 RPARM(2) = 0.16D-15
```

**Example 4:** This example finds the solution of the linear system Ax = b for the same sparse matrix A used in Example 3. However, matrix A is stored using upper-storage-by-rows in arrays AR, IA, and JA. The system is solved using the generalized minimum residual (GMRES), restarted after 5 steps and preconditioned with SSOR splitting. The iteration is stopped when the norm of the residual is less than the given threshold specified in RPARM(1). The algorithm is allowed to perform 20 iterations. The process converges after 12 iterations.

# Call Statement Input

```
AR
       = (2.0, -1.0, 2.0, -1.0, 2.0, -1.0, 2.0, -1.0, 2.0, -1.0,
          2.0, -1.0, 2.0, -1.0, 2.0, 2.0)
JA
       = (1, 3, 2, 4, 3, 5, 4, 6, 5, 7, 6, 8, 7, 9, 8, 9)
IΑ
       = (1, 3, 5, 7, 9, 11, 13, 15, 16, 17)
       Χ
       IPARM(1) = 20
IPARM(2) =
         3
IPARM(3) = 5
IPARM(4) = 3
IPARM(5) = 1
RPARM(1) = 1.D-7
RPARM(3) = 2.0
Output
      = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
IPARM(6) = 12
RPARM(2) = 0.33D-7
```

# DSMCG—Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Matrix Storage Mode

This subroutine solves a symmetric, positive definite or negative definite linear system, using the conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization, for a sparse matrix stored in compressed-matrix storage mode. Matrix **A** and vectors **x** and **b** are used:

$$Ax = b$$

where **A**, **x**, and **b** contain long-precision real numbers.

#### Notes:

- 1. These subroutines are provided only for migration purposes. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
- If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 99, you should first use the utility subroutine DSRSM to convert your sparse matrix to compressed-matrix storage mode. See "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979

# Syntax

Fortran	CALL DSMCG (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2)
C and C++	dsmcg (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2);
PL/I	CALL DSMCG (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2);

On Entry

m

is the order of the linear system Ax = b and the number of rows in sparse matrix A. Specified as: a fullword integer;  $m \ge 0$ .

nz

is the maximum number of nonzero elements in each row of sparse matrix A. Specified as: a fullword integer;  $nz \ge 0$ .

ac

is the array, referred to as AC, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode. Specified as: an *Ida* by (at least) *nz* array, containing long-precision real numbers.

ka

is the array, referred to as KA, containing the column numbers of the matrix  $\boldsymbol{A}$  elements stored in the corresponding positions in array AC. Specified as: an *Ida* by (at least) nz array, containing fullword integers, where  $1 \le$  (elements of KA)  $\le m$ .

lda

is the leading dimension of the arrays specified for ac and ka. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

b

is the vector  $\boldsymbol{b}$  of length m, containing the right-hand side of the matrix problem. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

Х

is the vector  $\mathbf{x}$  of length m, containing your initial guess of the solution of the linear system. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero. iparm

is an array of parameters, IPARM(i), where:

• IPARM(1) controls the number of iterations.

If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.

If IPARM(1) = 0, the following default values are used:

IPARM(1) = 300

IPARM(2) = 1

IPARM(3) = 0

 $RPARM(1) = 10^{-6}$ 

IPARM(2) is the flag used to select the stopping criterion.

If IPARM(2) = 0, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \|\mathbf{x}\|_2 < \varepsilon$$

where r = b-Ax is the residual, and  $\varepsilon$  is the desired relative accuracy.  $\varepsilon$  is stored in RPARM(1).

If IPARM(2) = 1, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \lambda \|\mathbf{x}\|_2 < \varepsilon$$

where  $\lambda$  is an estimate to the minimum eigenvalue of the iteration matrix.  $\lambda$  is computed adaptively by this program and, on output, is stored in RPARM(2).

If IPARM(2) = 2, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \lambda \|\mathbf{x}\|_2 < \varepsilon$$

where  $\lambda$  is a predetermined estimate to the minimum eigenvalue of the iteration matrix. This eigenvalue estimate, on input, is stored in RPARM(2) and may be obtained by an earlier call to this subroutine with the same matrix.

• IPARM(3) is the flag that determines whether the system is to be solved using the conjugate gradient method, preconditioned by an incomplete Cholesky factorization with no fill-in.

If IPARM(3) = 0, the system is not preconditioned.

If IPARM(3) = 10, the system is preconditioned by an incomplete Cholesky factorization.

If IPARM(3) = -10, the system is preconditioned by an incomplete Cholesky factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in aux2.

• IPARM(4), see "On Return" on page 645.

Specified as: an array of (at least) length 4, containing fullword integers, where:

 $IPARM(1) \ge 0$ 

IPARM(2) = 0, 1, or 2

IPARM(3) = 0, 10, or -10

#### rparm

is an array of parameters, RPARM(i), where  $\epsilon$  is stored in RPARM(1), and  $\lambda$  is stored in RPARM(2).

RPARM(1) > 0, is the relative accuracy  $\epsilon$  used in the stopping criterion.

RPARM(2) > 0, is the estimate of the smallest eigenvalue,  $\lambda$ , of the iteration matrix. It is only used when IPARM(2) = 2.

RPARM(3), see "On Return."

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

#### aux1

has the following meaning:

If naux1 = 0 and error 2015 is unrecoverable, aux1 is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers. naux1

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*. Specified as: a fullword integer, where:

If naux1 = 0 and error 2015 is unrecoverable, DSMCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, *naux1* must have at least the following value, where:

If IPARM(2) = 0 or 2, use  $naux1 \ge 3m$ .

If IPARM(2) = 1 and IPARM(1)  $\neq$  0, use  $naux1 \geq 3m+2(IPARM(1))$ .

If IPARM(2) = 1 and IPARM(1) = 0, use  $naux1 \ge 3m+600$ .

#### aux2

is a storage work area used by this subroutine. If IPARM(3) = -10, aux2 must contain the incomplete Cholesky factorization of matrix  $\boldsymbol{A}$ , computed in an earlier call to DSMCG. The size of aux2 is specified by naux2. Specified as: an area of storage, containing long-precision real numbers.

#### naux2

is the size of the work area specified by aux2—that is, the number of elements in aux2. Specified as: a fullword integer. When IPARM(3) = 10 or -10, naux2 must have at least the following value:  $naux2 \ge m(nz-1)1.5+2(m+6)$ .

# On Return

Х

is the vector  $\mathbf{x}$  of length m, containing the solution of the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . Returned as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

iparm

is an array of parameters, IPARM(i), where:

IPARM(1) is unchanged.

IPARM(2) is unchanged.

IPARM(3) is unchanged.

IPARM(4) contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers. rparm

is an array of parameters, RPARM(i), where:

RPARM(1) is unchanged.

RPARM(2) is unchanged if IPARM(2) = 0 or 2. If IPARM(2) = 1, RPARM(2) contains  $\lambda$ , an estimate of the smallest eigenvalue of the iteration matrix.

RPARM(3) contains the estimate of the error of the solution. If the process converged, RPARM(3)  $\leq \epsilon$ .

Returned as: a one-dimensional array of length 3, containing long-precision real numbers;  $\lambda > 0$ .

aux2

is the storage work area used by this subroutine.

If IPARM(3) = 10, *aux2* contains the incomplete Cholesky factorization of matrix **A**.

If IPARM(3) = -10, aux2 is unchanged.

See "Notes" for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

#### **Notes**

- When IPARM(3) = -10, this subroutine uses the incomplete Cholesky factorization in aux2, computed in an earlier call to this subroutine. When IPARM(3) = 10, this subroutine computes the incomplete Cholesky factorization and stores it in aux2.
- 2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify IPARM(3) = 10 on the first invocation. The incomplete factorization is stored in aux2. You may save computing time on subsequent calls by setting IPARM(3) = -10. In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of aux2 between calls.
- 3. Matrix **A** must have no common elements with vectors **x** and **b**; otherwise, results are unpredictable.
- 4. In the iterative solvers for sparse matrices, the relative accuracy ε (RPARM(1)) must be specified "reasonably" (10<sup>-4</sup> to 10<sup>-8</sup>). The algorithm computes a sequence of approximate solution vectors x that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|_2 / \lambda \|\boldsymbol{x}\|_2 < \varepsilon$$

where  $\lambda$  is an estimate of the minimum eigenvalue of the iteration matrix, which is either estimated adaptively or given by the user. As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

- 5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 93.
- 6. On output, array AC and vector **b** are not bitwise identical to what they were on input, because the matrix **A** and the right-hand side are scaled before starting the iterative process and are unscaled before returning control to the user. In addition, arrays AC and KA may be rearranged on output, but still contain a mathematically equivalent mapping of the elements in matrix **A**.
- 7. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The sparse positive definite or negative definite linear system:

Ax = b

is solved, where:

 $\boldsymbol{A}$  is a symmetric, positive definite or negative definite sparse matrix of order m, stored in compressed-matrix storage mode in AC and KA.

**x** is a vector of length *m*.

**b** is a vector of length m.

The system is solved using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization. In both cases, the matrix is scaled by the square root of the diagonal.

See references [59] and [62]. [36].

If your program uses a sparse matrix stored by rows and you want to use this subroutine, first convert your sparse matrix to compressed-matrix storage mode by using the subroutine DSRSM described on page 979.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux1 = 0, and unable to allocate work area.

Computational Errors: The following errors, with their corresponding return codes, can occur in this subroutine. Where a value of *i* is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

• For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector **x** contains the approximate solution computed at the last iteration.

- For error 2111, return code 2 indicates that aux2 contains an incorrect factorization. The subroutine has been called with IPARM(3) = −10, and aux2 contains an incomplete factorization of the input matrix A that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that aux2 has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2109, return code 3 indicates that the inner product (*y*, *Ay*) is negative in the iterative procedure after iteration *i*. This should not occur, because the input matrix is assumed to be positive or negative definite. Vector *x* contains the results of the last iteration. The value *i* is identified in the computational error message.
- For error 2108, return code 4 indicates that the matrix is not positive definite. AC is partially modified and does not represent the same matrix as on entry.

#### Input-Argument Errors

```
1. m < 0
```

- 2. Ida < 1
- 3. Ida < m
- 4. nz < 0
- 5. nz = 0 and m > 0
- 6. IPARM(1) < 0
- 7. IPARM(2)  $\neq$  0, 1, or 2
- 8. IPARM(3)  $\neq$  0, 10, or -10
- 9. RPARM(1) < 0
- 10. RPARM(2) < 0
- 11. Error 2015 is recoverable or *naux1*≠0, and *naux1* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
- 12. *naux2* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

**Example 1:** This example finds the solution of the linear system Ax = b for the sparse matrix A, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient method. Matrix A is:

```
2.0
           0.0 - 1.0
                       0.0
                            0.0
                                  0.0
                                        0.0
                                             0.0
0.0
      2.0 - 1.0
                 0.0
                       0.0
                            0.0
                                  0.0
                                        0.0
                                             0.0
0.0 -1.0 2.0
                 0.0
                     0.0
                            0.0
                                  0.0
                                        0.0
                                             0.0
-1.0
      0.0 0.0 2.0 -1.0
                            0.0
                                  0.0
                                             0.0
0.0
      0.0 0.0 -1.0 2.0 -1.0
                                  0.0
                                             0.0
                                        0.0
0.0
      0.0
          0.0
                 0.0 - 1.0
                            2.0
                                 -1.0
                                        0.0
                                             0.0
           0.0 0.0 0.0 -1.0
                                  2.0
                                      -1.0
                                             0.0
0.0
      0.0
                 0.0
0.0
      0.0
           0.0
                       0.0
                            0.0
                                 -1.0
                                        2.0
                                            -1.0
0.0
                 0.0
                       0.0
                            0.0
                                  0.0
```

**Note:** For input matrix KA, ( . ) indicates any value between 1 and 9.

#### Call Statement and Input

```
IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 0
RPARM(1) = 1.D-7
          2.0 -1.0
                    0.0
         2.0 -1.0
                   0.0
        -1.0 2.0
                   0.0
AC = \begin{vmatrix} 1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \\ -1.0 & 2.0 & -1.0 \end{vmatrix}
        -1.0 2.0 -1.0
        -1.0
               2.0 0.0
В
       Χ
        Output
        IPARM(4) = 5
RPARM(2) = 0
RPARM(3) = 0.351D-15
```

**Example 2:** This example finds the solution of the linear system Ax = b for the same sparse matrix A as in Example 1, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient method, preconditioned with an incomplete Cholesky factorization. The smallest eigenvalue of the iteration matrix is computed and used in stopping the computation.

Note: For input matrix KA, ( . ) indicates any value between 1 and 9.

Call Statement and Input

```
В
  Χ
  Output
  IPARM(4) = 1
RPARM(2) = 1
RPARM(3) = 0.100D-15
```

### DSDCG—Sparse Positive Definite or Negative Definite Symmetric Matrix Iterative Solve Using Compressed-Diagonal Storage Mode

This subroutine solves a symmetric, positive definite or negative definite linear system, using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization, for a sparse matrix stored in compressed-diagonal storage mode. Matrix **A** and vectors **x** and **b** are used:

$$Ax = b$$

where **A**, **x**, and **b** contain long-precision real numbers.

#### Syntax

Fortran	CALL DSDCG (iopt, m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2)	
C and C++	dsdcg (iopt, m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	
PL/I	CALL DSDCG (iopt, m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	

#### On Entry

iopt

indicates the type of storage used, where:

If iopt = 0, all the nonzero diagonals of the sparse matrix are stored in compressed-diagonal storage mode.

If iopt = 1, the sparse matrix, stored in compressed-diagonal storage mode, is symmetric. Only the main diagonal and one of each pair of identical diagonals are stored in array AD.

Specified as: a fullword integer; iopt = 0 or 1.

m

is the order of the linear system Ax = b and the number of rows in sparse matrix A. Specified as: a fullword integer;  $m \ge 0$ .

nd

is the number of nonzero diagonals stored in the columns of array AD, the number of columns in the array AD, and the number of elements in array LA. Specified as: a fullword integer; it must have the following value, where:

If m > 0, then nd > 0.

If m = 0, then  $nd \ge 0$ .

ad

is the array, referred to as AD, containing the values of the nonzero elements of the sparse matrix stored in compressed-diagonal storage mode. If iopt = 1, the main diagonal and one of each pair of identical diagonals is stored in this array.

Specified as: an *Ida* by (at least) *nd* array, containing long-precision real numbers.

Ida

is the leading dimension of the array specified for ad. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

la

is the array, referred to as LA, containing the diagonal numbers k for the diagonals stored in each corresponding column in array AD. For an explanation

of how diagonal numbers are assigned, see "Compressed-Diagonal Storage Mode" on page 94.

Specified as: a one-dimensional array of (at least) length nd, containing fullword integers, where  $1-m \le (\text{elements of LA}) \le m-1$ .

b

is the vector **b** of length m, containing the right-hand side of the matrix problem. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

Х

is the vector  $\mathbf{x}$  of length m, containing your initial guess of the solution of the linear system. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

iparm

is an array of parameters, IPARM(i), where:

IPARM(1) controls the number of iterations.

If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.

If IPARM(1) = 0, the following default values are used:

IPARM(1) = 300

IPARM(2) = 1

IPARM(3) = 0

 $RPARM(1) = 10^{-6}$ 

IPARM(2) is the flag used to select the stopping criterion.

If IPARM(2) = 0, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \|\mathbf{x}\|_2 < \varepsilon$$

where r = b - Ax is the residual and  $\varepsilon$  is the desired relative accuracy.  $\varepsilon$  is stored in RPARM(1).

If IPARM(2) = 1, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \lambda \|\mathbf{x}\|_2 < \varepsilon$$

where  $\lambda$  is an estimate to the minimum eigenvalue of the iteration matrix.  $\lambda$ is computed adaptively by this program and, on output, is stored in RPARM(2).

If IPARM(2) = 2, the conjugate gradient iterative procedure is stopped when:

$$\|\mathbf{r}\|_2 / \lambda \|\mathbf{x}\|_2 < \varepsilon$$

where  $\lambda$  is a predetermined estimate to the minimum eigenvalue of the iteration matrix. This eigenvalue estimate, on input, is stored in RPARM(2) and may be obtained by an earlier call to this subroutine with the same matrix.

• IPARM(3) is the flag that determines whether the system is to be solved using the conjugate gradient method, preconditioned by an incomplete Cholesky factorization with no fill-in.

If IPARM(3) = 0, the system is not preconditioned.

If IPARM(3) = 10, the system is preconditioned by an incomplete Cholesky factorization.

If IPARM(3) = -10, the system is preconditioned by an incomplete Cholesky factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in aux2.

• IPARM(4), see "On Return" on page 654.

Specified as: an array of (at least) length 4, containing fullword integers, where:

```
IPARM(1) = 0
```

IPARM(2) = 0, 1, or 2

IPARM(3) = 0, 10, or -10

#### rparm

is an array of parameters, RPARM(i), where  $\epsilon$  is stored in RPARM(1), and  $\lambda$  is stored in RPARM(2).

RPARM(1) > 0, is the relative accuracy  $\epsilon$  used in the stopping criterion.

RPARM(2) > 0, is the estimate of the smallest eigenvalue,  $\lambda$ , of the iteration matrix. It is only used when IPARM(2) = 2.

RPARM(3), see "On Return" on page 654.

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

#### aux1

has the following meaning:

If naux1 = 0 and error 2015 is unrecoverable, aux1 is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers. naux1

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*.

Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DSDCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have at least the following value, where:

```
If IPARM(2) = 0 or 2, use naux1 \ge 3m.
```

If IPARM(2) = 1 and IPARM(1)  $\neq$  0, use  $naux1 \geq 3m+2(IPARM(1))$ .

If IPARM(2) = 1 and IPARM(1) = 0, use  $naux1 \ge 3m+600$ .

#### aux2

is the storage work area used by this subroutine. If IPARM(3) = -10, aux2 must contain the incomplete Cholesky factorization of matrix A, computed in an

earlier call to DSDCG. Its size is specified by *naux2*. Specified as: an area of storage, containing long-precision real numbers.

#### naux2

is the size of the work area specified by aux2—that is, the number of elements in aux2. Specified as: a fullword integer. When IPARM(3) = 10 or -10, naux2 must have at least the following value, where:

If iopt = 0, use  $naux2 \ge m(1.5nd+2)1.5+2(m+6)$ .

If iopt = 1, use  $naux2 \ge m(3nd+2)+8$ .

#### On Return

Χ

is the vector  $\mathbf{x}$  of length m, containing the solution of the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . Returned as: a one-dimensional array, containing long-precision real numbers. iparm

As an array of parameters, IPARM(i), where:

IPARM(1) is unchanged.

IPARM(2) is unchanged.

IPARM(3) is unchanged.

IPARM(4) contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers. rparm

is an array of parameters, RPARM(i), where:

RPARM(1) is unchanged.

RPARM(2) is unchanged if IPARM(2) = 0 or 2. If IPARM(2) = 1, RPARM(2) contains  $\lambda$ , an estimate of the smallest eigenvalue of the iteration matrix.

RPARM(3) contains the estimate of the error of the solution. If the process converged, RPARM(3)  $\leq \epsilon$ .

Returned as: a one-dimensional array of length 3, containing long-precision real numbers;  $\lambda > 0$ .

#### aux2

is the storage work area used by this subroutine.

If IPARM(3) = 10, aux2 contains the incomplete Cholesky factorization of matrix A.

If IPARM(3) = -10, aux2 is unchanged.

See "Notes" for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

#### Notes

- 1. When IPARM(3) = -10, this subroutine uses the incomplete Cholesky factorization in *aux2*, computed in an earlier call to this subroutine. When IPARM(3) = 10, this subroutine computes the incomplete Cholesky factorization and stores it in *aux2*.
- 2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify IPARM(3) = 10 on the first invocation. The incomplete factorization is stored in aux2. You may save computing time on subsequent calls by setting

IPARM(3) = -10. In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of aux2 between calls.

- 3. Matrix **A** must have no common elements with vectors **x** and **b**; otherwise, results are unpredictable.
- 4. In the iterative solvers for sparse matrices, the relative accuracy  $\varepsilon$  (RPARM(1)) must be specified "reasonably" (10<sup>-4</sup> to 10<sup>-8</sup>). The algorithm computes a sequence of approximate solution vectors  $\mathbf{x}$  that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|_2 / \lambda \|\boldsymbol{x}\|_2 < \varepsilon$$

where  $\lambda$  is an estimate of the minimum eigenvalue of the iteration matrix, which is either estimated adaptively or given by the user. As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

- 5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 93.
- 6. On output, array AD and vector b are not bitwise identical to what they were on input, because the matrix A and the right-hand side are scaled before starting the iterative process and are unscaled before returning control to the user. In addition, arrays AD and LA may be rearranged on output, but still contain a mathematically equivalent mapping of the elements in matrix A.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

*Function:* The sparse positive definite or negative definite linear system:

$$Ax = b$$

is solved, where:

 ${\bf A}$  is a symmetric, positive definite or negative definite sparse matrix of order  ${\bf m}$ , stored in compressed-diagonal storage mode in arrays AD and LA.

**x** is a vector of length *m*.

**b** is a vector of length m.

The system is solved using the two-term conjugate gradient method, with or without preconditioning by an incomplete Cholesky factorization. In both cases, the matrix is scaled by the square root of the diagonal.

See references [59] and [62]. [36].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux1 = 0, and unable to allocate work area.

Computational Errors: The following errors, with their corresponding return codes, can occur in this subroutine. Where a value of *i* is indicated, it can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for that particular error code in the ESSL error option table; otherwise, the default value causes your program to terminate when the error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector **x** contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that *aux2* contains an incorrect factorization. The subroutine has been called with IPARM(3) = −10, and *aux2* contains an incomplete factorization of the input matrix *A* that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that *aux2* has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2109, return code 3 indicates that the inner product (*y*, *Ay*) is negative in the iterative procedure after iteration *i*. This should not occur, because the input matrix is assumed to be positive or negative definite. Vector *x* contains the results of the last iteration. The value *i* is identified in the computational error message.
- For error 2108, return code 4 indicates that the matrix is not positive definite. AC is partially modified and does not represent the same matrix as on entry.

#### Input-Argument Errors

- 1.  $iopt \neq 0 \text{ or } 1$
- 2. m < 0
- 3. Ida < 1
- 4. Ida < m
- 5. nd < 0
- 6. nd = 0 and m > 0
- 7.  $|\lambda(i)| > m-1$  for i = 1, nd
- 8. IPARM(1) < 0
- 9. IPARM(2)  $\neq$  0, 1, or 2
- 10. IPARM(3)  $\neq$  0, 10, or -10
- 11. RPARM(1) < 0
- 12. RPARM(2) < 0
- 13. Error 2015 is recoverable or *naux1*≠0, and *naux1* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
- 14. *naux2* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

**Example 1:** This example finds the solution of the linear system Ax = b for sparse matrix A, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the two-term conjugate gradient method. In this example, IOPT = 0.. Matrix A is:

```
2.0
                                                       0.0
       0.0
             -1.0
                     0.0
                            0.0
                                  0.0
                                         0.0
                                                0.0
0.0
       2.0
              0.0
                    -1.0
                            0.0
                                  0.0
                                         0.0
                                                0.0
                                                       0.0
-1.0
       0.0
              2.0
                     0.0
                           -1.0
                                   0.0
                                         0.0
                                                0.0
                                                       0.0
0.0
      -1.0
              0.0
                     2.0
                            0.0
                                 -1.0
                                         0.0
                                                0.0
                                                       0.0
0.0
       0.0
             -1.0
                     0.0
                            2.0
                                  0.0
                                        -1.0
                                                0.0
                                                       0.0
 0.0
       0.0
              0.0
                    -1.0
                            0.0
                                  2.0
                                         0.0
                                                       0.0
                                               -1.0
                          -1.0
                                  0.0
                                                      -1.0
0.0
       0.0
              0.0
                     0.0
                                         2.0
                                                0.0
 0.0
       0.0
              0.0
                     0.0
                            0.0
                                 -1.0
                                         0.0
                                                2.0
                                                       0.0
                                                0.0
 0.0
       0.0
              0.0
                     0.0
                            0.0
                                  0.0
                                        -1.0
                                                       2.0
```

#### Call Statement and Input

```
IOPT M
                ND AD LDA LA
                                     IPARM
                                            RPARM
                                                  AUX1
                                                      NAUX1 AUX2 NAUX2
CALL DSDCG( 0 , 9 , 3 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 283 , AUX2 ,
                IPARM(1) = 20
                IPARM(2) =
                         0
                IPARM(3) =
                         0
                RPARM(1) = 1.D-7
                        2.0
                             0.0
                                 -1.0
                        2.0
                             0.0
                                 -1.0
                        2.0
                            -1.0
                                 -1.0
                            -1.0
                        2.0
                                 -1.0
                AD
                        2.0
                            -1.0
                                 -1.0
                        2.0
                            -1.0
                                 -1.0
                        2.0
                            -1.0
                                 -1.0
                        2.0
                            -1.0
                                 0.0
                        2.0
                                  0.0
                LA
                          (0, -2, 2)
                          В
                Χ
                         Output
```

**Example 2:** This example finds the solution of the linear system Ax = b for the same sparse matrix A as in Example 1, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the two-term conjugate gradient method. In this example, IOPT = 1, indicating that the matrix is symmetric, and only the main diagonal and one of each pair of identical diagonals are stored in array AD.

#### Call Statement and Input

5

0 RPARM(3) = 0.46D-16

IPARM(4) =

RPARM(2) =

```
IOPT M
                    ND
                      AD LDA LA
                                             IPARM
                                                     RPARM
                                                            AUX1 NAUX1 AUX2 NAUX2
                                     В
                                         Χ
CALL DSDCG( 1
             , 9 , 2 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 283 , AUX2 , 80 )
```

```
IPARM(1) = 20
IPARM(2) = 0
IPARM(3) = 10
RPARM(1) = 1.D-7
        0.0
     2.0 0.0
     2.0 -1.0
     2.0 -1.0
     2.0 -1.0
AD
     2.0 -1.0
     2.0 -1.0
    2.0 -1.0
    2.0 -1.0
LA
     = (0, -2)
В
     Χ
     Output
     IPARM(4) = 1
RPARM(2) = 0
RPARM(3) = 0.89D-16
```

# DSMGCG—General Sparse Matrix Iterative Solve Using Compressed-Matrix Storage Mode

This subroutine solves a general sparse linear system of equations using an iterative algorithm, conjugate gradient squared or generalized minimum residual, with or without preconditioning by an incomplete LU factorization. The subroutine is suitable for positive real matrices—that is, when the symmetric part of the matrix,  $(A+A^T)/2$ , is positive definite. The sparse matrix is stored in compressed-matrix storage mode. Matrix A and vectors x and b are used:

Ax = b

where **A**, **x**, and **b** contain long-precision real numbers.

#### Notes:

- 1. These subroutines are provided only for migration purposes. You get better performance and a wider choice of algorithms if you use the DSRIS subroutine.
- If your sparse matrix is stored by rows, as defined in "Storage-by-Rows" on page 99, you should first use the utility subroutine DSRSM to convert your sparse matrix to compressed-matrix storage mode. See "DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode" on page 979.

#### Syntax

Fortran	CALL DSMGCG (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2)	
C and C++	dsmgcg (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	
PL/I	CALL DSMGCG (m, nz, ac, ka, lda, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	

On Entry

m

is the order of the linear system Ax = b and the number of rows in sparse matrix A. Specified as: a fullword integer;  $m \ge 0$ .

nz

is the maximum number of nonzero elements in each row of sparse matrix A. Specified as: a fullword integer;  $nz \ge 0$ .

ac

is the array, referred to as AC, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode. Specified as: an *Ida* by (at least) *nz* array, containing long-precision real numbers.

ka

is the array, referred to as KA, containing the column numbers of the matrix  $\boldsymbol{A}$  elements stored in the corresponding positions in array AC. Specified as: an *Ida* by (at least) nz array, containing fullword integers, where  $1 \le$  (elements of KA)  $\le m$ .

lda

is the leading dimension of the arrays specified for ac and ka. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

b

is the vector  $\boldsymbol{b}$  of length m, containing the right-hand side of the matrix problem. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

Х

is the vector  $\mathbf{x}$  of length m, containing your initial guess of the solution of the linear system. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

#### iparm

is an array of parameters, IPARM(i), where:

• IPARM(1) controls the number of iterations.

If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.

If IPARM(1) = 0, the following default values are used:

IPARM(1) = 300

IPARM(2) = 0

IPARM(3) = 10

 $RPARM(1) = 10^{-6}$ 

 IPARM(2) is the flag used to select the iterative procedure used in this subroutine.

If IPARM(2) = 0, the conjugate gradient squared method is used.

If IPARM(2) = k, the generalized minimum residual method, restarted after k steps, is used. Note that the size of the work area aux1 becomes larger as k increases. A value for k in the range of 5 to 10 is suitable for most problems.

• IPARM(3) is the flag that determines whether the system is to be preconditioned by an incomplete LU factorization with no fill-in.

If IPARM(3) = 0, the system is not preconditioned.

If IPARM(3) = 10, the system is preconditioned by an incomplete LU factorization.

If IPARM(3) = -10, the system is preconditioned by an incomplete LU factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in aux2.

IPARM(4), see "On Return" on page 661.

Specified as: an array of (at least) length 4, containing fullword integers, where:

 $IPARM(1) \ge 0$ 

 $IPARM(2) \ge 0$ 

IPARM(3) = 0, 10, or -10

#### rparm

is an array of parameters, RPARM(i), where:

RPARM(1) > 0, is the relative accuracy  $\epsilon$  used in the stopping criterion. The iterative procedure is stopped when:

$$\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x} \|_2 / \| \boldsymbol{x} \|_2 < \varepsilon$$

RPARM(2) is reserved.

RPARM(3), see "On Return" on page 661.

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

#### aux1

has the following meaning:

If naux1 = 0 and error 2015 is unrecoverable, aux1 is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers. naux1

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*. Specified as: a fullword integer, where:

If naux1 = 0 and error 2015 is unrecoverable, DSMGCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have at least the following value, where:

```
If IPARM(2) = 0, use naux1 \ge 7m.
```

If IPARM(2) > 0, use  $naux1 \ge (k+2)m+k(k+4)+1$ , where k = IPARM(2).

#### aux2

is the storage work area used by this subroutine. If IPARM(3) = -10, aux2 must contain the incomplete LU factorization of matrix A, computed in an earlier call to DSMGCG. The size of aux2 is specified by naux2.

Specified as: an area of storage, containing long-precision real numbers. naux2

is the size of the work area specified by aux2—that is, the number of elements in aux2. Specified as: a fullword integer. When IPARM(3) = 10, naux2 must have at least the following value:  $naux2 \ge 3+2m+1.5nz(m)$ .

#### On Return

Χ

is the vector  $\mathbf{x}$  of length m, containing the solution of the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . Returned as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

#### iparm

is an array of parameters, IPARM(i), where:

IPARM(1) is unchanged.

IPARM(2) is unchanged.

IPARM(3) is unchanged.

IPARM(4) contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers. *rparm* 

is an array of parameters, RPARM(i), where:

RPARM(1) is unchanged.

RPARM(2) is reserved.

RPARM(3) contains the estimate of the error of the solution. If the process converged, RPARM(3)  $\leq$  RPARM(1)

Returned as: a one-dimensional array of length 3, containing long-precision real numbers.

aux2

is the storage work area used by this subroutine.

If IPARM(3) = 10, aux2 contains the incomplete LU factorization of matrix A.

If IPARM(3) = -10, aux2 is unchanged.

See "Notes" for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

#### Notes

- 1. When IPARM(3) = -10, this subroutine uses the incomplete LU factorization in aux2, computed in an earlier call to this subroutine. When IPARM(3) = 10, this subroutine computes the incomplete LU factorization and stores it in aux2.
- 2. If you solve the same sparse linear system of equations several times with different right-hand sides using the preconditioned algorithm, specify IPARM(2) = 10 on the first invocation. The incomplete factorization is stored in *aux2*. You may save computing time on subsequent calls by setting IPARM(3) equal to –10. In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of *aux2* between calls.
- 3. Matrix **A** must have no common elements with vectors **x** and **b**; otherwise, results are unpredictable.
- 4. In the iterative solvers for sparse matrices, the relative accuracy  $\varepsilon$  (RPARM(1)) must be specified "reasonably" (10<sup>-4</sup> to 10<sup>-8</sup>). The algorithm computes a sequence of approximate solution vectors  $\mathbf{x}$  that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x} \|_2 / \| \boldsymbol{x} \|_2 < \varepsilon$$

As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

- 5. For a description of how sparse matrices are stored in compressed-matrix storage mode, see "Compressed-Matrix Storage Mode" on page 93.
- On output, array AC is not bitwise identical to what it was on input because the matrix A is scaled before starting the iterative process and is unscaled before returning control to the user.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

Function: The linear system:

$$Ax = b$$

is solved using either the conjugate gradient squared method or the generalized minimum residual method, with or without preconditioning by an incomplete LU factorization, where:

 ${\bf A}$  is a sparse matrix of order m, stored in compressed-matrix storage mode in arrays AC and KA.

**x** is a vector of length *m*.

**b** is a vector of length m.

See references [80] and [82]. [36].

If your program uses a sparse matrix stored by rows and you want to use this subroutine, first convert your sparse matrix to compressed-matrix storage mode by using the subroutine DSRSM described on page 979.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux1 = 0, and unable to allocate work area.

Computational Errors: The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see "What Can You Do about ESSL Computational Errors?" on page 48.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector **x** contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that aux2 contains an incorrect factorization. The subroutine has been called with IPARM(3) = −10, and aux2 contains an incomplete factorization of the input matrix A that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that aux2 has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2112, return code 3 indicates that the incomplete LU factorization of A could not be completed, because one pivot was 0.
- For error 2116, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain 0. Array AC is partially modified and does not represent the same matrix as on entry.

#### Input-Argument Errors

- 1. m < 0
- 2. Ida < 1
- 3. Ida < m
- 4. nz < 0
- 5. nz = 0 and m > 0
- 6. IPARM(1) < 0
- 7. IPARM(2) < 0
- 8. IPARM(3)  $\neq$  0, 10, or -10
- 9. RPARM(1) < 0
- 10. RPARM(2) < 0
- 11. Error 2015 is recoverable or naux1≠0, and naux1 is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

12. *naux2* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

**Example 1:** This example finds the solution of the linear system Ax = b for the sparse matrix A, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the conjugate gradient squared method. Matrix A is:

$$\begin{bmatrix} 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 2.0 \\ \end{bmatrix}$$

Note: For input matrix KA, ( . ) indicates any value between 1 and 9.

Call Statement and Input

$$AC = \begin{bmatrix} 2.0 & 0.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 1.0 & 2.0 & 0.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -1.0 \\ 1.0 & 2.0 & -0.0 \end{bmatrix}$$

#### Output

**Example 2:** This example finds the solution of the linear system Ax = b for the same sparse matrix A as in Example 1, which is stored in compressed-matrix storage mode in arrays AC and KA. The system is solved using the generalized minimum residual method, restarted after 5 steps and preconditioned with an incomplete LU factorization. Most of the input is the same as in Example 1.

Note: For input matrix KA, ( . ) indicates any value between 1 and 9.

#### Call Statement and Input

```
IPARM
                                                          NAUX1
                                                                 AUX2
           М
              NZ
                  AC
                       KΑ
                           LDA
                                В
                                              RPARM
                                                    AUX1
                                                                       NAUX2
CALL DSMGCG(9, 3, AC, KA, 9, B, X, IPARM, RPARM, AUX1, 109, AUX2, 46)
                 IPARM(1) =
                 IPARM(2) = 5
                 IPARM(3) = 10
                 RPARM(1) = 1.D-7
                 AC
                         =(same as input AC in Example 1)
                 KΑ
                         =(same as input KA in Example 1)
                 В
                         = (2.0, 1.0, 3.0, 2.0, 2.0, 2.0, 2.0, 2.0, 3.0)
                 Χ
                         Output
                         = (1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
                 IPARM(4) = 2
                 RPARM(3) = 0.290D-15
```

# DSDGCG—General Sparse Matrix Iterative Solve Using Compressed-Diagonal Storage Mode

This subroutine solves a general sparse linear system of equations using an iterative algorithm, conjugate gradient squared or generalized minimum residual, with or without preconditioning by an incomplete LU factorization. The subroutine is suitable for positive real matrices—that is, when the symmetric part of the matrix,  $(A+A^T)/2$ , is positive definite. The sparse matrix is stored in compressed-diagonal storage mode. Matrix A and vectors x and b are used:

$$Ax = b$$

where **A**, **x**, and **b** contain long-precision real numbers.

#### **Syntax**

Fortran	CALL DSDGCG (m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2)	
C and C++	dsdgcg (m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	
PL/I	CALL DSDGCG (m, nd, ad, lda, la, b, x, iparm, rparm, aux1, naux1, aux2, naux2);	

#### On Entry

m

is the order of the linear system Ax = b and the number of rows in sparse matrix A. Specified as: a fullword integer;  $m \ge 0$ .

nd

is the number of nonzero diagonals stored in the columns of array AD, the number of columns in array AD, and the number of elements in array LA. Specified as: a fullword integer; it must have the following value, where:

If m > 0, then nd > 0.

If m = 0, then  $nd \ge 0$ .

ad

is the array, referred to as AD, containing the values of the nonzero elements of the sparse matrix, stored in compressed-matrix storage mode. Specified as: an *Ida* by (at least) *nd* array, containing long-precision real numbers.

lda

is the leading dimension of the arrays specified for ad. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

la

is the array, referred to as LA, containing the diagonal numbers k for the diagonals stored in each corresponding column in array AD. For an explanation of how diagonal numbers are stored, see "Compressed-Diagonal Storage Mode" on page 94.

Specified as: a one-dimensional array of (at least) length nd, containing fullword integers, where  $1-m \le$  (elements of LA)  $\le$  (m-1).

b

is the vector  $\mathbf{b}$  of length m, containing the right-hand side of the matrix problem. Specified as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

Х

is the vector  $\mathbf{x}$  of length m, containing your initial guess of the solution of the linear system. Specified as: a one-dimensional array of (at least) length m,

containing long-precision real numbers. The elements can have any value, and if no guess is available, the value can be zero.

#### iparm

is an array of parameters, IPARM(i), where:

• IPARM(1) controls the number of iterations.

If IPARM(1) > 0, IPARM(1) is the maximum number of iterations allowed.

If IPARM(1) = 0, the following default values are used:

IPARM(1) = 300

IPARM(2) = 0

IPARM(3) = 10

 $RPARM(1) = 10^{-6}$ 

 IPARM(2) is the flag used to select the iterative procedure used in this subroutine.

If IPARM(2) = 0, the conjugate gradient squared method is used.

If IPARM(2) = k, the generalized minimum residual method, restarted after k steps, is used. Note that the size of the work area aux1 becomes larger as k increases. A value for k in the range of 5 to 10 is suitable for most problems.

• IPARM(3) is the flag that determines whether the system is to be preconditioned by an incomplete LU factorization with no fill-in.

If IPARM(3) = 0, the system is not preconditioned.

If IPARM(3) = 10, the system is preconditioned by an incomplete LU factorization.

If IPARM(3) = -10, the system is preconditioned by an incomplete LU factorization, where the factorization matrix was computed in an earlier call to this subroutine and is stored in *aux2*.

IPARM(4), see "On Return" on page 668.

Specified as: an array of (at least) length 4, containing fullword integers, where:

 $IPARM(1) \ge 0$ 

 $IPARM(2) \ge 0$ 

IPARM(3) = 0, 10, or -10

#### rparm

is an array of parameters, RPARM(i), where:

If RPARM(1) > 0, is the relative accuracy  $\epsilon$  used in the stopping criterion. The iterative procedure is stopped when:

$$\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x} \|_2 / \| \boldsymbol{x} \|_2 < \varepsilon$$

RPARM(2) is reserved.

RPARM(3), see "On Return" on page 668.

Specified as: a one-dimensional array of (at least) length 3, containing long-precision real numbers.

#### aux1

has the following meaning:

If naux1 = 0 and error 2015 is unrecoverable, aux1 is ignored.

Otherwise, it is a storage work area used by this subroutine, which is available for use by the calling program between calls to this subroutine. Its size is specified by *naux1*.

Specified as: an area of storage, containing long-precision real numbers. naux1

is the size of the work area specified by *aux1*—that is, the number of elements in *aux1*. Specified as: a fullword integer, where:

If naux1 = 0 and error 2015 is unrecoverable, DSDGCG dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, naux1 > 0 and must have at least the following value, where:

```
If IPARM(2) = 0, use naux1 \ge 7m.
```

```
If IPARM(2) > 0, use naux1 \ge (k+2)m+k(k+4)+1, where k = PARM(2). aux2
```

is a storage work area used by this subroutine. If IPARM(3) = -10, aux2 must contain the incomplete LU factorization of matrix  $\mathbf{A}$ , computed in an earlier call to DSDGCG. The size of aux2 is specified by naux2.

Specified as: an area of storage, containing long-precision real numbers. naux2

is the size of the work area specified by aux2—that is, the number of elements in aux2. Specified as: a fullword integer. When IPARM(3) = 10 or -10, naux2 must have at least the following value:  $naux2 \ge 3+2m+1.5nd(m)$ .

#### On Return

Χ

is the vector  $\mathbf{x}$  of length m, containing the solution of the system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . Returned as: a one-dimensional array of (at least) length m, containing long-precision real numbers.

#### iparm

is an array of parameters, IPARM(i), where:

IPARM(1) is unchanged.

IPARM(2) is unchanged.

IPARM(3) is unchanged.

IPARM(4) contains the number of iterations performed by this subroutine.

Returned as: a one-dimensional array of length 4, containing fullword integers. rparm

is an array of parameters, RPARM(i), where:

RPARM(1) is unchanged.

RPARM(2) is reserved.

RPARM(3) contains the estimate of the error of the solution. If the process converged, RPARM(3)  $\leq$  RPARM(1).

Returned as: a one-dimensional array of length 3, containing long-precision real numbers.

#### aux2

is the storage work area used by this subroutine.

If IPARM(3) = 10, aux2 contains the incomplete LU factorization of matrix **A**.

If IPARM(3) = -10, aux2 is unchanged.

See "Notes" for additional information on *aux2*. Returned as: an area of storage, containing long-precision real numbers.

#### Notes

- 1. When IPARM(3) = -10, this subroutine uses the incomplete LU factorization in aux2, computed in an earlier call to this subroutine. When IPARM(3) = 10, this subroutine computes the incomplete LU factorization and stores it in aux2.
- 2. If you solve the same sparse linear system of equations several times with different right-hand sides, using the preconditioned algorithm, specify IPARM(3) = 10 on the first invocation. The incomplete factorization is stored in aux2. You may save computing time on subsequent calls by setting IPARM(3) = -10. In this way, the algorithm reutilizes the incomplete factorization that was computed the first time. Therefore, you should not modify the contents of aux2 between calls.
- 3. Matrix **A** must have no common elements with vectors **x** and **b**; otherwise, results are unpredictable.
- 4. In the iterative solvers for sparse matrices, the relative accuracy  $\varepsilon$  (RPARM(1)) must be specified "reasonably" (10<sup>-4</sup> to 10<sup>-8</sup>). The algorithm computes a sequence of approximate solution vectors  $\mathbf{x}$  that converge to the solution. The iterative procedure is stopped when the norm of the residual is sufficiently small—that is, when:

$$\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x} \|_2 / \| \boldsymbol{x} \|_2 < \varepsilon$$

As a result, if you specify a larger  $\epsilon$ , the algorithm takes fewer iterations to converge to a solution. If you specify a smaller  $\epsilon$ , the algorithm requires more iterations and computer time, but converges to a more precise solution. If the value you specify is unreasonably small, the algorithm may fail to converge within the number of iterations it is allowed to perform.

- 5. For a description of how sparse matrices are stored in compressed-diagonal storage mode, see "Compressed-Diagonal Storage Mode" on page 94.
- 6. On output, array AD is not bitwise identical to what it was on input, because matrix **A** is scaled before starting the iterative process and is unscaled before returning control to the user.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

Function: The linear system:

$$Ax = b$$

is solved using either the conjugate gradient squared method or the generalized minimum residual method, with or without preconditioning by an incomplete LU factorization, where:

 ${\bf A}$  is a sparse matrix of order  ${\bf m}$ , stored in compressed-diagonal storage mode in arrays AD and LA.

**x** is a vector of length *m*.

**b** is a vector of length m.

See references [80] and [82]. [36].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux1 = 0, and unable to allocate work area.

Computational Errors: The following errors, with their corresponding return codes, can occur in this subroutine. For details on error handling, see "What Can You Do about ESSL Computational Errors?" on page 48.

- For error 2110, return code 1 indicates that the subroutine exceeded IPARM(1) iterations without converging. Vector **x** contains the approximate solution computed at the last iteration.
- For error 2111, return code 2 indicates that aux2 contains an incorrect factorization. The subroutine has been called with IPARM(3) = −10, and aux2 contains an incomplete factorization of the input matrix A that was computed by a previous call to the subroutine when IPARM(3) = 10. This error indicates that aux2 has been modified since the last call to the subroutine, or that the input matrix is not the same as the one that was factored. If the default action has been overridden, the subroutine can be called again with the same parameters, with the exception of IPARM(3) = 0 or 10.
- For error 2112, return code 3 indicates that the incomplete LU factorization of A could not be completed, because one pivot was 0.
- For error 2116, return code 4 indicates that the matrix is singular, because all elements in one row of the matrix contain 0. Array AC is partially modified and does not represent the same matrix as on entry.

#### Input-Argument Errors

- 1. m < 0
- 2. Ida < 1
- 3. Ida < m
- 4. nd < 0
- 5. nd = 0 and m > 0
- 6. IPARM(1) < 0
- 7. IPARM(2) < 0
- 8. IPARM(3)  $\neq$  0, 10, or -10
- 9. RPARM(1) < 1.D0
- 10. Error 2015 is recoverable or *naux1*≠0, and *naux1* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.
- 11. *naux2* is too small—that is, less than the minimum required value. Return code 5 is returned if error 2015 is recoverable.

**Example 1:** This example finds the solution of the linear system Ax = b for the sparse matrix A, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the conjugate gradient squared method. Matrix A is:

```
2.0
                                              0.0
                                                     0.0
     0.0
           -1.0
                   0.0
                          0.0
                                0.0
                                       0.0
0.0
     2.0
            0.0
                  -1.0
                          0.0
                                0.0
                                       0.0
                                              0.0
                                                     0.0
0.0
     0.0
            2.0
                   0.0
                         -1.0
                                0.0
                                       0.0
                                              0.0
                                                     0.0
0.0
     0.0
            0.0
                   2.0
                          0.0
                               -1.0
                                       0.0
                                              0.0
                                                     0.0
1.0
     0.0
            0.0
                   0.0
                          2.0
                                0.0
                                      -1.0
                                                     0.0
                                              0.0
0.0
     1.0
            0.0
                   0.0
                          0.0
                                2.0
                                       0.0
                                             -1.0
                                                     0.0
                                              0.0
0.0
     0.0
            1.0
                   0.0
                          0.0
                                0.0
                                       2.0
                                                    -1.0
0.0
     0.0
            0.0
                   1.0
                          0.0
                                0.0
                                       0.0
                                              2.0
                                                     0.0
0.0
     0.0
            0.0
                   0.0
                          1.0
                                0.0
                                       0.0
                                              0.0
                                                     2.0
```

#### Call Statement and Input

IPARM(1) = 20 IPARM(2) = 0 IPARM(3) = 0 RPARM(1) = 1.D-7

$$AD = \begin{bmatrix} 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 0.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & -1.0 & 1.0 \\ 2.0 & 0.0 & 1.0 \\ 2.0 & 0.0 & 1.0 \end{bmatrix}$$

LA = 
$$(0, 2, -4)$$
  
B =  $(1, 1, 1, 1, 2, 2, 2, 3, 3)$   
X =  $(0, 0, 0, 0, 0, 0, 0, 0, 0)$ 

#### Output

**Example 2:** This example finds the solution of the linear system Ax = b for the same sparse matrix A as in Example 1, which is stored in compressed-diagonal storage mode in arrays AD and LA. The system is solved using the generalized minimum residual method, restarted after 5 steps and preconditioned with an incomplete LU factorization. Most of the input is the same as in Example 1.

#### Call Statement and Input

М ND ADLDA LA В χ **IPARM RPARM** AUX1 NAUX1 AUX2 NAUX2 CALL DSDGCG(9, 3 , AD , 9 , LA , B , X , IPARM , RPARM , AUX1 , 109 , AUX2 , 46 )

```
IPARM(1) = 20
IPARM(2) = 5
IPARM(3) = 10
RPARM(1) = 1.D-7
AD
       =(same as input AD in Example 1)
LA
       =(same as input LA in Example 1)
В
       = (1, 1, 1, 1, 2, 2, 2, 3, 3)
χ
       = (0, 0, 0, 0, 0, 0, 0, 0)
Output
       IPARM(4) = 6
RPARM(3) = 0.250D-15
```

## **Linear Least Squares Subroutines**

This section contains the linear least squares subroutine descriptions.

## SGESVF and DGESVF—Singular Value Decomposition for a General Matrix

These subroutines compute the singular value decomposition of general matrix  $\mathbf{A}$  in preparation for solving linear least squares problems. To compute the minimal norm linear least squares solution of  $\mathbf{AX} \cong \mathbf{B}$ , follow the call to these subroutines with a call to SGESVS or DGESVS, respectively.

Table 114. Data Types	
<b>A</b> , <b>B</b> , <b>s</b> , aux	Subroutine
Short-precision real	SGESVF
Long-precision real	DGESVF

#### **Syntax**

Fortran	CALL SGESVF   DGESVF (iopt, a, Ida, b, Idb, nb, s, m, n, aux, naux)	
C and C++	sgesvf   dgesvf (iopt, a, Ida, b, Idb, nb, s, m, n, aux, naux);	
PL/I	CALL SGESVF   DGESVF (iopt, a, Ida, b, Idb, nb, s, m, n, aux, naux);	

#### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0 or 10, singular values are computed.

If iopt = 1 or 11, singular values and V are computed.

If iopt = 2 or 12, singular values, V, and  $U^TB$  are computed.

Specified as: a fullword integer; iopt = 0, 1, 2, 10, 11, or 12.

If *iopt* < 10, singular values are unordered.

If  $iopt \ge 10$ , singular values are sorted in descending order and, if applicable, the columns of **V** and the rows of **U**<sup>T</sup>**B** are swapped to correspond to the sorted singular values.

а

is the m by n general matrix A, whose singular value decomposition is to be computed. Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 114.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge \max(m, n)$ .

b

has the following meaning, where:

If iopt = 0, 1, 10, or 11, this argument is not used in the computation.

If iopt = 2 or 12, it is the m by nb matrix **B**.

Specified as: an *Idb* by (at least) *nb* array, containing numbers of the data type indicated in Table 114.

If this subroutine is followed by a call to SGESVS or DGESVS,  $\boldsymbol{B}$  should contain the right-hand side of the linear least squares problem,  $\boldsymbol{AX} \cong \boldsymbol{B}$ . (The nb column vectors of  $\boldsymbol{B}$  contain right-hand sides for nb distinct linear least

```
squares problems.) However, if the matrix U^{T} is desired on output, B should be
    equal to the identity matrix of order m.
ldb
    has the following meaning, where:
   If iopt = 0, 1, 10, or 11, this argument is not used in the computation.
   If iopt = 2 or 12, it is the leading dimension of the array specified for b.
   Specified as: a fullword integer. It must have the following values, where:
   If iopt = 0, 1, 10, or 11, Idb > 0.
   If iopt = 2 or 12, ldb > 0 and ldb \ge max(m, n).
nb
   has the following meaning, where:
   If iopt = 0, 1, 10, or 11, this argument is not used in the computation.
   If iopt = 2 or 12, it is the number of columns in matrix B.
   Specified as: a fullword integer; if iopt = 2 or 12, nb > 0.
    See "On Return."
m
   is the number of rows in matrices A and B. Specified as: a fullword integer;
   m \geq 0.
   is the number of columns in matrix A and the number of elements in vector s.
   Specified as: a fullword integer; n \ge 0.
aux
   has the following meaning:
   If naux = 0 and error 2015 is unrecoverable, aux is ignored.
   Otherwise, it is the storage work area used by this subroutine. Its size is
   specified by naux.
   Specified as: an area of storage, containing numbers of the data type indicated
   in Table 114 on page 674.
naux
   is the size of the work area specified by aux—that is, the number of elements
   in aux. Specified as: a fullword integer, where:
   If naux = 0 and error 2015 is unrecoverable, SGESVF and DGESVF
   dynamically allocate the work area used by the subroutine. The work area is
   deallocated before control is returned to the calling program.
   Otherwise, It must have the following value, where:
   If iopt = 0 or 10, naux \ge n + max(m, n).
   If iopt = 1 or 11, naux \ge 2n + max(m, n).
   If iopt = 2 or 12, naux \ge 2n + max(m, n, nb).
On Return
```

If iopt = 0, or 10, **A** is overwritten; that is, the original input is not preserved.

has the following meaning, where:

675

If iopt = 1, 2, 11, or 12, **A** contains the real orthogonal matrix **V**, of order *n*, in its first *n* rows and *n* columns. If iopt = 11 or 12, the columns of **V** are swapped to correspond to the sorted singular values. If m > n, rows n+1, n+2, ..., m of array A are overwritten; that is, the original input is not preserved.

Returned as: an *Ida* by (at least) *n* array, containing numbers of the data type indicated in Table 114 on page 674.

b

has the following meaning, where:

If iopt = 0, 1, 10, or 11, B is not used in the computation.

If iopt = 2 or 12, **B** is overwritten by the *n* by *nb* matrix  $U^TB$ .

If iopt = 12, the rows of  $U^TB$  are swapped to correspond to the sorted singular values. If m > n, rows n+1, n+2, ..., m of array B are overwritten; that is, the original input is not preserved.

Returned as: an *ldb* by (at least) *nb* array, containing numbers of the data type indicated in Table 114 on page 674.

s

is a the vector  $\mathbf{s}$  of length n, containing the singular values of matrix  $\mathbf{A}$ . Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 114 on page 674;  $s_i \ge 0$ , where:

If iopt < 10, the singular values are unordered in s.

If  $iopt \ge 10$ , the singular values are sorted in descending order in s; that is,  $s_1 \ge s_2 \ge ... \ge s_n \ge 0$ . If applicable, the columns of v and the rows of v are swapped to correspond to the sorted singular values.

#### **Notes**

- 1. The following items must have no common elements; otherwise, results are unpredictable: matrices **A** and **B**, vector **s**, and the data area specified for *aux*.
- 2. When you specify iopt = 0, 1, 10, or 11, you must also specify:
  - A dummy argument for b
  - · A positive value for Idb

See "Example" on page 561.

 You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The singular value decomposition of a real general matrix is computed as follows:

$$A = U \Sigma V^{T}$$

where:

$$U^{\mathsf{T}}U = V^{\mathsf{T}}V = VV^{\mathsf{T}} = I$$

**A** is an *m* by *n* real general matrix.

 $\boldsymbol{V}$  is a real general orthogonal matrix of order n. On output,  $\boldsymbol{V}$  overwrites the first n rows and n columns of  $\boldsymbol{A}$ .

 $U^T B$  is an n by nb real general matrix. On output,  $U^T B$  overwrites the first n rows and nb columns of B.

 $\Sigma$  is an n by n real diagonal matrix. The diagonal elements of  $\Sigma$  are the singular values of A, returned in the vector s.

If m or n is equal to 0, no computation is performed.

One of the following algorithms is used:

- 1. Golub-Reinsch Algorithm (See pages 134 to 151 in reference [93].)
  - a. Reduce the real general matrix A to bidiagonal form using Householder transformations.
  - b. Iteratively reduce the bidiagonal form to diagonal form using a variant of the QR algorithm.
- 2. Chan Algorithm (See reference [13].)
  - a. Compute the QR decomposition of matrix  $\boldsymbol{A}$  using Householder transformations; that is,  $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}$ .
  - b. Apply the Golub-Reinsch Algorithm to the matrix *R*.

If  $R = XWY^{T}$  is the singular value decomposition of R, the singular value decomposition of matrix A is given by:

$$A = Q \begin{bmatrix} X \\ 0 \end{bmatrix} W Y^{\mathsf{T}}$$

where:

$$\boldsymbol{U} = \boldsymbol{Q} \begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{0} \end{bmatrix}$$

$$\Sigma = W$$

$$V = Y$$

Also, see references [13], [55], [72], and pages 134 to 151 in reference [93]. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: Singular value (i) failed to converge after (x) iterations.

- The singular values  $(s_j, j = n, n-1, ..., i+1)$  are correct. If iopt < 10, they are unordered. Otherwise, they are ordered.
- a has been modified.
- If *iopt* = 2 or 12, then *b* has been modified.
- The return code is set to 1.
- *i* and *x* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2107 in the ESSL error option table;

otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

- 1.  $iopt \neq 0, 1, 2, 10, 11, or 12$
- $2. Ida \leq 0$
- 3. max(m, n) > Ida
- 4.  $ldb \le 0$  and iopt = 2, 12
- 5. max(m, n) > ldb and iopt = 2, 12
- 6.  $nb \le 0$  and iopt = 2, 12
- 7. m < 0
- 8. n < 0
- Error 2015 is recoverable or naux≠0, and naux is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to find only the singular values,  $\mathbf{s}$ , of a real long-precision general matrix  $\mathbf{A}$ , where:

- M is greater than N.
- NAUX is greater than or equal to N+max(M, N) = 7.
- LDB has been set to 1 to avoid a Fortran error message.
- DUMMY is a placeholder for argument *b*, which is not used in the computation.
- The singular values are returned in S.
- On output, matrix **A** is overwritten; that is, the original input is not preserved.

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 4.0 & 5.0 & 6.0 \\ 7.0 & 8.0 & 9.0 \\ 10.0 & 11.0 & 12.0 \end{bmatrix}$$

#### Output

$$S = (25.462, 1.291, 0.000)$$

**Example 2:** This example computes the singular values, s, of a real long-precision general matrix A and the matrix V, where:

- M is equal to N.
- NAUX is greater than or equal to 2N+max(M, N) = 9.
- LDB has been set to 1 to avoid a Fortran error message.
- DUMMY is a placeholder for argument *b*, which is not used in the computation.
- The singular values are returned in S.
- The matrix V is returned in A.

#### Call Statement and Input

$$A = \begin{bmatrix} 2.0 & 1.0 & 1.0 \\ 4.0 & 1.0 & 0.0 \\ -2.0 & 2.0 & 1.0 \end{bmatrix}$$

Output

$$A = \begin{bmatrix} -0.994 & 0.105 & -0.041 \\ -0.112 & -0.870 & 0.480 \\ -0.015 & -0.482 & -0.876 \end{bmatrix}$$

$$S = (4.922, 2.724, 0.597)$$

**Example 3:** This example computes the singular values, s, and computes matrices V and  $U^TB$  in preparation for solving the underdetermined system  $AX \cong B$ , where:

- M is less than N.
- NAUX is greater than or equal to 2N+max(M, N, NB) = 9.
- The singular values are returned in S.
- The matrix **V** is returned in A.
- The matrix **U**<sup>T</sup>**B** is returned in B.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 2.0 & 2.0 \\ 2.0 & 4.0 & 5.0 \\ & & & & \\ \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 \\ 4.0 \\ \cdot \end{bmatrix}$$

Output

$$A = \begin{bmatrix} -0.304 & -0.894 & 0.328 \\ -0.608 & 0.447 & 0.656 \\ -0.733 & 0.000 & -0.680 \end{bmatrix}$$

$$B = \begin{bmatrix} -4.061 \\ 0.000 \\ -0.714 \end{bmatrix}$$

$$S = (7.342, 0.000, 0.305)$$

**Example 4:** This example computes the singular values, s, and matrices V and  $U^TB$  in preparation for solving the overdetermined system  $AX \cong B$ , where:

- M is greater than N.
- NAUX is greater than or equal to 2N+max(M, N, NB) = 7.
- The singular values are returned in S.
- The matrix V is returned in A.
- The matrix **U**T**B** is returned in B.

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

#### Output

$$A = \begin{bmatrix} 0.922 & -0.386 \\ -0.386 & -0.922 \\ \cdot & \cdot \end{bmatrix}$$

$$B = \begin{bmatrix} -1.310 & -2.321 \\ -13.867 & -18.963 \\ \cdot & \cdot \end{bmatrix}$$

$$X = (0.773, 9.508)$$

**Example 5:** This example computes the singular values,  $\mathbf{s}$ , and matrices  $\mathbf{V}$  and  $\mathbf{U}^T\mathbf{B}$  in preparation for solving the overdetermined system  $\mathbf{AX} \cong \mathbf{B}$ . The singular values are sorted in descending order, and the columns of  $\mathbf{V}$  and the rows of  $\mathbf{U}^T\mathbf{B}$  are swapped to correspond to the sorted singular values.

- M is greater than N.
- NAUX is greater than or equal to 2N+max(M, N, NB) = 7.
- The singular values are returned in S.
- The matrix V is returned in A.
- The matrix **U**T**B** is returned in B.

#### Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

#### Output

$$A = \begin{bmatrix} -0.386 & 0.922 \\ -0.922 & -0.386 \\ & & & \end{bmatrix}$$

$$B = \begin{bmatrix} -13.867 & -18.963 \\ -1.310 & -2.321 \\ \cdot & \cdot \end{bmatrix}$$

$$S = (9.508, 0.773)$$

# SGESVS and DGESVS—Linear Least Squares Solution for a General Matrix Using the Singular Value Decomposition

These subroutines compute the minimal norm linear least squares solution of  $AX \cong B$ , where A is a general matrix, using the singular value decomposition computed by SGESVF or DGESVF.

Table 115. Data Types	
<b>V</b> , <b>UB</b> , <b>X</b> , <b>s</b> , τ	Subroutine
Short-precision real	SGESVS
Long-precision real	DGESVS

#### **Syntax**

Fortran	CALL SGESVS   DGESVS (v, ldv, ub, ldub, nb, s, x, ldx, m, n, tau)	
C and C++	sgesvs   dgesvs (v, ldv, ub, ldub, nb, s, x, ldx, m, n, tau);	
PL/I	CALL SGESVS   DGESVS (v, ldv, ub, ldub, nb, s, x, ldx, m, n, tau);	

#### On Entry

V

is the orthogonal matrix V of order n in the singular value decomposition of matrix A. It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument a.

Specified as: an *Idv* by (at least) *n* array, containing numbers of the data type indicated in Table 115.

ldv

is the leading dimension of the array specified for v. Specified as: a fullword integer; Idv > 0 and  $Idv \ge n$ .

ub

is an n by nb matrix, containing  $U^TB$ . It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument b. On output,  $U^TB$  is overwritten; that is, the original input is not preserved.

Specified as: an *Idub* by (at least) *nb* array, containing numbers of the data type indicated in Table 115.

Idub

is the leading dimension of the array specified for ub. Specified as: a fullword integer; ldub > 0 and  $ldub \ge n$ .

nb

is the number of columns in matrices  $\boldsymbol{X}$  and  $\boldsymbol{U}^{\mathsf{T}}\boldsymbol{B}$ . Specified as: a fullword integer; nb > 0.

s

is the vector  $\mathbf{s}$  of length n, containing the singular values of matrix  $\mathbf{A}$ . It is produced by a preceding call to SGESVF or DGESVF, where it corresponds to output argument  $\mathbf{s}$ .

Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 115;  $s_i \ge 0$ .

Χ

See "On Return" on page 683.

ldx

is the leading dimension of the array specified for x. Specified as: a fullword integer; ldx > 0 and  $ldx \ge n$ .

m

is the number of rows in matrix **A**. Specified as: a fullword integer;  $m \ge 0$ .

n

is the number of columns in matrix A, the order of matrix V, the number of elements in vector s, the number of rows in matrix UB, and the number of rows in matrix X. Specified as: a fullword integer;  $n \ge 0$ .

tau

is the error tolerance  $\tau$ . Any singular values in vector  $\boldsymbol{s}$  that are less than  $\tau$  are treated as zeros when computing matrix  $\boldsymbol{X}$ . Specified as: a number of the data type indicated in Table 115 on page 682;  $\tau \geq 0$ . For more information on the values for  $\tau$ , see "Notes."

#### On Return

Х

is an n by nb matrix, containing the minimal norm linear least solutions of  $AX \cong B$ . The nb column vectors of X contain minimal norm solution vectors for nb distinct linear least squares problems.

Returned as: an *ldx* by (at least) *nb* array, containing numbers of the data type indicated in Table 115 on page 682.

#### Notes

- V, X, s, and U<sup>T</sup>B can have no common elements; otherwise the results are unpredictable.
- 2. In problems involving experimental data,  $\tau$  should reflect the absolute accuracy of the matrix elements:

$$\tau \geq \max(|\Delta_{ii}|)$$

where  $\Delta_{ij}$  are the errors in  $a_{ij}$ . In problems where the matrix elements are known exactly or are only affected by roundoff errors:

$$\left[\tau \ge \varepsilon \left(\sqrt{mn}\right)\right] \max(s_j)$$
 for  $j = (1, ..., n)$ 

where:

 $\epsilon$  is equal to 0.11920E-06 for SGESVS and 0.22204D-15 for DGESVS. **s** is a vector containing the singular values of matrix **A**.

For more information, see references [13], [55], [72], and pages 134 to 151 in reference [93].

**Function:** The minimal norm linear least squares solution of  $AX \cong B$ , where A is a real general matrix, is computed using the singular value decomposition, produced by a preceding call to SGESVF or DGESVF. From SGESVF or DGESVF, the singular value decomposition of A is given by the following:

$$A = U \Sigma V^{T}$$

The linear least squares of solution X, for  $AX \subseteq B$ , is given by the following formula:

$$X = V \Sigma^+ U^T B$$

where:

 $\Sigma$  + is the diagonal matrix with elements  $\sigma_i^+$ , where:

$$\sigma_j^+ = 1.0 / \sigma_j$$
 if  $\sigma_j \ge \tau$  and  $\sigma_j \ne 0$   
 $\sigma_j^+ = 0$  for all other cases

If m or n is equal to 0, no computation is performed. See references [13], [55], [72], and pages 134 to 151 in reference [93]. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $Idv \leq 0$
- 2. n > ldv
- 3.  $Idub \leq 0$
- 4. n > Idub
- 5.  $Idx \leq 0$
- 6. n > ldx
- 7.  $nb \leq 0$
- 8. m < 09. n < 0
- 10. τ < 0

**Example 1:** This example finds the linear least squares solution for the underdetermined system  $AX \cong B$ , using the singular value decomposition computed by DGESVF. Matrix A is:

and matrix B is:

On output, matrix **U**<sup>T</sup>**B** is overwritten.

**Note:** This example corresponds to Example 3 of DGESVF on page 679.

Call Statement and Input

$$S = (7.342, 0.000, 0.305)$$
  
TAU = 0.3993D-14

Output

**Example 2:** This example finds the linear least squares solution for the overdetermined system  $AX \cong B$ , using the singular value decomposition computed by DGESVF. Matrix A is:

and where B is:

$$\left[\begin{array}{ccc} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{array}\right]$$

On output, matrix **U**<sup>T</sup>**B** is overwritten.

**Note:** This example corresponds to Example 4 of DGESVF on page 680.

Call Statement

Input

# **SGESVS and DGESVS**

$$V = \begin{bmatrix} 0.922 & -0.386 \\ -0.386 & -0.922 \\ & & & \end{bmatrix}$$

$$UB = \begin{bmatrix} -1.310 & -2.321 \\ -13.867 & -18.963 \\ \cdot & \cdot \end{bmatrix}$$

$$X = \begin{bmatrix} -1.000 & -2.000 \\ 2.000 & 3.000 \end{bmatrix}$$

# SGELLS and DGELLS—Linear Least Squares Solution for a General Matrix Using a QR Decomposition with Column Pivoting

These subroutines compute the minimal norm linear least squares solution of  $AX \cong B$ , using a QR decomposition with column pivoting.

Table 116. Data Types	
<b>A, B, X, rn,</b> τ, aux	Subroutine
Short-precision real	SGELLS
Long-precision real	DGELLS

# Syntax

Fortran	CALL SGELLS   DGELLS (iopt, a, Ida, b, Idb, x, Idx, rn, tau, m, n, nb, k, aux, naux)
C and C++	sgells   dgells (iopt, a, Ida, b, Idb, x, Idx, rn, tau, m, n, nb, k, aux, naux);
PL/I	CALL SGELLS   DGELLS (iopt, a, Ida, b, Idb, x, Idx, rn, tau, m, n, nb, k, aux, naux);

#### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0, X is computed.

If iopt = 1, X and the Euclidean Norm of the residual vectors are computed.

Specified as: a fullword integer; iopt = 0 or 1.

а

is the m by n coefficient matrix  $\boldsymbol{A}$ . On output,  $\boldsymbol{A}$  is overwritten; that is, the original input is not preserved. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 116.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge m$ .

b

is the m by nb matrix  $\boldsymbol{B}$ , containing the right-hand sides of the linear systems. The nb column vectors of  $\boldsymbol{B}$  contain right-hand sides for nb distinct linear least squares problems. On output,  $\boldsymbol{B}$  is overwritten; that is, the original input is not preserved.

Specified as: an *Idb* by (at least) *nb* array, containing numbers of the data type indicated in Table 116.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge m$ .

Χ

See "On Return" on page 688.

ldx

is the leading dimension of the array specified for x. Specified as: a fullword integer; ldx > 0 and  $ldx \ge n$ .

rn

See "On Return" on page 688.

tau is the tolerance  $\tau$ , used to determine the subset of the columns of **A** used in the solution. Specified as: a number of the data type indicated in Table 116;  $\tau \geq 0$ . For more information on how to select a value for  $\tau$ , see "Notes" on page 689. m is the number of rows in matrices **A** and **B**. Specified as: a fullword integer;  $m \geq 0$ . n is the number of columns in matrix A and the number of rows in matrix X. Specified as: a fullword integer;  $n \ge 0$ . nb is the number of columns in matrices **B** and **X** and the number of elements in vector rn. Specified as: a fullword integer; nb > 0. k See "On Return." aux has the following meaning: If naux = 0 and error 2015 is unrecoverable, aux is ignored. Otherwise, it is the storage work area used by this subroutine. Its size is specified by naux. Specified as: an area of storage, containing numbers of the data type indicated in Table 116 on page 687. On output, the contents of aux are overwritten. naux is the size of the work area specified by aux—that is, the number of elements in aux. Specified as: a fullword integer, where: If naux = 0 and error 2015 is unrecoverable, SGELLS and DGELLS dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program. Otherwise, It must have the following values:  $naux \ge 3n + max(n, nb)$  for SGELLS  $naux \ge [ceiling(2.5n) + max(n, nb)]$  for DGELLS On Return Χ is the solution matrix X, with n rows and nb columns, where: If  $k \neq 0$ , the *nb* column vectors of **X** contain minimal norm least squares solutions for *nb* distinct linear least squares problems. The elements in each solution vector correspond to the original columns of A. If k = 0, the *nb* column vectors of **X** are set to 0. Returned as: an *ldx* by (at least) *nb* array, containing numbers of the data type indicated in Table 116 on page 687. rn is the vector **rn** of length **nb**, where: If iopt = 0 or k = 0, rn is not used in the computation.

If iopt = 1,  $rn_i$  is the Euclidean Norm of the residual vector for the linear least

squares problem defined by the i-th column vector of **B**.

Returned as: a one-dimensional array of (at least) *nb*, containing numbers of the data type indicated in Table 116 on page 687.

k

is the number of columns of matrix  $\mathbf{A}$  used in the solution. Returned as: a fullword integer;  $\mathbf{k}=$  (the number of diagonal elements of matrix  $\mathbf{R}$  exceeding  $\tau$  in magnitude).

#### **Notes**

- 1. In your C program, argument *k* must be passed by reference.
- 2. If  $ldb \ge \max(m, n)$ , matrix X and matrix B can be the same; otherwise, matrix X and matrix B can have no common elements, or the results are unpredictable.
- 3. The following items must have no common elements; otherwise, results are unpredictable:
  - Matrices A and X, vector rn, and the data area specified for aux
  - Matrices **A** and **B**, vector **rn**, and the data area specified for **aux**.
- 4. If the relative uncertainty in the matrix **B** is  $\rho$ , then:

$$\tau \geq \rho \|\mathbf{A}\|_{\mathsf{F}}$$

See references [44 ], [59 ], and [72 ] for additional guidance on determining suitable values for  $\tau.$ 

- 5. When you specify iopt = 0, you must also specify a dummy argument for rn. For more details, see "Example 1" on page 690.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The minimal norm linear least squares solution of  $AX \cong B$  is computed using a QR decomposition with column pivoting, where:

**A** is an m by n real general matrix.

**B** is an *m* by *nb* real general matrix.

**X** is an *n* by *nb* real general matrix.

Optionally, the Euclidean Norms of the residual vectors can be computed. Following are the steps involved in finding the minimal norm linear least squares solution of AX = B. A is decomposed, using Householder transformations and column pivoting, into the following form:

$$AP = QR$$

where:

**P** is a permutation matrix.

**Q** is an orthogonal matrix.

**R** is an upper triangular matrix.

k is the first index, where:

$$|r_{k+1,k+1}| \le \tau$$

If k = n, the minimal norm linear least squares solution is obtained by solving  $RX = Q^TB$  and reordering X to correspond to the original columns of A.

If k < n, **R** has the following form:

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ 0 & 0 \end{bmatrix}$$

To find the minimal norm linear least squares solution, it is necessary to zero the submatrix  $R_{12}$  using Householder transformations. See references [44], [59], and [72]. If m or n is equal to 0, no computation is performed. These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

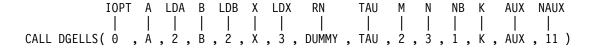
Computational Errors: None

Input-Argument Errors

- 1.  $iopt \neq 0$  or 1
- 2.  $Ida \leq 0$
- 3. m > Ida
- $4. Idb \leq 0$
- 5. m > ldb
- 6.  $Idx \leq 0$
- 7. n > ldx
- 8. m < 0
- 9. n < 0
- 10.  $nb \le 0$
- 11. τ < 0
- 12. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example solves the underdetermined system  $AX \cong B$ . On output, A and B are overwritten. DUMMY is used as a placeholder for argument rn, which is not used in the computation.

Call Statement and Input



$$A = \begin{bmatrix} 1.0 & 2.0 & 2.0 \\ 2.0 & 4.0 & 5.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 \\ 4.0 \end{bmatrix}$$

TAU = 
$$0.0$$

Output

$$X = \begin{bmatrix} -0.600 \\ -1.200 \\ 2.000 \end{bmatrix}$$

**Example 2:** This example solves the overdetermined system  $AX \cong B$ . On output, A and B are overwritten. DUMMY is used as a placeholder for argument rn, which is not used in the computation.

Call Statement and Input

$$A = \begin{bmatrix} 1.0 & 4.0 \\ 2.0 & 5.0 \\ 3.0 & 6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 7.0 & 10.0 \\ 8.0 & 11.0 \\ 9.0 & 12.0 \end{bmatrix}$$

Output

$$X = \begin{bmatrix} -1.000 & -2.000 \\ 2.000 & 3.000 \end{bmatrix}$$

**Example 3:** This example solves the overdetermined system  $AX \cong B$  and computes the Euclidean Norms of the residual vectors. On output, A and B are overwritten.

## Call Statement and Input

$$A = \begin{bmatrix} 1.1 & -4.3 \\ 2.0 & -5.0 \\ 3.0 & -6.0 \end{bmatrix}$$

$$B = \begin{bmatrix} -7.0 & 10.0 \\ -8.0 & 11.0 \\ -9.0 & 12.0 \end{bmatrix}$$

TAU = 
$$0.0$$

$$X = \begin{bmatrix} 0.543 & -1.360 \\ 1.785 & -2.699 \end{bmatrix}$$

$$RN = \begin{bmatrix} 0.196 \\ 0.275 \end{bmatrix}$$

# **Chapter 11. Eigensystem Analysis**

The eigensystem analysis subroutines are described in this chapter.

# **Overview of the Eigensystem Analysis Subroutines**

The eigensystem analysis subroutines provide solutions to the algebraic eigensystem analysis problem Az = wz and the generalized eigensystem analysis problem Az = wBz ( Table 117). Many of the eigensystem analysis subroutines use the algorithms presented in *Linear Algebra* by Wilkinson and Reinsch [93] or use adaptations of EISPACK routines, as described in the *EISPACK Guide Lecture Notes in Computer Science* in reference [81] or in the *EISPACK Guide Extension Lecture Notes in Computer Science* in reference [55]. (EISPACK is available from the sources listed in reference [49].)

Table 117. List of Eigensystem Analysis Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix	SGEEV CGEEV	DGEEV ZGEEV	696
Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPEV CHPEV	DSPEV ZHPEV	707
Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix	SSPSV CHPSV	DSPSV ZHPSV	716
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, Az=wBz, where A and B Are Real General Matrices	SGEGV	DGEGV	724
Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, Az=wBz, where A Is Real Symmetric and B Is Real Symmetric Positive Definite	SSYGV	DSYGV	730

# **Performance and Accuracy Considerations**

- The accuracy of the resulting eigenvalues and eigenvectors varies between the short- and long-precision versions of each subroutine. The degree of difference depends on the size and conditioning of the matrix computation. Some of the subroutines have examples illustrating this difference.
- 2. The short precision subroutines provide increased accuracy by accumulating intermediate results in long precision. Occasionally, for performance reasons, these intermediate results are stored.
- 3. If you want to compute 10% or fewer eigenvalues only, or you want to compute 30% or fewer eigenvalues and eigenvectors, you get better performance if you use \_SPSV and \_HPSV instead of \_SPEV and \_HPEV, respectively. For all other uses, you should use \_SPEV and \_HPEV.
- 4. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see

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"What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Eigensystem Analysis Subroutines**

This section contains the eigensystem analysis subroutine

# SGEEV, DGEEV, CGEEV, and ZGEEV—Eigenvalues and, Optionally, All or Selected Eigenvectors of a General Matrix

SGEEV and DGEEV compute the eigenvalues and, optionally, all or selected eigenvectors of real general matrix **A**. CGEEV and ZGEEV compute the eigenvalues and, optionally, all or selected eigenvectors of complex general matrix **A**. Eigenvalues are returned in complex vector **w**, and eigenvectors are returned in complex matrix **Z**:

Az = wz

Table 118. Data Types			
A	w, Z	aux	Subroutine
Short-precision real	Short-precision complex	Short-precision real	SGEEV
Long-precision real	Long-precision complex	Long-precision real	DGEEV
Short-precision complex	Short-precision complex	Short-precision real	CGEEV
Long-precision complex	Long-precision complex	Long-precision real	ZGEEV

#### Syntax

Fortran	CALL SGEEV   DGEEV   CGEEV   ZGEEV (iopt, a, Ida, w, z, Idz, select, n, aux, naux)
C and C++	sgeev   dgeev   cgeev   zgeev (iopt, a, Ida, w, z, Idz, select, n, aux, naux);
PL/I	CALL SGEEV   DGEEV   CGEEV   ZGEEV (iopt, a, Ida, w, z, Idz, select, n, aux, naux);

#### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0, eigenvalues only are computed.

If *iopt* = 1, eigenvalues and eigenvectors are computed.

If iopt = 2, eigenvalues and eigenvectors corresponding to selected eigenvalues are computed.

Specified as: a fullword integer; iopt = 0, 1, or 2.

а

is the real or complex general matrix  $\boldsymbol{A}$  of order n, whose eigenvalues and, optionally, eigenvectors are computed. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 118. On output, A is overwritten; that is, the original input is not preserved.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

W

See "On Return" on page 697.

Z

See "On Return" on page 697.

ldz

has the following meaning, where:

If iopt = 0, it is not used in the computation.

If iopt = 1 or 2, it is the leading dimension of the output array specified for z.

Specified as: a fullword integer. It must have the following values, where:

```
If iopt = 0, Idz > 0.
```

If iopt = 1 or 2, Idz > 0 and  $Idz \ge n$ .

#### select

has the following meaning, where:

If iopt = 0 or 1, it is not used in the computation.

If iopt = 2, it is the logical vector **select** of length n whose true elements indicate those eigenvalues whose corresponding eigenvectors are to be computed.

Specified as: a one-dimensional array of (at least) length n, containing logical data items. Element values can be true (.TRUE.) or false (.FALSE.).

n

is the order of matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 118 on page 696. On output, the contents are overwritten.

#### naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SGEEV, DGEEV, CGEEV, and ZGEEV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, it must have the following value, where:

```
For SGEEV and DGEEV:
```

```
If iopt = 0, naux \ge n.
```

If iopt = 1,  $naux \ge 2n$ .

If iopt = 2,

 $naux \ge n^2 + 4n$ .

For CGEEV and ZGEEV:

If iopt = 0,  $naux \ge 2n$ .

If iopt = 1,  $naux \ge 3n$ .

If iopt = 2,  $naux \ge 2n^2+5n$ .

On Return

и

is the vector  $\mathbf{w}$  of length n, containing the eigenvalues of  $\mathbf{A}$ . The eigenvalues are unordered. For SGEEV and DGEEV, complex conjugate pairs appear consecutively with the eigenvalue having the positive imaginary part first.

Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 118 on page 696.

z

has the following meaning, where:

If iopt = 0, it is not used in the computation.

If iopt = 1, it is the matrix Z of order n, containing the eigenvectors of matrix A. The eigenvector in column i of matrix Z corresponds to the eigenvalue  $w_i$ .

If iopt = 2, it is the n by m matrix Z, containing the m eigenvectors of matrix A, which correspond to the m selected eigenvalues in  $w_i$ ,

where m is the number of true elements in the logical vector **select**. The eigenvector in column i of matrix Z corresponds to the i-th selected eigenvalue. Any eigenvector that does not converge is set to 0.

Returned as: a two-dimensional array, containing numbers of the data type indicated in Table 118 on page 696, where:

If iopt = 1, the array must be ldz by (at least) n.

If iopt = 2, the array must be ldz by (at least) m.

#### **Notes**

- 1. When you specify iopt = 0, you must also specify:
  - A positive value for Idz
  - A dummy argument for z (see "Example 1" on page 701)
  - · A dummy argument for select.
- 2. When you specify *iopt* = 1, you must also specify a dummy argument for *select*.
- The following items must have no common elements: matrix A, matrix Z, vector w, vector select, and the data area specified for aux; otherwise, results are unpredictable. See "Concepts" on page 55.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The next two sections describe the methods used to compute the eigenvectors and eigenvalues for either a real general matrix or a complex general matrix. For more information on these methods, see references [39], [43], [45], [60], [81], [91], and [93]. If n is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. See the examples for an illustration of the difference in the results.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

Real General Matrix: The eigenvalues and, optionally, all or selected eigenvectors of a real general matrix **A** are computed as follows.

- For *iopt* = 0, the eigenvalues are computed as follows:
  - 1. Balance the real general matrix A.
  - 2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  - Compute the eigenvalues of the real upper Hessenberg matrix using the QR algorithm.

- 4. The eigenvalues are returned in vector w.
- For *iopt* = 1, the eigenvalues and eigenvectors are computed as follows:
  - 1. Balance the real general matrix **A**.
  - 2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  - 3. Accumulate the orthogonal similarity transformations used in the reduction of the real balanced matrix to upper Hessenberg form.
  - Compute the eigenvalues of the real upper Hessenberg matrix and the eigenvectors of the corresponding real balanced matrix using the QR algorithm.
  - 5. Back transform the eigenvectors of the balanced matrix to the eigenvectors of the original matrix.
  - 6. The eigenvalues are returned in vector **w**, and the eigenvectors are returned in matrix **Z**.
- For iopt = 2, the eigenvalues and selected eigenvectors are computed as follows:
  - 1. Balance the real general matrix **A**.
  - 2. Reduce the balanced matrix to a real upper Hessenberg matrix using orthogonal similarity transformations.
  - 3. Compute the eigenvalues of the real upper Hessenberg matrix using the QR algorithm.
  - 4. Compute the eigenvectors of the real upper Hessenberg matrix corresponding to selected eigenvalues, indicated in the logical vector **select**, using inverse iteration.
  - 5. Back transform the eigenvectors of the real upper Hessenberg matrix to the eigenvectors of the balanced matrix.
  - 6. Back transform the eigenvectors of the balanced matrix to the eigenvectors of the original matrix.
  - 7. The eigenvalues are returned in vector **w**, and the eigenvectors are returned in matrix **Z**.

Complex General Matrix: The eigenvalues and, optionally, all or selected eigenvectors of a complex general matrix **A** are computed as follows.

- For *iopt* = 0, the eigenvalues are computed as follows:
  - 1. Balance the complex general matrix **A**.
  - 2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
  - 3. Compute the eigenvalues of the complex upper Hessenberg matrix using a QR algorithm with implicit shift.
  - 4. The eigenvalues are returned in vector w.
- For *iopt* = 1, the eigenvalues and eigenvectors are computed as follows:
  - 1. Balance the complex general matrix **A**.
  - 2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
  - 3. Accumulate the unitary similarity transformations used in the reduction of the complex balanced matrix to complex upper Hessenberg form.
  - Compute the eigenvalues of the complex upper Hessenberg matrix and the eigenvectors of the complex balanced matrix using a QR algorithm with implicit shift.

- 5. Back transform the eigenvectors of the complex balanced matrix to the eigenvectors of the original matrix.
- 6. The eigenvalues are returned in vector **w**, and the eigenvectors are returned in matrix **Z**.
- For iopt = 2, the eigenvalues and selected eigenvectors are computed as follows:
  - 1. Balance the complex general matrix **A**.
  - 2. Reduce the complex balanced matrix to a complex upper Hessenberg matrix using unitary similarity transformations.
  - 3. Compute the eigenvalues of the complex upper Hessenberg matrix using a QR algorithm with implicit shift.
  - 4. Compute the eigenvectors of the complex upper Hessenberg matrix corresponding to selected eigenvalues, indicated in the logical vector *select*, using inverse iteration.
  - 5. Back transform the eigenvectors of the complex upper Hessenberg matrix to the eigenvectors of the complex balanced matrix.
  - 6. Back transform the eigenvectors of the complex balanced matrix to the eigenvectors of the original matrix.
  - 7. The eigenvalues are returned in vector  $\mathbf{w}$ , and the eigenvectors are returned in matrix  $\mathbf{z}$ .

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

#### Computational Errors

- 1. Eigenvalue (i) failed to converge after (xxx) iterations.
  - The eigenvalues  $(w_i, j = n, n-1, ..., i+1)$  are correct.
  - If *iopt* = 1, then z is modified, but no eigenvectors are correct.
  - a is modified.
  - The return code is set to 1.
  - *i* and *xxx* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.
- Eigenvector (yyy) failed to converge after (zzz) iterations. (The computational error message may occur multiple times with processing continuing after each error, because the number of allowable errors for error code 2102 is set to be unlimited in the ESSL error option table.)
  - All eigenvalues are correct.
  - The eigenvector that failed to converge is set to 0.
  - Any selected eigenvectors for which this message has not been issued are correct.
  - a is modified.
  - The return code is set to 2.
  - yyy and zzz for the last eigenvector that failed to converge can be
    determined at run time by use of the ESSL error-handling facilities. To
    obtain this information, you must use ERRSET to change the number of
    allowable errors for error 2199 in the ESSL error option table. See "What
    Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

- 1.  $iopt \neq 0, 1, or 2$
- 2. n < 0
- 3.  $Ida \leq 0$
- 4. n > Ida
- 5.  $Idz \le 0$  and  $iopt \ne 0$
- 6. n > ldz and  $iopt \neq 0$
- 7. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

Example 1: This example shows how to find the eigenvalues only of a real short-precision general matrix **A** of order 4, where:

- NAUX is equal to N.
- · AUX contains N elements.
- LDZ is set to avoid an error condition.
- DUMMY1 and DUMMY2 are used as placeholders for arguments z and select, which are not used in the computation.
- · On output, A has been overwritten.

**Note:** This matrix is used in Example 5.5 in referenced text [60].

Call Statement and Input

$$A = \begin{bmatrix} -2.0 & 2.0 & 2.0 & 2.0 \\ -3.0 & 3.0 & 2.0 & 2.0 \\ -2.0 & 0.0 & 4.0 & 2.0 \\ -1.0 & 0.0 & 0.0 & 5.0 \end{bmatrix}$$

Output

Example 2: This example shows how to find the eigenvalues and eigenvectors of a real short-precision general matrix **A** of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- DUMMY is used as a placeholder for argument select, which is not used in the computation.
- · On output, A has been overwritten.

**Note:** This matrix is used in Example 5.1 in referenced text [60].

Call Statement and Input

$$A = \begin{bmatrix} 33.0 & 16.0 & 72.0 \\ -24.0 & -10.0 & -57.0 \\ -8.0 & -4.0 & -17.0 \end{bmatrix}$$

#### Output

$$W = \begin{bmatrix} (3.000022, 0.000000) \\ (1.000019, 0.000000) \\ (1.999961, 0.000000) \end{bmatrix}$$

$$Z = \begin{bmatrix} (2.498781, 0.000000) & (76.837608, 0.000000) & (79.999451, 0.000000) \\ (-1.874081, 0.000000) & (-61.470169, 0.000000) & (-64.999649, 0.000000) \\ (-0.624695, 0.000000) & (-20.489990, 0.000000) & (-19.999886, 0.000000) \end{bmatrix}$$

Example 3: This example shows how to find the eigenvalues and eigenvectors of a real short-precision general matrix **A** of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- DUMMY is used as a placeholder for argument select, which is not used in the computation.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 5.4 in referenced text [60].

#### Call Statement and Input

A = 
$$\begin{vmatrix} 8.0 & -1.0 & -5.0 \\ -4.0 & 4.0 & -2.0 \\ 18.0 & -5.0 & -7.0 \end{vmatrix}$$

$$Z = \begin{bmatrix} (0.044710, 0.410578) & (0.044710, -0.410578) & (1.732048, 0.000000) \\ (-0.365868, 0.455287) & (-0.365868, -0.455287) & (3.464096, 0.000000) \\ (0.455287, 0.365868) & (0.455287, -0.365868) & (1.732049, 0.000000) \end{bmatrix}$$

**Example 4:** This example shows how to find the eigenvalues and selected eigenvectors of a real short-precision general matrix **A** of order 4, where:

- NAUX is equal to N<sup>2</sup>+4N.
- AUX contains NAUX elements.
- The first, third, and fourth eigenvectors are selected and appear in the first, second, and third columns of matrix Z, respectively.
- On output, A has been overwritten.

Note: This matrix is used in Example 5.5 in referenced text [60].

#### Call Statement and Input

$$A = \begin{bmatrix} -2.0 & 2.0 & 2.0 & 2.0 \\ -3.0 & 3.0 & 2.0 & 2.0 \\ -2.0 & 0.0 & 4.0 & 2.0 \\ -1.0 & 0.0 & 0.0 & 5.0 \end{bmatrix}$$

#### Output

$$W = \begin{bmatrix} (0.999999, & 0.000000) \\ (2.000001, & 0.000000) \\ (2.999996, & 0.000000) \\ (3.999999, & 0.000000) \end{bmatrix}$$

```
 Z = \begin{pmatrix} (1.000000, 0.000000) & (-0.674014, 0.000000) & (-0.474306, 0.000000) \\ (0.750000, 0.000000) & (-0.674014, 0.000000) & (-0.474306, 0.000000) \\ (0.500000, 0.000000) & (-0.674013, 0.000000) & (-0.474306, 0.000000) \\ (0.250000, 0.000000) & (-0.337006, 0.000000) & (-0.474305, 0.000000) \end{pmatrix}
```

**Example 5:** This example shows how to find the eigenvalues and selected eigenvectors of a real short-precision general matrix **A** of order 3, where:

- NAUX is equal to N<sup>2</sup>+4N.
- AUX contains NAUX elements.
- The first and second eigenvectors are selected and appear in the first and second columns of matrix Z, respectively.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 5.4 in referenced text [60].

Call Statement and Input

$$A = \begin{bmatrix} 8.0 & -1.0 & -5.0 \\ -4.0 & 4.0 & -2.0 \\ 18.0 & -5.0 & -7.0 \end{bmatrix}$$

#### Output

$$W = \begin{bmatrix} (1.999999, 3.999998) \\ (1.999999, -3.999998) \\ (0.999997, 0.000000) \end{bmatrix}$$

**Example 6:** This example shows how the results of Example 5 would differ if matrix A was a real long-precision general matrix. On output, A has been overwritten.

#### Call Statement and Input

#### Output

**Example 7:** This example shows how to find the eigenvalues only of a complex long-precision general matrix **A** of order 3, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- LDZ is set to avoid an error condition.

- DUMMY1 and DUMMY2 are used as placeholders for arguments z and select, which are not used in the computation.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 6.4 in referenced text [60].

#### Call Statement and Input

$$A = \begin{bmatrix} (1.0, 2.0) & (3.0, 4.0) & (21.0, 22.0) \\ (43.0, 44.0) & (13.0, 14.0) & (15.0, 16.0) \\ (5.0, 6.0) & (7.0, 8.0) & (25.0, 26.0) \end{bmatrix}$$

#### Output

**Example 8:** This example shows how to find the eigenvalues and eigenvectors of a complex long-precision general matrix **A** of order 4, where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- DUMMY is used as a placeholder for argument select, which is not used in the computation.
- On output, A has been overwritten.

**Note:** This matrix is used in Example 6.5 in referenced text [60].

### Call Statement and Input

$$A = \begin{bmatrix} (5.0, 9.0) & (5.0, 5.0) & (-6.0, -6.0) & (-7.0, -7.0) \\ (3.0, 3.0) & (6.0, 10.0) & (-5.0, -5.0) & (-6.0, -6.0) \\ (2.0, 2.0) & (3.0, 3.0) & (-1.0, 3.0) & (-5.0, -5.0) \\ (1.0, 1.0) & (2.0, 2.0) & (-3.0, -3.0) & (0.0, 4.0) \end{bmatrix}$$

```
 Z = \begin{pmatrix} (0.625817, \ 0.229776) & (0.333009, \ -0.729358) & (-1.535458, \ 1.519551) & (0.000000, \ 3.464102) \\ (0.625817, \ 0.229776) & (0.666017, \ -1.458715) & (-1.535458, \ 1.519551) & (0.000000, \ 1.732051) \\ (0.625817, \ 0.229776) & (0.333009, \ -0.729358) & (0.000000, \ 0.000000) & (0.000000, \ 1.732051) \\ (0.000000, \ 0.000000) & (0.333009, \ -0.729358) & (-1.535458, \ 1.519551) & (0.000000, \ 1.732051) \\ \end{pmatrix}
```

**Example 9:** This example shows how to find the eigenvalues and selected eigenvectors of a complex long-precision general matrix **A** of order 4, where:

- NAUX is equal to 2N<sup>2</sup>+5N.
- AUX contains NAUX elements.
- The first, third, and fourth eigenvectors are selected and appear in the first, second, and third columns of matrix Z, respectively.
- On output, A has been overwritten.

Note: This matrix is used in Example 6.5 in referenced text [60].

#### Call Statement and Input

A = 
$$\begin{bmatrix} (5.0, 9.0) & (5.0, 5.0) & (-6.0, -6.0) & (-7.0, -7.0) \\ (3.0, 3.0) & (6.0, 10.0) & (-5.0, -5.0) & (-6.0, -6.0) \\ (2.0, 2.0) & (3.0, 3.0) & (-1.0, 3.0) & (-5.0, -5.0) \\ (1.0, 1.0) & (2.0, 2.0) & (-3.0, -3.0) & (0.0, 4.0) \end{bmatrix}$$

# SSPEV, DSPEV, CHPEV, and ZHPEV—Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix

SSPEV and DSPEV compute the eigenvalues and, optionally, the eigenvectors of real symmetric matrix  $\boldsymbol{A}$ , stored in lower- or upper-packed storage mode. CHPEV and ZHPEV compute the eigenvalues and, optionally, the eigenvectors of complex Hermitian matrix  $\boldsymbol{A}$ , stored in lower- or upper-packed storage mode. Eigenvalues are returned in vector  $\boldsymbol{w}$ , and eigenvectors are returned in matrix  $\boldsymbol{Z}$ :

$$Az = wz$$

where  $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$  or  $\mathbf{A} = \mathbf{A}^{\mathsf{H}}$ .

Table 119. Data Types		
A, z	<b>w</b> , aux	Subroutine
Short-precision real	Short-precision real	SSPEV
Long-precision real	Long-precision real	DSPEV
Short-precision complex	Short-precision real	CHPEV
Long-precision complex	Long-precision real	ZHPEV

**Note:** For compatibility with earlier releases of ESSL, you can use the names SSLEV, DSLEV, CHLEV, and ZHLEV for SSPEV, DSPEV, CHPEV, and ZHPEV, respectively.

#### Syntax

Fortran	CALL SSPEV   DSPEV   CHPEV   ZHPEV (iopt, ap, w, z, ldz, n, aux, naux)
C and C++	sspev   dspev   chpev   zhpev (iopt, ap, w, z, ldz, n, aux, naux);
PL/I	CALL SSPEV   DSPEV   CHPEV   ZHPEV (iopt, ap, w, z, ldz, n, aux, naux);

#### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0 or 20, eigenvalues only are computed.

If iopt = 1 or 21, eigenvalues and eigenvectors are computed.

Specified as: a fullword integer; iopt = 0, 1, 20, or 21.

ар

is the real symmetric or complex Hermitian matrix  $\boldsymbol{A}$  of order n, whose eigenvalues and, optionally, eigenvectors are computed. It is stored in an array, referred to as AP, where:

If iopt = 0 or 1, it is stored in lower-packed storage mode.

If iopt = 20 or 21, it is stored in upper-packed storage mode.

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 119. On output, for SSPEV and DSPEV if iopt = 0 or 20, and for CHPEV and ZHPEV, AP is overwritten; that is, the original input is not preserved.

```
W
    See "On Return" on page 708.
    See "On Return."
ldz
   has the following meaning, where:
   If iopt = 0 or 20, it is not used in the computation.
   If iopt = 1 or 21, it is the leading dimension of the output array specified for z.
    Specified as: a fullword integer. It must have the following value, where:
   If iopt = 0 or 20, Idz > 0.
   If iopt = 1 or 21, Idz > 0 and Idz \ge n.
n
   is the order of matrix A. Specified as: a fullword integer; n \ge 0.
aux
   has the following meaning:
   If naux = 0 and error 2015 is unrecoverable, aux is ignored.
    Otherwise, it is a storage work area used by this subroutine. Its size is specified
   by naux.
    Specified as: an area of storage, containing numbers of the data type indicated
   in Table 119 on page 707. On output, the contents are overwritten.
naux
   is the size of the work area specified by aux—that is, the number of elements
   in aux. Specified as: a fullword integer, where:
   If naux = 0 and error 2015 is unrecoverable, SSPEV, DSPEV, CHPEV, and
   ZHPEV dynamically allocate the work area used by the subroutine. The work
   area is deallocated before control is returned to the calling program.
    Otherwise, It must have the following value, where:
   For SSPEV and DSPEV:
        If iopt = 0 or 20, naux \ge n.
        If iopt = 1 or 21, naux \ge 2n.
   For CHPEV and ZHPEV:
        If iopt = 0 or 20, naux \ge 3n.
        If iopt = 1 or 21, naux \ge 4n.
On Return
W
   is the vector \mathbf{w} of length n, containing the eigenvalues of \mathbf{A} in ascending order.
   Returned as: a one-dimensional array of (at least) length n, containing numbers
   of the data type indicated in Table 119 on page 707.
   has the following meaning, where:
   If iopt = 0 or 20, it is not used in the computation.
   If iopt = 1 or 21, it is the matrix Z of order n, containing the orthonormal
    eigenvectors of matrix A. The eigenvector in column i of matrix Z corresponds
   to the eigenvalue w_i.
```

Returned as: an ldz by (at least) n array, containing numbers of the data type indicated in Table 119 on page 707.

#### **Notes**

- 1. When you specify iopt = 0 or 20, you must specify:
  - A positive value for Idz
  - A dummy argument for z (see "Example 1" on page 711)
- The following items must have no common elements: matrix A, matrix Z, vector w, and the data area specified for aux; otherwise, results are unpredictable.
   See "Concepts" on page 55.
- 3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.
- 4. For a description of how real symmetric matrices are stored in lower- or upper-packed storage mode, see "Lower-Packed Storage Mode" on page 66 or "Upper-Packed Storage Mode" on page 67, respectively.
  - For a description of how complex Hermitian matrices are stored in lower- or upper-packed storage mode, see "Complex Hermitian Matrix" on page 70.
- You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The next two sections describe the methods used to compute the eigenvalues and, optionally, the eigenvectors for either a real symmetric matrix or a complex Hermitian matrix. For more information on these methods, see references [39], [43], [60], [81], [91], and [93]. If n is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. See "Example 3" on page 712 and "Example 4" on page 713 for an illustration of the difference in results. Eigenvalues computed using equivalent *iopt* values are mathematically equivalent, but are not guaranteed to be bitwise identical. For example, the results computed using iopt = 0 and iopt = 20 are mathematically equivalent, but are not necessarily bitwise identical.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

*Real Symmetric Matrix:* The eigenvalues and, optionally, the eigenvectors of a real symmetric matrix **A** are computed as follows:

- For *iopt* = 0 or 20, the eigenvalues are computed as follows:
  - 1. Reduce the real symmetric matrix **A** to a real symmetric tridiagonal matrix using orthogonal similarity transformations.
  - 2. Compute the eigenvalues of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  - 3. The eigenvalues are ordered and returned in vector  $\mathbf{w}$ .
- For *iopt* = 1 or 21, the eigenvalues and eigenvectors are computed as follows:
  - 1. Reduce the real symmetric matrix **A** to a real symmetric tridiagonal matrix using and accumulating orthogonal similarity transformations.

- 2. Compute the eigenvalues of the real symmetric tridiagonal matrix and the eigenvectors of the real symmetric matrix using the implicit QL algorithm.
- 3. The eigenvalues are ordered and returned in vector **w**, and the corresponding eigenvectors are returned in matrix **Z**.

Complex Hermitian Matrix: The eigenvalues and, optionally, the eigenvectors of a complex Hermitian matrix **A** are computed as follows:

- For *iopt* = 0 or 20, the eigenvalues are computed as follows:
  - 1. Reduce the complex Hermitian matrix **A** to a real symmetric tridiagonal matrix using unitary similarity transformations.
  - 2. Compute the eigenvalues of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  - 3. The eigenvalues are ordered and returned in vector w.
- For *iopt* = 1 or 21, the eigenvalues and eigenvectors are computed as follows:
  - 1. Reduce the complex Hermitian matrix **A** to a real symmetric tridiagonal matrix using unitary similarity transformations.
  - 2. Compute the eigenvalues and eigenvectors of the real symmetric tridiagonal matrix using the implicit QL algorithm.
  - 3. Back transform the eigenvectors of the real symmetric tridiagonal matrix to those of the original complex Hermitian matrix.
  - 4. The eigenvalues are ordered and returned in vector **w**, and the corresponding eigenvectors are returned in matrix **Z**.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: Eigenvalue (i) failed to converge after (xxx) iterations:

- The eigenvalues  $(w_i, j = 1, 2, ..., i-1)$  are correct, but are unordered.
- If iopt = 1 or 21, then z is modified, but no eigenvectors are correct.
- If iopt = 0 or 20 for SSPEV and DSPEV, ap is modified.
- For CHPEV and ZHPEV, ap is modified.
- The return code is set to 1.
- *i* and *xxx* can be determined at run time by use of the ESSL error-handling-facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.

#### Input-Argument Errors

- 1.  $iopt \neq 0, 1, 20, or 21$
- 2. n < 0
- 3.  $Idz \le 0$  and iopt = 1 or 21
- 4. n > Idz and iopt = 1 or 21
- 5. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to find the eigenvalues only of a real short-precision symmetric matrix A of order 3, stored in lower-packed storage mode Matrix A is:

$$\begin{bmatrix}
1.0 & -1.0 & 0.0 \\
-1.0 & 2.0 & -1.0 \\
0.0 & -1.0 & 1.0
\end{bmatrix}$$

#### where:

- NAUX is equal to N.
- AUX contains N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument z, which is not used in the computation.
- On output, AP has been overwritten.

#### Call Statement and Input

#### Output

$$W = \begin{bmatrix} 0.000000 \\ 1.000000 \\ 3.000000 \end{bmatrix}$$

Example 2: This example shows how to find the eigenvalues and eigenvectors of a real short-precision symmetric matrix A of order 4, stored in upper-packed storage mode. Matrix A is:

# where:

- NAUX is equal to 2N.
- AUX contains 2N elements.

Note: This matrix is used in Example 4.1 in referenced text [60].

### Call Statement and Input

# SSPEV, DSPEV, CHPEV, and ZHPEV

#### Output

Example 3: This example shows how to find the eigenvalues and eigenvectors of a real short-precision symmetric matrix **A**, stored in lower-packed storage mode, which has an eigenvalue of multiplicity 2. Matrix A is:

#### where:

- NAUX is equal to 2N.
- · AUX contains 2N elements.

**Note:** This matrix is used in Example 4.2 in referenced text [60].

## Call Statement and Input

**Example 4:** This example shows how the results of Example 3 differ if matrix **A** is a real long-precision symmetric matrix.

# Call Statement and Input

#### Output

$$W = \begin{bmatrix} -1.000000 \\ 5.000000 \\ 5.000000 \\ 15.000000 \end{bmatrix}$$

Example 5: This example shows how to find the eigenvalues and eigenvectors of a complex Hermitian matrix **A** of order 2, stored in lower-packed storage mode. Matrix A is:

$$\left[ \begin{array}{cccc} (1.0, 0.0) & (0.0, -1.0) \\ (0.0, 1.0) & (1.0, 0.0) \end{array} \right]$$

#### where:

- NAUX is equal to 4N.
- AUX contains 4N elements.
- On output, AP has been overwritten.

Note: This matrix is used in Example 6.1 in referenced text [60].

## Call Statement and Input

$$Z = \begin{bmatrix} (0.000000, -0.707107) & (0.000000, -0.707107) \\ (-0.707107, 0.000000) & (0.707107, 0.000000) \end{bmatrix}$$

**Example 6:** This example shows how to find the eigenvalues only of a complex Hermitian matrix **A** of order 4, stored in upper-packed storage mode. Matrix **A** is:

$$\begin{bmatrix} (3.0, 0.0) & (1.0, 0.0) & (0.0, 0.0) & (0.0, 2.0) \\ (1.0, 0.0) & (3.0, 0.0) & (0.0, -2.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 2.0) & (1.0, 0.0) & (1.0, 0.0) \\ (0.0, -2.0) & (0.0, 0.0) & (1.0, 0.0) & (1.0, 0.0) \\ \end{bmatrix}$$

#### where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument z, which is not used in the computation.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.6 in referenced text [60].

Call Statement and Input

Output

**Example 7:** This example shows how to find the eigenvalues and eigenvectors of a complex Hermitian matrix **A** of order 2, stored in lower-packed storage mode. Matrix A is:

$$\left[ \begin{array}{cccc}
(1.0, 0.0) & (1.0, -1.0) \\
(1.0, 1.0) & (1.0, 0.0)
\end{array} \right]$$

#### where:

- NAUX is equal to 4N.
- AUX contains 4N elements.
- On output, AP has been overwritten.

Note: This matrix is used in Example 6.2 in referenced text [60].

# Call Statement and Input

$$W = \begin{bmatrix} -0.414214 \\ 2.414214 \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.500000, -0.500000) & (0.500000, -0.500000) \\ (-0.707107, & 0.000000) & (0.707107, & 0.000000) \end{bmatrix}$$

# SSPSV, DSPSV, CHPSV, and ZHPSV—Extreme Eigenvalues and, Optionally, the Eigenvectors of a Real Symmetric Matrix or a Complex Hermitian Matrix

SSPSV and DSPSV compute the extreme eigenvalues and, optionally, the eigenvectors of real symmetric matrix  $\boldsymbol{A}$ , stored in lower- or upper-packed storage mode. CHPSV and ZHPSV compute the extreme eigenvalues and, optionally, the eigenvectors of complex Hermitian matrix  $\boldsymbol{A}$ , stored in lower- or upper-packed storage mode. The extreme eigenvalues are returned in vector  $\boldsymbol{w}$ , and the corresponding eigenvectors are returned in matrix  $\boldsymbol{Z}$ :

$$Az = wz$$

where  $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$  or  $\mathbf{A} = \mathbf{A}^{\mathsf{H}}$ .

Table 120. Data Types		
A, z	<b>w</b> , aux	Subroutine
Short-precision real	Short-precision real	SSPSV
Long-precision real	Long-precision real	DSPSV
Short-precision complex	Short-precision real	CHPSV
Long-precision complex	Long-precision real	ZHPSV

**Note:** If you want to compute 10% or fewer eigenvalues only, or you want to compute 30% or fewer eigenvalues and eigenvectors, you get better performance if you use \_SPSV and \_HPSV instead of \_SPEV and \_HPEV, respectively. For all other uses, you should use \_SPEV and \_HPEV.

#### **Syntax**

Fortran	CALL SSPSV   DSPSV   CHPSV   ZHPSV (iopt, ap, w, z, ldz, n, m, aux, naux)	
C and C++	sspsv   dspsv   chpsv   zhpsv (iopt, ap, w, z, ldz, n, m, aux, naux);	
PL/I	CALL SSPSV   DSPSV   CHPSV   ZHPSV (iopt, ap, w, z, ldz, n, m, aux, naux);	

#### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0 or 20, the m smallest eigenvalues only are computed.

If iopt = 1 or 21, the m smallest eigenvalues and the eigenvectors are computed.

If iopt = 10 or 30, the m largest eigenvalues only are computed.

If iopt = 11 or 31, the m largest eigenvalues and the eigenvectors are computed.

Specified as: a fullword integer; iopt = 0, 1, 10, 11, 20, 21, 30, or 31.

ар

is the real symmetric or complex Hermitian matrix  $\mathbf{A}$  of order n, whose m smallest or largest eigenvalues and, optionally, the corresponding eigenvectors are computed. It is stored in an array, referred to as AP, where:

If iopt = 0, 1, 10, or 11, it is stored in lower-packed storage mode.

```
If iopt = 20, 21, 30, or 31, it is stored in upper-packed storage mode.
```

Specified as: a one-dimensional array of (at least) length n(n+1)/2, containing numbers of the data type indicated in Table 120 on page 716. On output, AP is overwritten; that is, the original input is not preserved.

W

See "On Return."

Ζ

See "On Return."

ldz

has the following meaning, where:

If iopt = 0, 10, 20, or 30, it is not used in the computation.

If iopt = 1, 11, 21, or 31, it is the leading dimension of the output array specified for z.

Specified as: a fullword integer. It must have the following value, where:

If iopt = 0, 10, 20, or 30, Idz > 0.

If  $iopt = 1, 11, 21, or 31, Idz > 0 and Idz \ge n$ .

n

is the order of matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

n

is the number of eigenvalues and, optionally, eigenvectors to be computed. Specified as: a fullword integer;  $0 \le m \le n$ .

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 120 on page 716. On output, the contents are overwritten.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SSPSV, DSPSV, CHPSV, and ZHPSV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, It must have the following value, where:

For SSPSV and DSPSV:

```
If iopt = 0, 10, 20, or 30, naux \ge 3n.
If iopt = 1, 11, 21, or 31, naux \ge 9n.
```

For CHPSV and ZHPSV:

```
If iopt = 0, 10, 20, or 30, naux \ge 5n.
If iopt = 1, 11, 21, or 31, naux \ge 11n.
```

On Return

W

is the vector  $\mathbf{w}$  of length n, containing in the first m positions of either the m smallest eigenvalues of  $\mathbf{A}$  in ascending order or the m largest eigenvalues of  $\mathbf{A}$  in descending order.

Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 120 on page 716.

Z

has the following meaning, where:

If iopt = 0, 10, 20, or 30, it is not used in the computation.

If iopt = 1, 11, 21, or 31, it is the n by m matrix Z, containing m orthonormal eigenvectors of matrix A. The eigenvector in column i of matrix Z corresponds to the eigenvalue  $w_i$ .

Returned as: an *Idz* by (at least) *m* array, containing numbers of the data type indicated in Table 120 on page 716.

#### **Notes**

- 1. When you specify iopt = 0, 10, 20, or 30, you must specify:
  - A positive value for *ldz*
  - A dummy argument for z (see "Example 4" on page 722)
- The following items must have no common elements: matrix A, matrix Z, vector w, and the data area specified for aux; otherwise, results are unpredictable.
   See "Concepts" on page 55.
- 3. On input, the imaginary parts of the diagonal elements of the complex Hermitian matrix **A** are assumed to be zero, so you do not have to set these values.
- 4. For a description of how real symmetric matrices are stored in lower- or upper-packed storage mode, see "Lower-Packed Storage Mode" on page 66 or "Upper-Packed Storage Mode" on page 67, respectively.
  - For a description of how complex Hermitian matrices are stored in lower- or upper-packed storage mode, see "Complex Hermitian Matrix" on page 70.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The methods used to compute the extreme eigenvalues and, optionally, the eigenvectors for either a real symmetric matrix or a complex Hermitian matrix are described in the steps below. For more information on these methods, see references [39], [43], [60], [81], [91], and [93]. If n or m is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy. Eigenvalues computed using equivalent *iopt* values are mathematically equivalent, but are not guaranteed to be bitwise identical. For example, the results computed using iopt = 0 and iopt = 20 are mathematically equivalent, but are not necessarily bitwise identical.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

The extreme eigenvalues and, optionally, the eigenvectors of a real symmetric matrix  $\mathbf{A}$  or complex Hermitian matrix  $\mathbf{A}$  are computed as follows:

- For iopt = 0, 10, 20, or 30, the eigenvalues are computed as follows:
  - Reduce the real symmetric matrix A (for SSPSV and DSPSV) or complex Hermitian matrix A (for CHPSV and ZHPSV) to a real symmetric tridiagonal matrix using orthogonal similarity transformations (for SSPSV and DSPSV) or unitary similarity transforms (for CHPSV and ZHPSV).
  - 2. Compute the *m* smallest eigenvalues or *m* largest eigenvalues of the real symmetric tridiagonal matrix using a rational variant of the QR method with Newton corrections.
  - 3. The eigenvalues are returned in vector **w** in the first *m* positions, where the *m* smallest are placed in ascending order, or the *m* largest are placed in descending order.
- For *iopt* = 1, 11, 21, or 31, the eigenvalues and eigenvectors are computed as follows:
  - Reduce the real symmetric matrix A (for SSPSV and DSPSV) or complex Hermitian matrix A (for CHPSV and ZHPSV) to a real symmetric tridiagonal matrix using orthogonal similarity transformations (for SSPSV and DSPSV) or unitary similarity transforms (for CHPSV and ZHPSV).
  - 2. Compute the *m* smallest eigenvalues or *m* largest eigenvalues of the real symmetric tridiagonal matrix using a rational variant of the QR method with Newton corrections.
  - 3. Compute the corresponding eigenvectors of the real symmetric tridiagonal matrix using inverse iteration.
  - 4. Back transform the eigenvectors of the real symmetric tridiagonal matrix to those of the original matrix.
  - 5. The eigenvalues are returned in vector **w** in the first **m** positions, where the **m** smallest are placed in ascending order, or the **m** largest are placed in descending order. The corresponding eigenvectors are returned in matrix **Z**.

# **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

#### Computational Errors

- 1. Eigenvalue (i) failed to converge after (xxx) iterations. (The computational error message may occur multiple times with processing continuing after each error, because the number of allowable errors for error code 2114 is set to be unlimited in the ESSL error option table.)
  - The eigenvalue,  $w_i$ , is the best estimate obtained. Any eigenvalues for which this message has not been issued are correct.
  - ap is modified.
  - The return code is set to 1.
  - *i* and *xxx* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error 2199 in the ESSL error option table. See "What Can You Do about ESSL Computational Errors?" on page 48.
- 2. Eigenvector (i) failed to converge after (xxx) iterations. (The computational error message may occur multiple times with processing continuing after each error, because the number of allowable errors for error code 2102 is set to be unlimited in the ESSL error option table.)

- · All eigenvalues are correct.
- The eigenvector that failed to converge is set to zero; however, any selected eigenvectors for which this message is not issued are correct.
- ap is modified.
- The return code is set to 2.
- i and xxx can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error 2199 in the ESSL error option table.
   See "What Can You Do about ESSL Computational Errors?" on page 48.

# Input-Argument Errors

- 1.  $iopt \neq 0, 1, 10, 11, 20, 21, 30, or 31$
- 2. n < 0
- 3. m < 0
- 4. m > n
- 5.  $Idz \le 0$  and iopt = 1, 11, 21, or 31
- 6. n > Idz and iopt = 1, 11, 21, or 31
- 7. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to find the two smallest eigenvalues and corresponding eigenvectors of a real long-precision symmetric matrix **A** of order 4, stored in upper-packed storage mode. Matrix **A** is:

# where:

- NAUX is equal to 9N.
- AUX contains 9N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 4.1 in referenced text [60].

# Call Statement and Input

# Output

$$Z = \begin{bmatrix} -0.707107 & 0.000000 \\ 0.707107 & 0.000000 \\ 0.000000 & -0.707107 \\ 0.000000 & 0.707107 \end{bmatrix}$$

Example 2: This example shows how to find the three largest eigenvalues and corresponding eigenvectors of a real long-precision symmetric matrix **A** of order 4, stored in lower-packed storage mode, having an eigenvalue of multiplicity two. Matrix A is:

# where:

- NAUX is equal to 9N.
- AUX contains 9N elements.
- · On output, AP has been overwritten.

Note: This matrix is used in Example 4.2 in referenced text [60].

Call Statement and Input

Output

**Example 3:** This example shows how to find the largest eigenvalue and the corresponding eigenvector of a complex Hermitian matrix A of order 2, stored in lower-packed storage mode. Matrix A is:

#### where:

- NAUX is equal to 11N.
- AUX contains 11N elements.
- On output, AP has been overwritten.

**Note:** This matrix is used in Example 6.1 in referenced text [60].

Call Statement and Input

## Output

$$W = \begin{bmatrix} 2.000000 \\ \cdot \end{bmatrix}$$

$$Z = \begin{bmatrix} (0.000000, -0.707107) \\ (0.707107, 0.000000) \end{bmatrix}$$

Example 4: This example shows how to find the two smallest eigenvalues only of a complex Hermitian matrix **A** of order 4, stored in upper-packed storage mode. Matrix A is:

$$\begin{bmatrix} (3.0, 0.0) & (1.0, 0.0) & (0.0, 0.0) & (0.0, 2.0) \\ (1.0, 0.0) & (3.0, 0.0) & (0.0, -2.0) & (0.0, 0.0) \\ (0.0, 0.0) & (0.0, 2.0) & (1.0, 0.0) & (1.0, 0.0) \\ (0.0, -2.0) & (0.0, 0.0) & (1.0, 0.0) & (1.0, 0.0) \end{bmatrix}$$

# where:

- NAUX is equal to 5N.
- AUX contains 5N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument z, which is not used in the computation.
- On output, AP has been overwritten.

Note: This matrix is used in Example 6.6 in referenced text [60].

Call Statement and Input

# Output

$$W = \begin{bmatrix} -0.828427 \\ 0.000000 \\ \vdots \\ \vdots \end{bmatrix}$$

# SGEGV and DGEGV—Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Eigensystem, Az=wBz, where A and B Are Real General Matrices

These subroutines compute the eigenvalues and, optionally, the eigenvectors of a generalized real eigensystem, where  $\boldsymbol{A}$  and  $\boldsymbol{B}$  are real general matrices.

Eigenvalues **w** are based on the two parts returned in vectors  $\alpha$  and  $\beta$ , such that  $w_i = \alpha/\beta_i$  for  $\beta_i \neq 0$ , and  $w_i = \infty$  for  $\beta_i = 0$ . Eigenvectors are returned in matrix **Z**:

$$Az = wBz$$

Table 121. Data Types		
<b>A</b> , <b>B</b> , β, aux	α, <b>Ζ</b>	Subroutine
Short-precision real	Short-precision complex	SGEGV
Long-precision real	Long-precision complex	DGEGV

# Syntax

Fortran	CALL SGEGV   DGEGV (iopt, a, Ida, b, Idb, alpha, beta, z, Idz, n, aux, naux)	
C and C++	sgegv   dgegv (iopt, a, Ida, b, Idb, alpha, beta, z, Idz, n, aux, naux);	
PL/I	CALL SGEGV   DGEGV (iopt, a, Ida, b, Idb, alpha, beta, z, Idz, n, aux, naux);	

### On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0, eigenvalues only are computed.

If iopt = 1, eigenvalues and eigenvectors are computed.

Specified as: a fullword integer; iopt = 0 or 1.

а

is the real general matrix  $\mathbf{A}$  of order n. Specified as: an Ida by (at least) n array, containing numbers of the data type indicated in Table 121. On output, A is overwritten; that is, the original input is not preserved.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

h

is the real general matrix  $\boldsymbol{B}$  of order n. Specified as: an ldb by (at least) n array, containing numbers of the data type indicated in Table 121. On output, B is overwritten; that is, the original input is not preserved.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

alpha

See "On Return" on page 725.

beta

See "On Return" on page 725.

Z

See "On Return" on page 725.

ldz

has the following meaning, where:

If iopt = 0, it is not used in the computation.

If iopt = 1, it is the leading dimension of the output array specified for z.

Specified as: a fullword integer. It must have the following value, where:

If iopt = 0, Idz > 0.

If iopt = 1, Idz > 0 and  $Idz \ge n$ .

n

is the order of matrices **A** and **B**. Specified as: a fullword integer;  $n \ge 0$ .

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 121 on page 724. On output, the contents are overwritten.

#### naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SGEGV and DGEGV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge 3n$ .

## On Return

#### alpha

is the vector  $\alpha$  of length n, containing the numerators of the eigenvalues of the generalized real eigensystem Az = wBz. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 121 on page 724.

#### beta

is the vector  $\beta$  of length n, containing the denominators of the eigenvalues of the generalized real eigensystem Az = wBz. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 121 on page 724.

Ζ

has the following meaning, where:

If iopt = 0, it is not used in the computation.

If iopt = 1, it is the matrix Z of order n, containing the eigenvectors of the generalized real eigensystem, Az = wBz. The eigenvector in column i of matrix Z corresponds to the eigenvalue  $w_i$ , computed using the  $\alpha_i$  and  $\beta_i$  values. Each eigenvector is normalized so that the modulus of its largest element is 1.

Returned as: an *ldz* by (at least) *n* array, containing numbers of the data type indicated in Table 121 on page 724.

#### Notes

- 1. When you specify iopt = 0, you must specify:
  - A positive value for Idz
  - A dummy argument for z (see "Example 1" on page 727)
- 2. Matrices A, B, and Z, vectors  $\alpha$  and  $\beta$ , and the work area specified for *aux* must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The following steps describe the methods used to compute the eigenvalues and, optionally, the eigenvectors of a generalized real eigensystem, Az = wBz, where A and B are real general matrices. The methods are based upon Moler and Stewart's QZ algorithm. You must calculate the resulting eigenvalues w based on the two parts returned in vectors  $\alpha$  and  $\beta$ . Each eigenvalue is calculated as follows:  $w_i = \alpha/\beta_i$  for  $\beta_i \neq 0$  and  $w_i = \infty$  for  $\beta_i = 0$ . Eigenvalues are unordered, except that complex conjugate pairs appear consecutively with the eigenvalue having the positive imaginary part first.

- For *iopt* = 0, the eigenvalues are computed as follows:
  - Simultaneously reduce A to upper Hessenberg form and B to upper triangular form using orthogonal transformations.
  - 2. Reduce **A** from upper Hessenberg form to quasi-upper triangular form while maintaining the upper triangular form of **B** using orthogonal transformations.
  - 3. Compute the eigenvalues of the generalized real eigensystem with **A** in quasi-upper triangular form and **B** in upper triangular form using orthogonal transformations.
  - 4. The numerators and denominators of the eigenvalues are returned in vectors  $\alpha$  and  $\beta$ , respectively.
- For *iopt* = 1, the eigenvalues and eigenvectors are computed as follows:
  - 1. Simultaneously reduce **A** to upper Hessenberg form and **B** to upper triangular form using and accumulating orthogonal transformations.
  - Reduce A from upper Hessenberg form to quasi-upper triangular form while maintaining the upper triangular form of B using and accumulating orthogonal transformations.
  - 3. Compute the eigenvalues of the generalized real eigensystem with **A** in quasi-upper triangular form and **B** in upper triangular form using and accumulating orthogonal transformations.
  - 4. Compute the eigenvectors of the generalized real eigensystem with **A** in quasi-upper triangular form and **B** in upper triangular form using back substitution.
  - 5. The numerators and denominators of the eigenvalues are returned in vectors  $\alpha$  and  $\beta$ , respectively, and the eigenvectors are returned in matrix  $\boldsymbol{Z}$ .

For more information on these methods, see references [39], [43], [55], [77], [60], [59], [81], [91], and [93]. If n is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: Eigenvalue (i) failed to converge after (xxx) iterations:

- The eigenvalues  $(w_i, j = i+1, i+2, ..., n)$  are correct.
- If *iopt* = 1, then **Z** is modified, but no eigenvectors are correct.
- A and B have been modified.
- The return code is set to 1.
- i and xxx can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.

# Input-Argument Errors

- 1.  $iopt \neq 0$  or 1
- 2. n < 0
- $3. Ida \leq 0$
- 4. n > Ida
- 5. Idb < 0
- 6. n > ldb
- 7.  $Idz \le 0$  and iopt = 1
- 8. n > Idz and iopt = 1
- 9. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 2 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to find the eigenvalues only of a real generalized eigensystem problem, AZ = wBZ, where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument z, which is not used in the computation.
- On output, matrices A and B are overwritten.

Note: These matrices are from page 257 in referenced text [59].

# Call Statement and Input



$$A = \begin{bmatrix} 10.0 & 1.0 & 2.0 \\ 1.0 & 3.0 & -1.0 \\ 1.0 & 1.0 & 2.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 4.0 & 5.0 & 6.0 \\ 7.0 & 8.0 & 9.0 \end{bmatrix}$$

Output

ALPHA = 
$$\begin{bmatrix} (4.778424, 0.000000) \\ (-4.760580, 0.000000) \\ (2.769466, 0.000000) \end{bmatrix}$$

BETA = 
$$\begin{bmatrix} 0.000000 \\ 0.934851 \\ 15.446215 \end{bmatrix}$$

**Example 2:** This example shows how to find the eigenvalues and eigenvectors of a real generalized eigensystem problem, AZ = wBZ, where:

- NAUX is equal to 3N.
- AUX contains 3N elements.
- On output, matrices A and B are overwritten.

**Note:** These matrices are from page 263 in referenced text [59].

Call Statement and Input

$$A = \begin{bmatrix} 2.0 & 3.0 & 4.0 & 5.0 & 6.0 \\ 4.0 & 4.0 & 5.0 & 6.0 & 7.0 \\ 0.0 & 3.0 & 6.0 & 7.0 & 8.0 \\ 0.0 & 0.0 & 2.0 & 8.0 & 9.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 10.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 1.0 & -1.0 & -1.0 & -1.0 & -1.0 \\ 0.0 & 1.0 & -1.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 1.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

Output

```
(7.950050, 0.000000)
           (-0.277338, 0.000000)
            (2.149669, 0.000000)
            (6.720718, 0.000000)
           (10.987556, 0.000000)
           0.374183
           1.480299
BETA =
           1.636872
           1.213574
           0.908837
          (1.000000, 0.000000)
                                 (-0.483408, 0.000000)
                                                         (0.540696, 0.000000)
          (0.565497, 0.000000)
                                (1.000000, 0.000000)
                                                         (0.684441, 0.000000)
Ζ
         (0.180429, 0.000000)
                                 (-0.661372, 0.000000)
                                                        (-1.000000, 0.000000)
         (0.034182, 0.000000)
                                 (0.180646, 0.000000)
                                                         (0.363671, 0.000000)
                                 (-0.017732, 0.000000)
          (0.003039, 0.000000)
                                                        (-0.041865, 0.000000)
                                                (-1.000000, 0.000000)
                           (1.000000, 0.000000)
                           (0.722065, 0.000000)
                                                (-0.610415, 0.000000)
                                                 (-0.116987, 0.000000)
                          (-0.089003, 0.000000)
                          (-0.223599, 0.000000)
                                                  (0.038979, 0.000000)
```

(0.050111, 0.000000)

(0.018653, 0.000000)

# SSYGV and DSYGV—Eigenvalues and, Optionally, the Eigenvectors of a Generalized Real Symmetric Eigensystem, Az=wBz, where A Is Real Symmetric and B Is Real Symmetric Positive Definite

These subroutines compute the eigenvalues and, optionally, the eigenvectors of a generalized real symmetric eigensystem, where **A** is a real symmetric matrix, and **B** is a real positive definite symmetric matrix. Both **A** and **B** are stored in lower storage mode in two-dimensional arrays. Eigenvalues are returned in vector **w**, and eigenvectors are returned in matrix **Z**:

$$Az = wBz$$

where  $\mathbf{A} = \mathbf{A}^{\mathsf{T}}$ ,  $\mathbf{B} = \mathbf{B}^{\mathsf{T}}$ , and  $\mathbf{x}^{\mathsf{T}}\mathbf{B}\mathbf{x} > 0$ .

Table 122. Data Types	
<b>A</b> , <b>B</b> , <b>w</b> , <b>Z</b> , aux	Subroutine
Short-precision real	SSYGV
Long-precision real	DSYGV

# **Syntax**

Fortran CALL SSYGV   DSYGV (iopt, a, Ida, b, Idb, w, z, Idz, n, aux, naux)		
C and C++	ssygv   dsygv (iopt, a, Ida, b, Idb, w, z, Idz, n, aux, naux);	
PL/I	CALL SSYGV   DSYGV (iopt, a, Ida, b, Idb, w, z, Idz, n, aux, naux);	

# On Entry

iopt

indicates the type of computation to be performed, where:

If iopt = 0, eigenvalues only are computed.

If iopt = 1, eigenvalues and eigenvectors are computed.

Specified as: a fullword integer; iopt = 0 or 1.

а

is the real symmetric matrix  $\boldsymbol{A}$  of order n. It is stored in lower storage mode. Specified as: an lda by (at least) n array, containing numbers of the data type indicated in Table 122. On output, the data in the lower triangle of  $\boldsymbol{A}$  is overwritten; that is, the original input is not preserved.

lda

is the leading dimension of the array specified for a. Specified as: a fullword integer; Ida > 0 and  $Ida \ge n$ .

b

is the real positive definite symmetric matrix  $\mathbf{B}$  of order n. It is stored in lower storage mode. Specified as: an ldb by (at least) n array, containing numbers of the data type indicated in Table 122. On output, the data in the lower triangle of  $\mathbf{B}$  is overwritten; that is, the original input is not preserved.

ldb

is the leading dimension of the array specified for b. Specified as: a fullword integer; ldb > 0 and  $ldb \ge n$ .

```
See "On Return" on page 731.

Z
See "On Return."

Idz
has the following meaning, where:
If iopt = 0, it is not used in the computation.

If iopt = 1, it is the leading dimension of the output array specified for z. Specified as: a fullword integer. It must have the following value, where:

If iopt = 0, Idz > 0.

If iopt = 1, Idz > 0 and Idz \ge n.

n
is the order of matrices A and B. Specified as: a fullword integer; n \ge 0.

aux
```

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 122 on page 730. On output, the contents are overwritten.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SSYGV and DSYGV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, It must have the following value, where:

```
If iopt = 0, naux \ge n.
If iopt = 1, naux \ge 2n.
```

# On Return

W

is the vector  $\mathbf{w}$  of length n, containing the eigenvalues of the generalized real symmetric eigensystem  $\mathbf{A}\mathbf{z} = w\mathbf{B}\mathbf{z}$  in ascending order. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 122 on page 730.

Z

has the following meaning, where:

If iopt = 0, it is not used in the computation.

If iopt = 1, it is the matrix Z of order n, containing the eigenvectors of the generalized real symmetric eigensystem, Az = wBz. The eigenvectors are normalized so that  $Z^TBZ = I$ . The eigenvector in column i of matrix Z corresponds to the eigenvalue  $w_i$ .

Returned as: an Idz by (at least) n array, containing numbers of the data type indicated in Table 122 on page 730.

#### Notes

- 1. When you specify iopt = 0, you must specify:
  - A positive value for Idz
  - A dummy argument for z (see "Example 1" on page 733)
- 2. Matrices **A** and **Z** may coincide. Matrices **A** and **B**, vector **w**, and the data area specified for aux must have no common elements; otherwise, results are unpredictable. Matrices Z and B, vector w, and the data area specified for auxmust also have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. For a description of how real symmetric matrices are stored in lower storage mode, see "Lower Storage Mode" on page 68.
- 4. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The following steps describe the methods used to compute the eigenvalues and, optionally, the eigenvectors of a generalized real symmetric eigensystem, Az = wBz, where A is a real symmetric matrix, and B is a real positive definite symmetric matrix. Both A and B are stored in lower storage mode in two-dimensional arrays.

1. Compute the Cholesky Decomposition of **B**:

$$B = LL^{T}$$

For a description of methods used in this computation, see "SPPF, DPPF, SPOF, DPOF, CPOF, and ZPOF—Positive Definite Real Symmetric or Complex Hermitian Matrix Factorization" on page 492.

2. Compute C:

$$C = L^{-1}AL^{-T}$$

In this computation, **C** overwrites **A**.

3. Solve the real symmetric eigensystems analysis problem, computing the eigenvalues w and, optionally, the eigenvectors Y:

$$CY = wY$$

where:

$$Y = L^{T}Z$$

For a description of the methods used for this computation, see "Real Symmetric Matrix" on page 709. In this computation, Y overwrites Z.

4. If eigenvectors are requested (with iopt = 1), transform the eigenvectors Y into the eigenvectors **Z** of the original system, Az = wBz, by solving  $L^{T}Z = Y$  for **Z**:

$$Z = L^{-T}Y$$

For more information on these methods, see references [39], [43], [55], [60], [59], [81], [91], and [93]. If n is 0, no computation is performed. The results of the computations using short- and long-precision data can vary in accuracy.

These algorithms have a tendency to generate underflows that may hurt overall performance. The system default is to mask underflow, which improves the performance of these subroutines.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

# Computational Errors

- 1. The **B** matrix is not positive definite. The leading minor of order *i* has a nonpositive determinant.
  - **B** is modified, but no eigenvalues or eigenvectors are correct.
  - The return code is set to 1.
  - *i* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2115 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.
- 2. Eigenvalue (i) failed to converge after (xxx) iterations:
  - The eigenvalues  $(w_i, j = 1, 2, ..., i-1)$  are correct, but are unordered.
  - If iopt = 1, then z is modified, but no eigenvectors are correct.
  - A and B have been modified.
  - The return code is set to 2.
  - *i* and *xxx* can be determined at run time by use of the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2101 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. See "What Can You Do about ESSL Computational Errors?" on page 48.

# Input-Argument Errors

- 1.  $iopt \neq 0$  or 1
- 2. n < 0
- $3. Ida \leq 0$
- 4. n > Ida
- 5.  $ldb \leq 0$
- 6. n > ldb
- 7.  $Idz \le 0$  and iopt = 1
- 8. n > Idz and iopt = 1
- 9. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 3 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to find the eigenvalues only of a real symmetric generalized eigensystem problem, AZ = wBZ, where:

- NAUX is equal to N.
- AUX contains N elements.
- LDZ is set to 1 to avoid an error condition.
- DUMMY is used as a placeholder for argument z, which is not used in the computation.
- On output, the lower triangle of A and B is overwritten.

Note: These matrices are used in Example 8.6.2 in referenced text [59].

# Call Statement and Input

$$A = \begin{bmatrix} 229.0 & . \\ 163.0 & 116.0 \end{bmatrix}$$

$$B = \begin{bmatrix} 81.0 & . \\ 59.0 & 43.0 \end{bmatrix}$$

# Output

$$W = \begin{bmatrix} -0.500000 \\ 5.000000 \end{bmatrix}$$

**Example 2:** This example shows how to find the eigenvalues and eigenvectors of a real symmetric generalized eigensystem problem, AZ = wBZ, where:

- NAUX is equal to 2N.
- AUX contains 2N elements.
- On output, the lower triangle of A and B is overwritten.

**Note:** These matrices are from page 67 in referenced text [55].

# Call Statement and Input

$$A = \begin{vmatrix} -1.0 & . & . \\ 1.0 & 1.0 & . \\ -1.0 & -1.0 & 1.0 \end{vmatrix}$$

$$B = \begin{bmatrix} 2.0 & . & . \\ 1.0 & 2.0 & . \\ 0.0 & 1.0 & 2.0 \end{bmatrix}$$

# Output

$$W = \begin{bmatrix} -1.500000 \\ 0.000000 \\ 2.000000 \end{bmatrix}$$

$$Z = \begin{bmatrix} 0.866025 & 0.000000 & 0.000000 \\ -0.577350 & -0.408248 & -0.707107 \\ 0.288675 & -0.408248 & 0.707107 \end{bmatrix}$$

# SSYGV and DSYGV

# **Chapter 12. Fourier Transforms, Convolutions and Correlations, and Related Computations**

The signal processing subroutines, provided in three areas, are described in this chapter.

# **Overview of the Signal Processing Subroutines**

This section describes the subroutines in each of the three signal processing areas:

- Fourier transform subroutines (Table 123)
- Convolution and correlation subroutines (Table 124)
- Related-computation subroutines (Table 125)

# **Fourier Transforms Subroutines**

The Fourier transform subroutines perform mixed-radix transforms in one, two, and three dimensions.

Table 123. List of Fourier Transform Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Complex Fourier Transform	SCFT SCFTP§	DCFT	747
Real-to-Complex Fourier Transform	SRCFT	DRCFT	755
Complex-to-Real Fourier Transform	SCRFT	DCRFT	763
Cosine Transform	SCOSF SCOSFT§	DCOSF	771
Sine Transform	SSINF	DSINF	778
Complex Fourier Transform in Two Dimensions	SCFT2 SCFT2P§	DCFT2	785
Real-to-Complex Fourier Transform in Two Dimensions	SRCFT2	DRCFT2	792
Complex-to-Real Fourier Transform in Two Dimensions	SCRFT2	DCRFT2	799
Complex Fourier Transform in Three Dimensions	SCFT3 SCFT3P§	DCFT3	807
Real-to-Complex Fourier Transform in Three Dimensions	SRCFT3	DRCFT3	813
Complex-to-Real Fourier Transform in Three Dimensions	SCRFT3	DCRFT3	819
	•	<u> </u>	

<sup>§</sup> This subroutine is provided only for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutine is no longer provided.

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# **Convolution and Correlation Subroutines**

The convolution and correlation subroutines provide the choice of using Fourier methods or direct methods. The Fourier-method subroutines contain a high-performance mixed-radix capability. There are also several direct-method subroutines that provide decimated output.

Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Convolution or Correlation of One Sequence with One or More Sequences	SCON§ SCOR§		826
Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method	SCOND SCORD		832
Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method	SCONF SCORF		838
Convolution or Correlation with Decimated Output Using a Direct Method	SDCON SDCOR	DDCON DDCOR	847
Autocorrelation of One or More Sequences	SACOR§		851
Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method	SACORF		855

<sup>§</sup> These subroutines are provided only for migration from earlier releases of ESSL and are not intended for use in new programs.

# **Related-Computation Subroutines**

The related-computation subroutines consist of a group of computations that can be used in general signal processing applications. They are similar to those provided on the IBM 3838 Array Processor; however, the ESSL subroutines generally solve a wider range of problems.

able 125. List of Related-Computation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Evaluation	SPOLY	DPOLY	861
I-th Zero Crossing	SIZC	DIZC	864
Time-Varying Recursive Filter	STREC	DTREC	867
Quadratic Interpolation	SQINT	DQINT	870
Wiener-Levinson Filter Coefficients	SWLEV	DWLEV	874

# Fourier Transforms, Convolutions, and Correlations Considerations

This section describes some global information applying to the Fourier transform, convolution, and correlation subroutines.

# **Use Considerations**

This section provides some key points about using the Fourier transform, convolution, and correlation subroutines.

# Understanding the Terminology and Conventions Used for Your Array Data

These subroutines use the term "sequences," rather than vectors and matrices, to describe the data that is stored in the arrays. The conventions used for representing sequences are defined in "Sequences" on page xxvi.

Some of the sequences used in these computations use a zero origin rather than a one-origin. For example,  $x_j$  can be expressed with j = 0, 1, ..., n-1 rather than j = 1, 2, ..., n. When using the formulas provided in this book to calculate array sizes or offsets into arrays, you need to be careful that you substitute the correct values. For example, the number of  $x_j$  elements in the sequence is n, not n-1.

# **Concerns about Lengths of Transforms**

The length of the transform you can use in your program depends on the limits of the addressability of your processor.

# **Determining an Acceptable Length of a Transform**

To determine acceptable lengths of the transforms in the Fourier transform subroutines, you have several choices. First, you can use the formula or table of values in "Acceptable Lengths for the Transforms" to choose a value. Second, ESSL's input-argument error recovery provides a means of determining an acceptable length of the transform. It uses the optionally-recoverable error 2030. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

# Acceptable Lengths for the Transforms

Use the following formula to determine acceptable transform lengths:

$$n = (2^h)(3^i)(5^j)(7^k)(11^m)$$
 for  $n \le 37748736$ 

where:

$$h = 1, 2, ..., 25$$
  
 $i = 0, 1, 2$   
 $j, k, m = 0, 1$ 

Figure 13 on page 740 lists all the acceptable values for transform lengths in the Fourier transform subroutines.

2	4	6	8	10	12	14	16	18
20	22	24	28	30	32	36	40	42
44	48	56	60	64	66	70	72	80
84	88	90	96	110	112	120	126	128
132	140	144	154	160	168	176	180	192
198	210	220	224	240	252	256	264	280
288	308	320	330	336	352	360	384	396
420	440	448	462	480	504	512	528	560
576	616	630	640	660	672	704	720	768
770	792	840	880	896	924	960	990	1008
1024	1056	1120	1152	1232	1260	1280	1320	1344
1386	1408	1440	1536	1540	1584	1680	1760	1792
1848	1920	1980	2016	2048	2112	2240	2304	2310
2464	2520	2560	2640	2688	2772	2816	2880	3072
3080	3168	3360	3520	3584	3696	3840	3960	4032
4096	4224	4480	4608	4620	4928	5040	5120	5280
5376	5544	5632	5760	6144	6160	6336	6720	6930
7040	7168	7392	7680	7920	8064	8192	8448	8960
9216	9240	9856	10080	10240	10560	10752	11088	11264
11520	12288	12320	12672	13440	13860	14080	14336	14784
15360	15840	16128	16384	16896	17920	18432	18480	19712
20160	20480	21120	21504	22176	22528	23040	24576	24640
25344	26880	27720	28160	28672	29568	30720	31680	32256
32768	33792	35840	36864	36960	39424	40320	40960	42240
43008	44352	45056	46080	49152	49280	50688	53760	55440
56320	57344	59136	61440	63360	64512	65536	67584	71680
73728	73920	78848	80640	81920	84480	86016	88704	90112
92160	98304	98560	101376	107520	110880	112640	114688	118272
122880	126720	129024	131072	135168	143360	147456	147840	157696
161280	163840	168960	172032	177408	180224	184320	196608	197120
202752	215040	221760	225280	229376	236544	245760	253440	258048
262144	270336	286720	294912	295680	315392	322560	327680	337920
344064	354816	360448	368640	393216	394240	405504	430080	443520
450560	458752	473088	491520	506880	516096	524288	540672	573440
589824	591360	630784	645120	655360	675840	688128	709632	720896
737280	786432	788480	811008	860160	887040	901120	917504	946176
983040	1013760	1032192	1048576	1081344	1146880	1179648	1182720	1261568
1290240	1310720	1351680	1376256	1419264	1441792	1474560	1572864	1576960
1622016	1720320	1774080	1802240	1835008	1892352	1966080	2027520	2064384
2097152	2162688	2293760	2359296	2365440	2523136	2580480	2621440	2703360
2752512	2838528	2883584	2949120	3145728	3153920	3244032	3440640	3548160
3604480	3670016	3784704	3932160	4055040	4128768	4194304	4325376	4587520
4718592	4730880	5046272	5160960	5242880	5406720	5505024	5677056	5767168
5898240	6291456	6307840	6488064	6881280	7096320	7208960	7340032	7569408
7864320	8110080	8257536	8388608	8650752	9175040	9437184	9461760	10092544
10321920	10485760	10813440	11010048	11354112	11534336	11796480	12582912	12615680
12976128	13762560	14192640	14417920	14680064	15138816	15728640	16220160	16515072
16777216	17301504	18350080	18874368	18923520	20185088	20643840	20971520	21626880
22020096	22708224	23068672	23592960	25165824	25231360	25952256	27525120	28385280
28835840	29360128	30277632	31457280	32440320	33030144	33554432	34603008	36700160
37748736								

Figure 13. Table of Acceptable Lengths for the Transforms

# **Understanding Auxiliary Working Storage Requirements**

Auxiliary working storage is required by the Fourier transform subroutines and by the SCONF, SCORF, and SACORF subroutines. This storage is provided through the calling sequence arguments *aux*, *aux1*, and *aux2*. The sizes of these storage areas are specified by the calling sequence arguments *naux*, *naux1*, and *naux2*, respectively.

**AUX1:** The *aux1* array is used for storing tables and other parameters when you call a Fourier transform, convolution, or correlation subroutine for initialization with init = 1. The initialized *aux1* array is then used on succeeding calls with init = 0, when the computation is actually done. You should not use this array between the initialization and the computation.

**AUX and AUX2:** The *aux* and *aux2* arrays are used for temporary storage during the running of the subroutine and are available for use by your program between calls to the subroutine.

**AUX3:** The aux3 argument is provided for migration purposes only and is ignored.

# **Initializing Auxiliary Working Storage**

In many of those subroutines requiring aux1 auxiliary working storage, two invocations of the subroutines are necessary. The first invocation initializes the working storage in aux1 for the subroutine, and the second performs the computations. (For an explanation of auxiliary working storage, see Understanding Auxiliary Working Storage Requirements.) As a result, the working storage in aux1 should not be used by the calling program between the two calls to the subroutine. However, it can be reused after intervening calls to the subroutine with different arguments.

If you plan to repeat a computation many times using the same set of arguments, you only need to do one initialization of the *aux1* array; that is, the initialized *aux1* array can be saved and reused as many times as needed for the computation.

If you plan to perform different computations, with different sets of arguments (except for input argument x), you need to do an initialization for each different computation; that is, you initialize the various aux1 arrays for use with the different computations, saving and reusing them until they are not needed any more.

# **Determining the Amount of Auxiliary Working Storage That You Need**

To determine the size of auxiliary storage, you have several choices. First, you can use the formulas provided in each subroutine description. Second, ESSL's input-argument error recovery provides a means of determining the minimum size you need for auxiliary storage. It uses the optionally-recoverable error 2015. For details, see "Using Auxiliary Storage in ESSL" on page 31. Third, you can have ESSL dynamically allocate *aux* and *aux2*. For details, see "Dynamic Allocation of Auxiliary Storage" on page 32.

# **Performance and Accuracy Considerations**

The following sections explain the performance and accuracy considerations for the Fourier transforms, convolution, and correlation subroutines. For further details about performance and accuracy, see Chapter 2 on page 25.

# When Running on the Workstation Processors

There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Defining Arrays**

The stride arguments, inc1h, inc1x, inc1y, inc2x, inc2y, inc3x, and inc3y, provide great flexibility in defining the input and output data arrays. The arrangement of data in storage, however, can have an effect upon cache performance. By using strides, you can have data scattered in storage. Best performance is obtained with data closely spaced in storage and with elements of the sequence in contiguous locations. The optimum values for inc1h, inc1x, and inc1y are 1.

In writing the calling program, you may find it convenient to declare X or Y as a two-dimensional array. For example, you can declare X in a DIMENSION statement as X(INC2X,M).

# **Fourier Transform Considerations**

This section describes some ways to optimize performance in the Fourier transform subroutines.

# Setting Up Your Data

Many of the Fourier transform, convolution, and correlation subroutines provide the facility for processing many sequences in one call. For short sequences, for example 1024 elements or less, this facility should be used as much as possible. This provides improved performance compared to processing only one sequence at a time.

If possible, you should use the same array for input and output. In addition, the requirements for the strides of the input and output arrays are explained in the Notes for each subroutine.

For improved performance, small values of inc1x and inc1y should be used, where applicable, preferably inc1x = 1 and inc1y = 1. A stride of 1 means the sequence elements are stored contiguously. Also, if possible, the sequences should be stored close to each other. For all the Fourier transform subroutines except RCFT and CRFT, you should use the STRIDE subroutine to determine the optimal stride(s) for your input or output data. Complete instructions on how to use STRIDE for each of these subroutines is included in "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969.

To obtain the best performance in the three-dimensional Fourier transform subroutines, you should use strides, inc2 and inc3, provided by the STRIDE subroutine and declare your three-dimensional data structure as a one-dimensional array. The three-dimensional Fourier transform subroutines assume that inc1 for the array is 1. Therefore, each element  $x_{ijk}$  for i=0,1,...,n1-1,j=0,1,...,n2-1, and k=0,1,...,n3-1 of the three-dimensional data structure of dimensions n1 by n2 by n3 is stored in a one-dimensional array X(0:L) at location X(I), where I=i+inc2(j)+inc3(k). The minimum required value of L is calculated by inserting the maximum values for i,j, and k in the above equation, giving L=(n1-1)+inc2(n2-1)+inc3(n3-1). The minimum total size of array X is L+1. To ensure that this mapping is unique so no two elements  $x_{ijk}$  occupy the same array element, X(I), the subroutines have the following restriction:  $inc2 \ge n1$  and  $inc3 \ge (inc2)(n2)$ . This arrangement of array data in storage leaves some blank space between successive planes of the array X. By determining the best size for this space, specifying an optimum inc3 stride, the third dimension of the array does not create conflicts in the 3090 storage hierarchy.

If the *inc3* stride value returned by the STRIDE subroutine turns out to be a multiple of *inc2*, the array X can be declared as a three-dimensional array as X(inc2,inc3/inc2,n3); otherwise, it can be declared as either a one-dimensional array, X(0:L), as described above, or a two-dimensional array X(0:inc3-1,0:n3-1), where  $X_{iik}$  is stored in X(l,k) where I = i+(inc2)(j).

# Using the Scale Argument

If you must multiply either the input or the output sequences by a common factor, you can avoid the multiplication by letting the *scale* argument contain the factor. The subroutines multiply the sine and cosine values by the scale factor during the initialization. Thus, scaling takes no time after the initialization of the Fourier transform calculations.

# How the Fourier Transform Subroutines Achieve High Performance

There are two levels of optimization for the fast Fourier transforms (FFTs) in the ESSL library. For sequences with a large power of 2 length, we provide efficient radix-2 and radix-8 transform implementations where cache use is optimized. The cache optimization includes ordering of operations to maximize stride-1 data access and prefetching cache lines.

Similar optimization techniques are used for sequence lengths which are not a power of 2 and mixed-radix FFT's are performed. Many short sequence FFT's have sequence size specific optimizations. Some of these optimizations were originally developed for a vector machine and have been adapted for cache based RISC machines (see references [1], [5], and [7])

The other optimization in the FFT routine is to treat multiple sequences as efficiently as possible. Techniques here include blocking sequences to fit into available CPU cache and transposing sequences to ensure stride-1 access. Whenever possible, the highest performance can be obtained when multiple sequences are transformed in a single call.

# **Convolution and Correlation Considerations**

This section describes some ways to optimize performance in the convolution and correlation subroutines.

# Performance Tradeoffs between Subroutines

The subroutines SCON, SCOR, SACOR, SCOND, SCORD, SDCON, SDCOR, DDCON, and DDCOR compute convolutions, correlations, and autocorrelations using essentially the same methods. They make a decision, based on estimated timings, to use one of two methods:

- · A direct method that is most efficient when one or both of the input sequences are short
- A direct method that is most efficient when the output sequence is short

Using this approach has the following advantages:

- In most cases, improved performance can be achieved for direct methods because:
  - No initialization is required.
  - No working storage or padding of sequences is necessary.
- In some cases, greater accuracy may be available.
- Negative strides can be used.

In general, using SCONF, SCORF, and SACORF provides the best performance, because the mixed-radix Fourier transform subroutines are used. However, if you can determine from your arguments that a direct method is preferred, you should use SCOND and SCORD instead. These give you better performance for the direct methods, and also give you additional capabilities.

In cases where there is doubt as to the best choice of a subroutine, perform timing experiments.

# Special Uses of SCORD

The subroutine SCORD can perform the functions of SCON and SACOR; that is, it can compute convolutions and autocorrelations. To compute a convolution, you must specify a negative stride for h (see Example 4 in SCORD). To compute the autocorrelation, you must specify the two input sequences to be the same (see Example 5 in SCORD).

# Special Uses of \_DCON and \_DCOR

The \_DCON and \_DCOR subroutines compute convolutions and correlations, respectively, by the direct method with decimated output. Setting the decimation interval id = 1 in SDCON and SDCOR provides the same function as SCOND and SCORD, respectively. Doing the same in DDCON and DDCOR provides long-precision versions of SCOND and SCORD, respectively, which are not otherwise available.

# Accuracy When Direct Methods Are Used

The direct methods used by the convolution and correlation subroutines use vector operations to accumulate sums of products. The products are computed and accumulated in long precision. As a result, higher accuracy can be obtained in the final results for some types of data. For example, if input data consists only of integers, and if no intermediate and final numbers become too large (larger than 2<sup>24</sup>–1 for short-precision computations and larger than 2<sup>56</sup>–1 for long-precision computations), the results are exact.

# **Accuracy When Fourier Methods Are Used**

The Fourier methods used by the convolution and correlation subroutines compute Fourier transforms of input data that is multiplied element-by-element in short-precision arithmetic. The inverse Fourier transform is then computed. There are internally generated rounding errors in the Fourier transforms. It has been shown in references [ 90] and [ 79] that, in the case of white noise data, the relative root mean square (RMS) error of the Fourier transform is proportional to  $log_2n$  with a very small proportionality factor. In general, with random, evenly distributed data, this is better than the RMS error of the direct method. However, one must keep in mind the fact that, while the Fourier method may yield a smaller root mean square error, there can be points with large relative errors. Thus, it can happen that some points, usually at the ends of the output sequence, can be obtained with greater relative accuracy with direct methods.

# **Convolutions and Correlations by Fourier Methods**

The convolution and correlation subroutines that use the Fourier methods determine a sequence length n, whose Fourier transform is computed using ESSL subroutines. In the simple case where iy0 = 0 for convolution or iy0 = -nh+1 for correlation, n is chosen as a value greater than or equal to the following, which is also acceptable to the Fourier transform subroutines:

```
nt = min(nh+nx-1, ny) for convolution and correlation nt = min(nx+nx-1, ny) for autocorrelation
```

which is also acceptable to the Fourier subroutines.

# **Related Computation Considerations**

This section describes some key points about using the related-computation subroutines.

# **Accuracy Considerations**

- Many of the subroutines performing short-precision computations provide increased accuracy by accumulating results in long precision. This is noted in the functional description for each subroutine.
- There are ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Fourier Transform Subroutines**

This section contains the Fourier transform subroutine descriptions.

# **SCFT and DCFT—Complex Fourier Transform**

These subroutines compute a set of m complex discrete n-point Fourier transforms of complex data.

Table 126. Data Types				
X, Y	scale	Subroutine		
Short-precision complex	Short-precision real	SCFT		
Long-precision complex	Long-precision real	DCFT		

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

# Syntax

Fortran	CALL SCFT   DCFT (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2)
C and C++	scft   dcft (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SCFT   DCFT (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);

### On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m sequences of length n. Specified as: an array of (at least) length 1+(n-1)inc1x+(m-1)inc2x, containing numbers of the data type indicated in Table 126.

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. (If m=1, this argument is ignored.) Specified as: a fullword integer; inc2x > 0.

У

See "On Return" on page 749.

inc1y

is the stride between the elements within each sequence in array Y. Specified as: a fullword integer; inc1y > 0.

inc2y

is the stride between the first elements of each sequence in array Y. (If m = 1, this argument is ignored.) Specified as: a fullword integer; inc2y > 0.

n

is the length of each sequence to be transformed. Specified as: a fullword integer;  $n \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument, as well as in the optionally-recoverable error 2030. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

m

is the number of sequences to be transformed. Specified as: a fullword integer; m > 0.

# isign

controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:

If isign = positive value, lsign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

#### scale

is the scaling constant scale. See "Function" on page 750 for its usage. Specified as: a number of the data type indicated in Table 126 on page 747, where scale > 0.0 or scale < 0.0

#### aux1

is the working storage for this subroutine, where:

If *init*  $\neq$  0, the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer; naux1 > 7 and  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 7 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCFT and DCFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of the results of the m discrete Fourier transforms, each of length n.

Returned as: an array of (at least) length 1+(n-1)inc1y+(m-1)inc2y, containing numbers of the data type indicated in Table 126 on page 747. This array must be aligned on a doubleword boundary.

#### aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- For optimal performance, the preferred value for *inc1x* and *inc1y* is 1. This
  implies that the sequences are stored with stride 1. The preferred value for *inc2x* and *inc2y* is n. This implies that sequences are stored one after another
  without any gap.

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case, inc2x (or inc2y) = 1 and inc1x (or inc1y) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of inc1x and inc1y for \_CFT, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969. Example 1 in the STRIDE subroutine description explains how it is used for \_CFT.

If you specify the same array for X and Y, then inc1x and inc1y must be equal, and inc2x and inc2y must be equal. In this case, output overwrites input. If m = 1, the inc2x and inc2y values are not used by the subroutine. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

# Processor-Independent Formulas for SCFT for NAUX1 and NAUX2

# NAUX1 Formulas:

```
If n \le 8192, use naux1 = 20000.
If n > 8192, use naux1 = 20000+1.14n.
```

#### NAUX2 Formulas:

```
If n \le 8192, use naux2 = 20000.

If n > 8192, use naux2 = 20000+1.14n.

For the transposed case, where inc2x = 1 or inc2y = 1, and where n \ge 252, add the following to the above storage requirements: (n+256)(\min(64, m)).
```

# Processor-Independent Formulas for DCFT for NAUX1 and NAUX2

## NAUX1 Formulas:

```
If n \le 2048, use naux1 = 20000.
If n > 2048, use naux1 = 20000+2.28n.
```

# NAUX2 Formulas:

```
If n \le 2048, use naux2 = 20000.

If n > 2048, use naux2 = 20000+2.28n.

For the transposed case, where inc2x = 1 or inc2y = 1, and where n \ge 252, add the following to the above storage requirements: (2n+256)(\min(64, m)).
```

**Function:** The set of m complex discrete n-point Fourier transforms of complex data in array X, with results going into array Y, is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n-1} x_{ji} W_n^{(Isign)jk}$$

for:

$$k = 0, 1, ..., n-1$$
  
 $i = 1, 2, ..., m$ 

where:

$$W_n = e^{-2\pi\left(\sqrt{-1}\right)/n}$$

# and where:

 $x_{ji}$  are elements of the sequences in array X.  $y_{ki}$  are elements of the sequences in array Y. *Isign* is + or – (determined by argument *isign*). *scale* is a scalar value.

For *scale* = 1.0 and *isign* being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with *scale* = 1.0/*n* and *isign* being negative. See references [1], [3], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

# **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. n > 37748736
- 2. inc1x, inc2x, inc1y, or  $inc2y \le 0$
- $3. m \leq 0$
- 4. isign = 0
- 5. scale = 0.0
- 6. The subroutine has not been initialized with the present arguments.
- 7. The length of the transform in *n* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 8.  $naux1 \leq 7$
- 9. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 10. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows an input array X with a set of four short-precision complex sequences:

$$e^{2\pi\left(\sqrt{-1}\right)jk/n}$$

for j = 0, 1, ..., n-1 with n = 8, and the single frequencies k = 0, 1, 2, and 3. The arrays are declared as follows:

```
COMPLEX*8 X(0:1023),Y(0:1023)
REAL*8 AUX1(1693),AUX2(4096)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input



INIT = 1(for initialization) INIT = 0(for computation)

SCALE = 1.0

# X contains the following four sequences:

```
(1.0000, 0.0000)
                   (1.0000, 0.0000)
                                                             (1.0000, 0.0000)
                                        (1.0000,
                                                  0.0000)
(1.0000, 0.0000)
                   (0.7071,
                             0.7071)
                                        (0.0000,
                                                  1.0000)
                                                            (-0.7071, 0.7071)
                                                             (0.0000, -1.0000)
(1.0000, 0.0000)
                             1.0000)
                                       (-1.0000, 0.0000)
                   (0.0000,
                                                             (0.7071, 0.7071)
(1.0000, 0.0000)
                                        (0.0000, -1.0000)
                  (-0.7071,
                             0.7071)
                                                  0.0000)
(1.0000, 0.0000)
                  (-1.0000, 0.0000)
                                        (1.0000,
                                                            (-1.0000, 0.0000)
(1.0000, 0.0000)
                  (-0.7071, -0.7071)
                                        (0.0000, 1.0000)
                                                             (0.7071, -0.7071)
(1.0000, 0.0000)
                   (0.0000, -1.0000)
                                       (-1.0000, 0.0000)
                                                             (0.0000, 1.0000)
(1.0000, 0.0000)
                   (0.7071, -0.7071)
                                        (0.0000, -1.0000)
                                                            (-0.7071, -0.7071)
```

# Output: Y contains the following four sequences:

```
(8.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (8.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (8.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (8.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
                                      (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
```

**Example 2:** This example shows an input array X with a set of four input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of the transform in Example 1 by using a negative *isign*, giving as output the four sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

## Call Statement and Input

Output

Y =(same as input X in Example 1)

**Example 3:** This example shows an input array X with a set of four short-precision complex sequences

$$e^{2\pi(\sqrt{-1})jk/n}$$

for j = 0, 1, ..., n-1 with n = 12, and the single frequencies k = 0, 1, 2, and 3. Also, inc1x = inc1y = m and inc2x = inc2y = 1 to show how the input and output arrays can be stored in the transposed form. The arrays are declared as follows:

```
COMPLEX*8 X (4,0:11),Y(4,0:11)
REAL*8 AUX1(10000),AUX2(10000)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

INIT = 1(for initialization)
INIT = 0(for computation)

SCALE = 1.0

# X contains the following four sequences:

```
(1.0000, 0.0000)
                    (1.0000, 0.0000)
                                        (1.0000, 0.0000)
                                                            (1.0000, 0.0000)
(1.0000, 0.0000)
                    (0.8660, 0.5000)
                                        (0.5000, 0.8660)
                                                            (0.0000, 1.0000)
(1.0000, 0.0000)
                    (0.5000, 0.8660)
                                       (-0.5000, 0.8660)
                                                           (-1.0000, 0.0000)
(1.0000, 0.0000)
                    (0.0000, 1.0000)
                                      (-1.0000, 0.0000)
                                                           (0.0000, -1.0000)
(1.0000, 0.0000)
                  (-0.5000, 0.8660)
                                     (-0.5000, -0.8660)
                                                            (1.0000, 0.0000)
(1.0000, 0.0000)
                                      (0.5000, -0.8660)
                  (-0.8660, 0.5000)
                                                            (0.0000, 1.0000)
(1.0000, 0.0000)
                  (-1.0000, 0.0000)
                                        (1.0000, 0.0000)
                                                           (-1.0000, 0.0000)
(1.0000, 0.0000)
                 (-0.8660, -0.5000)
                                        (0.5000, 0.8660)
                                                           (0.0000, -1.0000)
(1.0000, 0.0000)
                 (-0.5000, -0.8660)
                                       (-0.5000, 0.8660)
                                                            (1.0000, 0.0000)
                                                            (0.0000, 1.0000)
(1.0000, 0.0000)
                  (0.0000, -1.0000)
                                       (-1.0000, 0.0000)
(1.0000, 0.0000)
                  (0.5000, -0.8660) (-0.5000, -0.8660) (-1.0000, 0.0000)
(1.0000, 0.0000)
                  (0.8660, -0.5000)
                                      (0.5000, -0.8660)
                                                          (0.0000, -1.0000)
```

#### Output: Y contains the following four sequences:

```
(0.0000, 0.0000)
(12.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                    (12.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                        (12.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                            (12.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
 (0.0000, 0.0000)
                     (0.0000, 0.0000)
                                         (0.0000, 0.0000)
                                                             (0.0000, 0.0000)
```

**Example 4:** This example shows an input array X with a set of four input spike sequences exactly equal to the output of Example 3. This shows how you can compute the inverse of the transform in Example 3 by using a negative *isign*, giving as output the four sequences listed in the input for Example 3. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

```
INIT X INC1X INC2X Y INC1Y INC2Y N M ISIGN SCALE
                                                                 AUX1 NAUX1 AUX2 NAUX2
CALL SCFT(INIT, X , 4 , 1 , Y , 4 , 1 , 12 , 4 , -1 , SCALE , AUX1, 10000, AUX2, 10000)
                    INIT
                             = 1(for initialization)
                    INIT
                             = 0(for computation)
                    SCALE
                             = 1.0/12.0
                    Χ
                             =(same as output Y in Example 3)
```

# Output

Υ =(same as input X in Example 3)

**Example 5:** This example shows how to compute a transform of a single long-precision complex sequence. It uses isign = 1 and scale = 1.0. The arrays are declared as follows:

```
COMPLEX*16 X(0:7), Y(0:7)
REAL*8
            AUX1(26), AUX2(12)
```

The input in X is an impulse at zero, and the output in Y is constant for all frequencies. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

```
AUX1 NAUX1 AUX2 NAUX2
         INIT X INC1X INC2X Y INC1Y INC2Y N M ISIGN SCALE
CALL DCFT(INIT, X , 1 , 0 , Y , 1 , 0 , 8 , 1 , 1 , SCALE , AUX1 , 26 , AUX2 , 12)
```

= 1(for initialization) INIT INIT 0(for computation)

SCALE = 1.0

#### X contains the following sequence:

(1.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)(0.0000, 0.0000)

# Output:

(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)(1.0000, 0.0000)

## SRCFT and DRCFT—Real-to-Complex Fourier Transform

These subroutines compute a set of *m* complex discrete *n*-point Fourier transforms of real data.

Table 127. Data Types		
X, scale	Y	Subroutine
Short-precision real	Short-precision complex	SRCFT
Long-precision real	Long-precision complex	DRCFT

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

## Syntax

Fortran	CALL SRCFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3)
	CALL DRCFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2)
C and C++	srcft (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	drcft (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SRCFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	CALL DRCFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);

On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m sequences of length n, which are to be transformed. The sequences are assumed to be stored with stride 1. Specified as: an array of (at least) length n+(m-1)inc2x, containing numbers of the data type indicated in Table 127. See "Notes" on page 757 for more details. (It can be declared as X(inc2x,m).)

inc2x

is the stride between the first elements of the sequences in array X. (If m = 1, this argument is ignored.) Specified as: a fullword integer;  $inc2x \ge n$ .

y

See "On Return" on page 757.

inc2y

is the stride between the first elements of the sequences in array Y. (If m = 1, this argument is ignored.) Specified as: a fullword integer;  $inc2y \ge (n/2)+1$ .

n

is the length of each sequence to be transformed. Specified as: a fullword integer;  $n \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

m

is the number of sequences to be transformed. Specified as: a fullword integer; m > 0.

isign

controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:

If isign = positive value, Isign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

scale

is the scaling constant *scale*. See "Function" on page 758 for its usage. Specified as: a number of the data type indicated in Table 127 on page 755, where scale > 0.0 or scale < 0.0.

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in *aux1*. Specified as: a fullword integer; *naux1* > 14 and *naux1* ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 14 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31. *aux2* 

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SRCFT and DRCFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge (minimum value required for successful processing)$ . To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of

having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

aux3

this argument is provided for migration purposes only and is ignored.

Specified as: an area of storage, containing *naux3* long-precision real numbers. *naux3* 

this argument is provided for migration purposes only and is ignored.

Specified as: a fullword integer.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of the results of the m complex discrete Fourier transforms, each of length n. The sequences are stored with the stride 1. Due to complex conjugate symmetry, only the first (n/2) + 1 elements of each sequence are given in the output—that is,  $y_{ki}$ , k = 0, 1, ..., n/2, i = 1, 2, ..., m.

Returned as: an array of (at least) length n/2+1+(m-1)inc2y, containing numbers of the data type indicated in Table 127 on page 755. This array must be aligned on a doubleword boundary. (It can be declared as Y(inc2y,m).) aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. In these subroutines, the elements in each sequence in x and y are assumed to be stored in contiguous storage locations, using a stride of 1; therefore, inc1x and inc1y values are not a part of the argument list. For optimal performance, the inc2x and inc2y values should be close to their respective minimum values, which are given below:

```
min(inc2x) = n

min(inc2y) = n/2+1
```

If you specify the same array for X and Y, then inc2x must equal 2(inc2y). In this case, output overwrites input. If m=1, the inc2x and inc2y values are not used by the subroutine. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

3. Be sure to align array X on a doubleword boundary, and specify an even number for *inc2x*, if possible.

#### Processor-Independent Formulas for SRCFT for NAUX1 and NAUX2

#### NAUX1 Formulas

```
If n \le 16384, use naux1 = 25000.
If n > 16384, use naux1 = 20000+0.82n.
```

#### NAUX2 Formulas

```
If n \le 16384, use naux2 = 20000.
If n > 16384, use naux2 = 20000+0.57n.
```

#### Processor-Independent Formulas for DRCFT for NAUX1 and NAUX2

#### NAUX1 Formulas

```
If n \le 4096, use naux1 = 22000.
If n > 4096, use naux1 = 20000+1.64n.
```

#### NAUX2 Formulas

```
If n \le 4096, use naux2 = 20000.
If n > 4096, use naux2 = 20000+1.14n.
```

**Function:** The set of m complex conjugate even discrete n-point Fourier transforms of real data in array X, with results going into array Y, is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n-1} x_{ji} W_n^{(Isign)jk}$$

for:

$$k = 0, 1, ..., n-1$$
  
 $i = 1, 2, ..., m$ 

where:

$$W_n = e^{-2\pi\left(\sqrt{-1}\right)/n}$$

and where:

 $x_{ji}$  are elements of the sequences in array X.  $y_{ki}$  are elements of the sequences in array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

The output in array Y is complex. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/n and isign being negative. See references [1], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With  $init \neq 0$ , the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n > 37748736
- 2.  $m \le 0$
- 3. inc2x < n
- 4. inc2y < n/2+1
- 5. isign = 0
- 6. scale = 0.0
- 7. The subroutine has not been initialized with the present arguments.
- 8. The length of the transform in *n* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 9.  $naux1 \le 14$
- 10. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 11. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows an input array X with a set of m cosine sequences  $\cos(2\pi jk/n)$ , j=0,1,...,15 with the single frequencies k=0,1,2,3. The Fourier transform of the cosine sequence with frequency k=0 or n/2 has 1.0 in the 0 or n/2 position, respectively, and zeros elsewhere. For all other k, the Fourier transform has 0.5 in the k position and zeros elsewhere. The arrays are declared as follows:

```
REAL*4 X(0:65535)
COMPLEX*8 Y(0:32768)
REAL*8 AUX1(41928), AUX2(35344), AUX3(1)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

X contains the following four sequences:

```
1.0000
         1.0000
                   1.0000
                             1.0000
1.0000
         0.9239
                   0.7071
                             0.3827
1.0000
         0.7071
                   0.0000
                            -0.7071
1.0000
         0.3827
                  -0.7071
                            -0.9239
         0.0000
                  -1.0000
1.0000
                             0.0000
1.0000
        -0.3827
                  -0.7071
                             0.9239
1.0000
        -0.7071
                   0.0000
                             0.7071
1.0000
        -0.9239
                   0.7071
                            -0.3827
1.0000
        -1.0000
                   1.0000
                            -1.0000
        -0.9239
                   0.7071
                            -0.3827
1.0000
        -0.7071
                   0.0000
                             0.7071
1.0000
1.0000
        -0.3827
                  -0.7071
                             0.9239
1.0000
         0.0000
                  -1.0000
                             0.0000
                  -0.7071
1.0000
         0.3827
                            -0.9239
1.0000
         0.7071
                   0.0000
                            -0.7071
1.0000
         0.9239
                   0.7071
                             0.3827
```

#### Output: Y contains the following four sequences:

```
(1.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.5000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.5000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.5000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
                   (0.0000, 0.0000)
(0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                   (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
```

**Example 2:** This example shows another transform computation with different data using the same initialized array AUX1 as in Example 1. The input is also a set of four cosine sequences  $\cos(2\pi jk/n)$ , j=0,1,...,15 with the single frequencies k=8,9,10,11, thus including the middle frequency k=8. The middle frequency has the value 1.0. For other frequencies, the transform has zeros, except for frequencies k and n-k. Only the values for j=n-k are given in the output.

#### Call Statement and Input

**SCALE** 

X contains the following four sequences:

= 1.0/16

```
1.0000
          1.0000
                   1.0000
                            1.0000
-1.0000
         -0.9239
                  -0.7071
                           -0.3827
1.0000
                   0.0000
                           -0.7071
         0.7071
-1.0000
         -0.3827
                   0.7071
                            0.9239
1.0000
          0.0000
                 -1.0000
                            0.0000
                   0.7071
-1.0000
          0.3827
                           -0.9239
         -0.7071
                   0.0000
1.0000
                            0.7071
-1.0000
                  -0.7071
         0.9239
                            0.3827
1.0000
         -1.0000
                  1.0000
                           -1.0000
-1.0000
         0.9239
                  -0.7071
                            0.3827
                   0.0000
1.0000
         -0.7071
                            0.7071
                   0.7071
-1.0000
         0.3827
                           -0.9239
1.0000
         0.0000 - 1.0000
                            0.0000
-1.0000
         -0.3827
                   0.7071
                            0.9239
1.0000
         0.7071
                   0.0000
                           -0.7071
-1.0000
        -0.9239
                 -0.7071
                           -0.3827
```

#### Output: Y contains the following four sequences:

```
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
                                      (0.0000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.0000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.0000, 0.0000)
                                                         (0.5000, 0.0000)
(0.0000, 0.0000)
                  (0.0000, 0.0000)
                                      (0.5000, 0.0000)
                                                         (0.0000, 0.0000)
                  (0.5000, 0.0000)
                                                        (0.0000, 0.0000)
(0.0000, 0.0000)
                                     (0.0000, 0.0000)
(1.0000, 0.0000)
                  (0.0000, 0.0000)
                                     (0.0000, 0.0000)
                                                        (0.0000, 0.0000)
```

## **Example 3:** This example uses the mixed-radix capability. The arrays are declared as follows:

```
REAL*8 X(0:11)
COMPLEX*16 Y(0:6)
REAL*8 AUX1(50),AUX2(50)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

Output: Y contains the following sequence:

## **SRCFT and DRCFT**

(12.0000, 0.0000) (0.0000 , 0.0000) (0.0000 , 0.0000) (0.0000 , 0.0000) (0.0000, 0.0000)(0.0000 , 0.0000) (0.0000 , 0.0000)

## SCRFT and DCRFT—Complex-to-Real Fourier Transform

These subroutines compute a set of m real discrete n-point Fourier transforms of complex conjugate even data.

Table 128. Data Types		
X	Y, scale	Subroutine
Short-precision complex	Short-precision real	SCRFT
Long-precision complex	Long-precision real	DCRFT

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

## Syntax

Fortran	CALL SCRFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3)
	CALL DCRFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2)
C and C++	scrft (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	dcrft (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SCRFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	CALL DCRFT (init, x, inc2x, y, inc2y, n, m, isign, scale, aux1, naux1, aux2, naux2);

On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m sequences. Due to complex conjugate symmetry, the input consists of only the first (n/2)+1 elements of each sequence; that is,  $x_{ji}$ , j=0,1,...,n/2, i=1,2,...,m. The sequences are assumed to be stored with stride 1.

Specified as: an array of (at least) length n/2+1+(m-1)inc2x, containing numbers of the data type indicated in Table 128. This array must be aligned on a doubleword boundary. (It can be declared as X(inc2x,m).)

inc2x

is the stride between the first elements of the sequences in array X. (If m = 1, this argument is ignored.) Specified as: a fullword integer;  $inc2x \ge (n/2)+1$ .

See "On Return" on page 765.

inc2y

is the stride between the first elements of the sequences in array Y. (If m = 1, this argument is ignored.) Specified as: a fullword integer;  $inc2y \ge n$ .

n

is the length of each sequence to be transformed. Specified as: a fullword integer;  $n \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

m

is the number of sequences to be transformed. Specified as: a fullword integer; m > 0.

#### isign

controls the direction of the transform, determining the sign *Isign* of the exponent of  $W_n$ , where:

If isign = positive value, lsign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

#### scale

is the scaling constant scale. See "Function" on page 766 for its usage. Specified as: a number of the data type indicated in Table 128 on page 763, where scale > 0.0 or scale < 0.0.

#### aux1

is the working storage for this subroutine, where:

If *init*  $\neq$  0, the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer; naux1 > 13 and  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 13 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine that is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCRFT and DCRFT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

aux3

this argument is provided for migration purposes only and is ignored.

Specified as: an area of storage, containing *naux3* long-precision real numbers. *naux3* 

this argument is provided for migration purposes only and is ignored.

Specified as: a fullword integer.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of the results of the m discrete Fourier transforms of the complex conjugate even data, each of length n. The sequences are stored with stride 1.

Returned as: an array of (at least) length n+(m-1)inc2y, containing numbers of the data type indicated in Table 128 on page 763. See "Notes" for more details. (It can be declared as Y(inc2y,m).)

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with init ≠ 0 and init = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. The elements in each sequence in x and y are assumed to be stored in contiguous storage locations—that is, with a stride of 1. Therefore, inc1x and inc1y values are not a part of the argument list. For optimal performance, the inc2x and inc2y values should be close to their respective minimum values, which are given below:

```
min(inc2y) = n

min(inc2x) = n/2+1
```

If you specify the same array for X and Y, then inc2y must equal 2(inc2x). In this case, output overwrites input. If m=1, the inc2x and inc2y values are not used by the subroutine. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

3. Be sure to align array Y on a doubleword boundary, and specify an even number for *inc2y*, if possible.

#### Processor-Independent Formulas for SCRFT for NAUX1 and NAUX2

#### NAUX1 Formulas

```
If n \le 16384, use naux1 = 25000.
If n > 16384, use naux1 = 20000+0.82n.
```

#### NAUX2 Formulas

```
If n \le 16384, use naux2 = 20000.
If n > 16384, use naux2 = 20000+0.57n.
```

#### Processor-Independent Formulas for DCRFT for NAUX1 and NAUX2

#### NAUX1 Formulas

```
If n \le 4096, use naux1 = 22000.
If n > 4096, use naux1 = 20000+1.64n.
```

#### NAUX2 Formulas

If 
$$n \le 4096$$
, use  $naux2 = 20000$ .  
If  $n > 4096$ , use  $naux2 = 20000+1.14n$ .

**Function:** The set of m real discrete n-point Fourier transforms of complex conjugate even data in array X, with results going into array Y, is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n-1} x_{ji} W_n^{(Isign)jk}$$

for:

$$k = 0, 1, ..., n-1$$
  
 $i = 1, 2, ..., m$ 

where:

$$W_n = e^{-2\pi\left(\sqrt{-1}\right)/n}$$

and where:

 $x_{ji}$  are elements of the sequences in array X.  $y_{ki}$  are elements of the sequences in array Y. *Isign* is + or – (determined by argument *isign*). *scale* is a scalar value.

Because of the symmetry, Y has real data. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/n and isign being negative. See references [1], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n > 37748736
- $2. m \leq 0$
- 3. inc2x < n/2+1
- 4. inc2y < n
- 5. scale = 0.0
- 6. isign = 0
- 7. The subroutine has not been initialized with the present arguments.
- 8. The length of the transform in *n* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 9. naux1 ≤ 13
- 10. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 11. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example uses the mixed-radix capability and shows how to compute a single transform. The arrays are declared as follows:

```
COMPLEX*8 X(0:6)

REAL*8 AUX1(50), AUX2(50), AUX3(1)

REAL*4 Y(0:11)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

**Note:** X shows the n/2+1 = 7 elements used in the computation.

#### Call Statement and Input

X contains the following sequence:

(1.0, 0.0)(0.0, 0.0)(0.0, 0.0)(0.0, 0.0)(0.0, 0.0)(0.0, 0.0)(0.0, 0.0)

#### Output

Example 2: This example shows another transform computation with different data using the same initialized array AUX1 as in Example 1.

#### Call Statement and Input

SCALE = 1.0

X contains the following sequence:

(1.0, 0.0)

(1.0, 0.0)

(1.0, 0.0)

(1.0, 0.0)

(1.0, 0.0)

(1.0, 0.0)

(1.0, 0.0)

#### Output

```
0.0 , 0.0 , 0.0 , 0.0)
```

**Example 3:** This example shows how to compute many transforms simultaneously. The arrays are declared as follows:

```
COMPLEX*8 X(0:8,2)
REAL*8
           AUX1(50), AUX2(16), AUX3(1)
REAL*4
           Y(0:15,2)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

```
INIT X INC2X Y INC2Y
                                       M ISIGN SCALE AUX1 NAUX1 AUX2 NAUX2 AUX3 NAUX3
CALL SCRFT(INIT, X , 9 , Y , 16 , 16 , 2 , 1 , SCALE, AUX1 , 50 , AUX2 , 16 , AUX3 , 0 )
                     INIT
                                 1(for initialization)
                                 0(for computation)
                     INIT
                     SCALE
                              = 1.0
```

X contains the following two sequences:

```
    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (0.0, 0.0)

    (1.0, 0.0)
    (1.0, 0.0)
```

Output: Y contains the following two sequences:

```
16.0
     1.0
0.0 - 1.0
0.0
     1.0
0.0 - 1.0
0.0 1.0
0.0 - 1.0
0.0 1.0
0.0 - 1.0
0.0
     1.0
0.0 - 1.0
0.0 1.0
0.0 - 1.0
0.0
     1.0
0.0 - 1.0
0.0 1.0
0.0 - 1.0
```

**Example 4:** This example shows the same array being used for input and output. The arrays are declared as follows:

```
COMPLEX*16 X(0:8,2)
REAL*8 AUX1(50), AUX2(16)
REAL*8 Y(0:17,2)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

```
EQUIVALENCE (X,Y)
```

This requires INC2Y = 2(INC2X). First, initialize AUX1 using the calling sequence shown below with INIT  $\neq 0$ . Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input

X contains the following two sequences:

#### **SCRFT and DCRFT**

```
(1.0, 0.0)
              (1.0, 0.0)
 (0.0, 1.0)
               (0.0, -1.0)
(-1.0, 0.0)
             (-1.0, 0.0)
              (0.0, 1.0)
 (0.0, -1.0)
 (1.0, 0.0)
               (1.0, 0.0)
(0.0, 1.0)
(-1.0, 0.0)
               (0.0, -1.0)
              (-1.0, 0.0)
 (0.0, -1.0)
               (0.0, 1.0)
 (1.0, 0.0)
               (1.0,0.0)
```

## Output: Y contains the following two sequences:

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

## SCOSF and DCOSF—Cosine Transform

These subroutines compute a set of *m* real even discrete *n*-point Fourier transforms of cosine sequences of real even data.

Table 129. Data Types	
X, Y, scale	Subroutine
Short-precision real	SCOSF
Long-precision real	DCOSF

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

## Syntax

Fortran	CALL SCOSF   DCOSF (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2)
C and C++	scosf   dcosf (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SCOSF   DCOSF (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2);

#### On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m sequences of length n/2+1. Specified as: an array of (at least) length 1+(n/2)inc1x+(m-1)inc2x, containing numbers of the data type indicated in Table 129.

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. (If m=1, this argument is ignored.) Specified as: a fullword integer; inc2x > 0.

y

See "On Return" on page 773.

inc1y

is the stride between the elements within each sequence in array Y. Specified as: a fullword integer; inc1y > 0.

inc2y

is the stride between the first elements of the sequences in array Y. (If m = 1, this argument is ignored.) Specified as: a fullword integer; inc2y > 0.

n

is the transform length. However, due to symmetry, only the first n/2+1 values are given in the input and output. Specified as: a fullword integer;  $n \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

m

is the number of sequences to be transformed. Specified as: a fullword integer; m > 0.

#### scale

is the scaling constant scale. See "Function" on page 774 for its usage. Specified as: a number of the data type indicated in Table 129 on page 771, where scale > 0.0 or scale < 0.0.

#### aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer;  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCOSF and DCOSF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of the results of the m discrete Fourier transforms, where each Fourier transform is real and of length n. However, due to symmetry, only the first n/2+1 values are given in the output—that is,  $y_{ki}$ , k = 0, 1, ..., n/2 for each i = 1, 2, ..., m.

Returned as: an array of (at least) length 1+(n/2)inc1y+(m-1)inc2y, containing numbers of the data type indicated in Table 129 on page 771.

#### aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with init ≠ 0 and init = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. For optimal performance, the preferred value for *inc1x* and *inc1y* is 1. This implies that the sequences are stored with stride 1. In addition, *inc2x* and *inc2y* should be close to *n*/2+1.

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case, inc2x (or inc2y) = 1 and inc1x (or inc1y) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of inc1x and inc1y for \_COSF, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969. Example 2 in the STRIDE subroutine description explains how it is used for COSF.

If you specify the same array for X and Y, then inc1x and inc1y must be equal, and inc2x and inc2y must be equal. In this case, output overwrites input. If m=1, the inc2x and inc2y values are not used by the subroutine. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

#### Processor-Independent Formulas for SCOSF for NAUX1 and NAUX2

#### NAUX1 Formulas:

```
If n \le 16384, use naux1 = 40000.
If n > 16384, use naux1 = 20000+.30n.
```

## NAUX2 Formulas:

```
If n \le 16384, use naux2 = 25000.
If n > 16384, use naux2 = 20000+.32n.
```

For the transposed case, where inc2x = 1 or inc2y = 1, and where  $n \ge 252$ , add the following to the above storage requirements:  $(n/4+257)(\min(128, m)).$ 

#### Processor-Independent Formulas for DCOSF for NAUX1 and NAUX2

#### NAUX1 Formulas:

```
If n \le 16384, use naux1 = 35000.
If n > 16384, use naux1 = 20000+.60n.
```

#### NAUX2 Formulas:

If  $n \le 16384$ , use naux2 = 20000. If n > 16384, use naux2 = 20000 + .64n. For the transposed case, where inc2x = 1 or inc2y = 1, and where  $n \ge 252$ , add the following to the above storage requirements:  $(n/2+257)(\min(128, m)).$ 

Function: The set of m real even discrete n-point Fourier transforms of the cosine sequences of real data in array X, with results going into array Y, is expressed as follows:

$$y_{ki} = scale \left( .5x_{0,i} + .5(-1)^k x_{n/2,i} + \sum_{j=1}^{n/2-1} x_{ji} \cos(jk(2\pi/n)) \right)$$

for:

$$k = 0, 1, ..., n/2$$
  
 $i = 1, 2, ..., m$ 

#### where:

 $x_{ii}$  are elements of the sequences in array X, where each sequence contains the n/2+1 real nonredundant data  $x_{ij}$ , j = 0, 1, ..., n/2.  $y_{ki}$  are elements of the sequences in array Y, where each sequence contains the n/2+1 real nonredundant data  $y_{ki}$ , k = 0, 1, ..., n/2. scale is a scalar value.

You can obtain the inverse cosine transform by specifying scale = 4.0/n. Thus, if an X input is used with scale = 1.0, and its output is used as input on a subsequent call with scale = 4.0/n, the original X is obtained. See references [1], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init*  $\neq$  0, the subroutine tests and initializes arguments of the program, setting up the aux1 working storage.
- 2. With init = 0, the subroutine checks that the initialization arguments in the aux1 working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n > 37748736
- 2. inc1x or  $inc1y \le 0$
- 3. inc2x or  $inc2y \le 0$
- $4. m \leq 0$
- 5. scale = 0.0
- 6. The subroutine has not been initialized with the present arguments.
- 7. The length of the transform in *n* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 8. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 9. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows an input array X with a set of m cosine sequences of length n/2+1,  $\cos(jk(2\pi/n))$ , j=0,1,...,n/2, with the single frequencies k=0,1,2,3. The Fourier transform of the cosine sequence with frequency k=0 or n/2 has n/2 in the 0-th or n/2-th position, respectively, and zeros elsewhere. For all other k, the Fourier transform has n/4 in position k and zeros elsewhere. The arrays are declared as follows:

```
REAL*4 X(0:71),Y(0:71)
REAL*8 AUX1(414),AUX2(8960)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

## Call Statement and Input

INIT = 1(for initialization)
INIT = 0(for computation)
SCALE = 1.0

X contains the following four sequences:

```
1.0000
                   1.0000
                            1.0000
1.0000
1.0000
         0.9808
                   0.9239
                            0.8315
1.0000
         0.9239
                   0.7071
                            0.3827
1.0000
         0.8315
                   0.3827
                           -0.1951
1.0000
         0.7071
                   0.0000
                           -0.7071
                  -0.3827
                           -0.9808
1.0000
         0.5556
         0.3827
                  -0.7071
                           -0.9239
1.0000
1.0000
                  -0.9239
         0.1951
                           -0.5556
1.0000
         0.0000
                 -1.0000
                            0.0000
1.0000
        -0.1951
                 -0.9239
                            0.5556
        -0.3827
                  -0.7071
                            0.9239
1.0000
        -0.5556
                 -0.3827
1.0000
                            0.9808
1.0000
        -0.7071
                   0.0000
                            0.7071
1.0000
        -0.8315
                   0.3827
                            0.1951
1.0000
        -0.9239
                   0.7071
                           -0.3827
1.0000
        -0.9808
                   0.9239
                           -0.8315
1.0000
        -1.0000
                   1.0000
                           -1.0000
```

Output: Y contains the following four sequences:

```
16.0000
        0.0000
                0.0000 0.0000
0.0000
        8.0000
                0.0000
                        0.0000
0.0000
        0.0000
                8.0000 0.0000
0.0000
        0.0000
                0.0000 8.0000
0.0000
        0.0000
                0.0000
                        0.0000
                0.0000
0.0000
        0.0000
                       0.0000
0.0000 \quad 0.0000
                0.0000 0.0000
0.0000
        0.0000
                0.0000
                        0.0000
                0.0000
0.0000
        0.0000
                        0.0000
0.0000
        0.0000
                0.0000
                         0.0000
0.0000
        0.0000
                0.0000
                         0.0000
0.0000
        0.0000
                0.0000
                        0.0000
                0.0000
0.0000
        0.0000
                        0.0000
        0.0000
                0.0000
0.0000
                        0.0000
0.0000
        0.0000
                0.0000
                        0.0000
0.0000
        0.0000
                0.0000
                        0.0000
0.0000 0.0000 0.0000
                        0.0000
```

**Example 2:** This example shows an input array X with a set of four input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of the transform in Example 1 by using scale = 4.0/n, giving as output the four sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq 0$ . Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

```
INIT X INC1X INC2X Y INC1Y INC2Y
                                               N
                                                        SCALE
                                                               AUX1
                                                                     NAUX1
                                                                            AUX2
                                                                                  NAUX2
                                                   Μ
CALL SCOSF(INIT, X , 1 , 18 , Y , 1 , 18 , 32 , 4 , SCALE, AUX1 , 414 , AUX2 , 8960)
                     INIT
                                 1(for initialization)
                     INIT
                                 0(for computation)
                     SCALE
                                 4.0/32
                     χ
                              =(same sequences as in output Y in Example 1)
```

## Output

Y =(same sequences as in output X in Example 1)

**Example 3:** This example shows another computation using the same arguments initialized in Example 1 and using different input sequence data. The data for this example has frequencies k = 14, 15, 16, 17. Because only the sequence data has changed, initialization does not have to be done again.

#### Call Statement and Input

SCALE = 1.0

#### X contains the following four sequences:

```
1.0000
          1.0000
                   1.0000
                            1.0000
-0.9239
         -0.9808
                  -1.0000
                            -0.9808
0.7071
          0.9239
                   1.0000
                            0.9239
                  -1.0000
-0.3827
         -0.8315
                            -0.8315
          0.7071
0.0000
                   1.0000
                            0.7071
0.3827
         -0.5556
                 -1.0000
                            -0.5556
-0.7071
          0.3827
                   1.0000
                            0.3827
0.9239
                  -1.0000
         -0.1951
                            -0.1951
-1.0000
          0.0000
                  1.0000
                            0.0000
                 -1.0000
0.9239
          0.1951
                            0.1951
                   1.0000
-0.7071
         -0.3827
                            -0.3827
                 -1.0000
0.3827
          0.5556
                            0.5556
         -0.7071
0.0000
                   1.0000
                            -0.7071
-0.3827
          0.8315
                  -1.0000
                            0.8315
0.7071
         -0.9239
                   1.0000
                            -0.9239
-0.9239
          0.9808
                  -1.0000
                            0.9808
1.0000 -1.0000
                   1.0000
                           -1.0000
```

#### Output: Y contains the following four sequences:

```
0.0000
0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                          0.0000
0.0000
        0.0000
                 0.0000
                          0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
0.0000
        0.0000
                 0.0000
                          0.0000
0.0000
        0.0000
                 0.0000
                         0.0000
                 0.0000
0.0000
        0.0000
                         0.0000
8.0000
        0.0000
                 0.0000
                         0.0000
        8.0000
0.0000
                 0.0000
                         8.0000
0.0000
        0.0000
                16.0000
                         0.0000
```

## **SSINF and DSINF—Sine Transform**

These subroutines compute a set of m real even discrete n-point Fourier transforms of sine sequences of real even data.

Table 130. Data Types	
X, Y, scale	Subroutine
Short-precision real	SSINF
Long-precision real	DSINF

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

## Syntax

Fortran	CALL SSINF   DSINF (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2)
C and C++	ssinf   dsinf (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SSINF   DSINF (init, x, inc1x, inc2x, y, inc1y, inc2y, n, m, scale, aux1, naux1, aux2, naux2);

#### On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transforms of the given sequences are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Х

is the array X, consisting of m sequences of length n/2. Specified as: an array of (at least) length 1+(n/2-1)inc1x+(m-1)inc2x, containing numbers of the data type indicated in Table 130. The first element in X must have a value of 0.0 (otherwise, incorrect results may occur).

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. (If m=1, this argument is ignored.) Specified as: a fullword integer; inc2x > 0.

y See "On Return" on page 780.

inc1y

is the stride between the elements within each sequence in array Y. Specified as: a fullword integer; inc1y > 0.

inc2y

is the stride between the first elements of the sequences in array Y. (If m = 1, this argument is ignored.) Specified as: a fullword integer; inc2y > 0.

n

is the transform length. However, due to symmetry, only the first n/2 values are given in the input and output. Specified as: a fullword integer;  $n \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

m

is the number of sequences to be transformed. Specified as: a fullword integer; m > 0.

scale

is the scaling constant scale. See "Function" on page 781 for its usage. Specified as: a number of the data type indicated in Table 130 on page 778, where scale > 0.0 or scale < 0.0.

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer;  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SSINF and DSINF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of the results of the m discrete Fourier transforms, where each Fourier transform is real and of length n. However, due to symmetry, only the first n/2 values are given in the output—that is,  $y_{ki}$ , k = 0, 1, ..., n/2-1 for each i = 1, 2, ..., m.

Returned as: an array of (at least) length 1+(n/2-1)inc1y+(m-1)inc2y, containing numbers of the data type indicated in Table 130 on page 778. aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with init ≠ 0 and init = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. For optimal performance, the preferred value for *inc1x* and *inc1y* is 1. This implies that the sequences are stored with stride 1. In addition, *inc2x* and *inc2y* should be close to *n*/2.

It is possible to specify sequences in the transposed form—that is, as rows of a two-dimensional array. In this case, inc2x (or inc2y) = 1 and inc1x (or inc1y) is equal to the leading dimension of the array. One can specify either input, output, or both in the transposed form by specifying appropriate values for the stride parameters. For selecting optimal values of inc1x and inc1y for \_SINF, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969. Example 3 in the STRIDE subroutine description explains how it is used for SINF.

If you specify the same array for X and Y, then inc1x and inc1y must be equal, and inc2x and inc2y must be equal. In this case, output overwrites input. If m=1, the inc2x and inc2y values are not used by the subroutine. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

#### Processor-Independent Formulas for SSINF for NAUX1 and NAUX2

#### NAUX1 Formulas:

```
If n \le 16384, use naux1 = 60000.
If n > 16384, use naux1 = 20000+.30n.
```

## NAUX2 Formulas:

```
If n \le 16384, use naux2 = 25000.
If n > 16384, use naux2 = 20000+.32n.
```

For the transposed case, where inc2x = 1 or inc2y = 1, and where  $n \ge 252$ , add the following to the above storage requirements:  $(n/4+257)(\min(128, m))$ .

#### Processor-Independent Formulas for DSINF for NAUX1 and NAUX2

#### NAUX1 Formulas:

```
If n \le 16384, use naux1 = 50000.
If n > 16384, use naux1 = 20000+.60n.
```

#### NAUX2 Formulas:

If  $n \le 16384$ , use naux2 = 20000. If n > 16384, use naux2 = 20000+.64n. For the transposed case, where inc2x = 1 or inc2y = 1, and where  $n \ge 252$ , add the following to the above storage requirements:  $(n/2+257)(\min(128, m))$ .

**Function:** The set of m real even discrete n-point Fourier transforms of the sine sequences of real data in array X, with results going into array Y, is expressed as follows:

$$y_{ki} = scale \sum_{j=0}^{n/2-1} x_{ji} \sin(jk(2\pi/n))$$

for:

$$k = 0, 1, ..., n/2-1$$
  
 $i = 1, 2, ..., m$ 

#### where:

 $x_{0i} = 0.0$ 

 $x_{ji}$  are elements of the sequences in array X, where each sequence contains the n/2 real nonredundant data  $x_{ji}$ , j=0,1,...,n/2-1.

 $y_{ki}$  are elements of the sequences in array Y, where each sequence contains the n/2 real nonredundant data  $y_{ki}$ , k=0,1,...,n/2-1. scale is a scalar value.

You can obtain the inverse sine transform by specifying scale = 4.0/n. Thus, if an X input is used with scale = 1.0, and its output is used as input on a subsequent call with scale = 4.0/n, the original X is obtained. See references [1], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transforms.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n > 37748736
- 2. inc1x or  $inc1y \le 0$
- 3. inc2x or  $inc2y \le 0$
- $4. m \leq 0$
- 5. scale = 0.0
- 6. The subroutine has not been initialized with the present arguments.
- 7. The length of the transform in n is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 8. naux1 is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 9. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows an input array X with a set of m sine sequences of length n/2,  $\sin(jk(2\pi/n))$ , j = 0, 1, ..., n/2-1, with the single frequencies k = 1, 2,3. The Fourier transform of the sine sequence has n/4 in position k and zeros elsewhere. The arrays are declared as follows:

```
REAL*4
           X(0:53), Y(0:53)
REAL*8
           AUX1(414), AUX2(8960)
```

First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

```
INIT X INC1X INC2X Y INC1Y INC2Y N
                                                      SCALE AUX1 NAUX1 AUX2
                                                                                  NAUX2
                                                  М
CALL SSINF(INIT, X , 1 , 18 , Y , 1 , 18 , 32 , 3 , SCALE, AUX1 , 414 , AUX2 , 8960)
                     INIT
                              = 1(for initialization)
                     INIT
                                0(for computation)
                     SCALE
                                1.0
```

X contains the following three sequences:

```
0.0000
0.0000
                  0.0000
0.1951
         0.3827
                  0.5556
0.3827
         0.7071
                  0.9239
0.5556
         0.9239
                  0.9808
0.7071
         1.0000
                  0.7071
0.8315
         0.9239
                  0.1951
0.9239
         0.7071
                 -0.3827
0.9808
         0.3827
                 -0.8315
1.0000
         0.0000
                 -1.0000
0.9808
        -0.3827
                 -0.8315
        -0.7071
0.9239
                 -0.3827
        -0.9239
0.8315
                  0.1951
0.7071
        -1.0000
                  0.7071
0.5556
       -0.9239
                  0.9808
0.3827
        -0.7071
                  0.9239
0.1951 -0.3827
                  0.5556
```

Output: Y contains the following three sequences:

```
0.0000
       0.0000 0.0000
8.0000
       0.0000 0.0000
0.0000
       8.0000 0.0000
0.0000
       0.0000 8.0000
       0.0000
0.0000
              0.0000
       0.0000
0.0000
              0.0000
0.0000
      0.0000 0.0000
0.0000
       0.0000 0.0000
       0.0000
0.0000
              0.0000
0.0000
       0.0000
               0.0000
0.0000
       0.0000
               0.0000
0.0000
       0.0000
              0.0000
0.0000
       0.0000
              0.0000
0.0000
       0.0000
              0.0000
0.0000
       0.0000
               0.0000
0.0000 0.0000
               0.0000
```

**Example 2:** This example shows an input array X with a set of three input spike sequences equal to the output of Example 1. This shows how you can compute the inverse of the transform in Example 1 by using scale = 4.0/n, giving as output the three sequences listed in the input for Example 1. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq 0$ . Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

```
INIT X INC1X INC2X Y INC1Y INC2Y N M SCALE AUX1 NAUX1 AUX2 NAUX2

CALL SSINF(INIT, X , 1 , 18 , Y , 1 , 18 , 32 , 3 , SCALE, AUX1 , 414 , AUX2 , 8960)

INIT = 1(for initialization)
INIT = 0(for computation)
SCALE = 4.0/32
X = (same sequences as in output Y in Example 1)
```

#### Output

Y =(same sequences as in output X in Example 1)

**Example 3:** This example shows another computation using the same arguments initialized in Example 1 and using different input sequence data. The data for this example has frequencies k = 14, 15, 17. Because only the sequence data has changed, initialization does not have to be done again.

#### Call Statement and Input

SCALE = 1.0

X contains the following three sequences:

```
0.0000
         0.0000
                  0.0000
0.3827
         0.1951 -0.1951
-0.7071 -0.3827
                 0.3827
0.9239
         0.5556 -0.5556
-1.0000 -0.7071
                 0.7071
0.9239
        0.8315 -0.8315
-0.7071 -0.9239
                 0.9239
         0.9808 -0.9808
0.3827
0.8573 -1.0000
                 1.0000
-0.3827
        0.9808 -0.9808
0.7071 - 0.9239
                 0.9239
-0.9239
        0.8315 -0.8315
1.0000 -0.7071
                 0.7071
-0.9239
        0.5556 -0.5556
0.7071 -0.3827
                  0.3827
-0.3827
         0.1951 -0.1951
```

Output: Y contains the following three sequences:

```
0.0000
                0.0000
0.0000
       0.0000
0.0000
                0.0000
0.0000
       0.0000
                0.0000
0.0000 0.0000
                0.0000
0.0000 0.0000
                0.0000
0.0000 0.0000
                0.0000
0.0000
       0.0000
                0.0000
0.0000
       0.0000
                0.0000
0.0000 0.0000
                0.0000
0.0000 \quad 0.0000
                0.0000
0.0000 0.0000
                0.0000
       0.0000
0.0000
                0.0000
0.0000 0.0000
                0.0000
8.0000 0.0000
                0.0000
0.0000 8.0000
                -8.0000
0.0000 0.0000
                0.0000
```

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# SCFT2 and DCFT2—Complex Fourier Transform in Two Dimensions

These subroutines compute the two-dimensional discrete Fourier transform of complex data.

Table 131. Data Types		
Х, Ү	scale	Subroutine
Short-precision complex	Short-precision real	SCFT2
Long-precision complex	Long-precision real	DCFT2

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

## Syntax

Fortran	CALL SCFT2   DCFT2 (init, x, inc1x, inc2x, y, inc1y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2)
C and C++	scft2   dcft2 (init, x, inc1x, inc2x, y, inc1y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SCFT2   DCFT2 (init, x, inc1x, inc2x, y, inc1y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);

On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, containing the two-dimensional data to be transformed, where each element  $x_{j1,j2}$ , using zero-based indexing, is stored in X(j1(inc1x)+j2(inc2x)) for j1=0,1,...,n1-1 and j2=0,1,...,n2-1.

Specified as: an array of (at least) length 1+(n1-1)inc1x+(n2-1)inc2x, containing numbers of the data type indicated in Table 131. This array must be aligned on a doubleword boundary, and:

If inc1x = 1, the input array is stored in normal form, and  $inc2x \ge n1$ .

If inc2x = 1, the input array is stored in transposed form, and  $inc1x \ge n2$ .

See "Notes" on page 788 for more details.

inc1x

is the stride between the elements in array X for the first dimension.

If the array is stored in the normal form, inc1x = 1.

If the array is stored in the transposed form, inc1x is the leading dimension of the array and  $inc1x \ge n2$ . Specified as: a fullword integer; inc1x > 0. If inc2x = 1, then  $inc1x \ge n2$ . inc2x is the stride between the elements in array X for the second dimension. If the array is stored in the transposed form, inc2x = 1. If the array is stored in the normal form, inc2x is the leading dimension of the array and  $inc2x \ge n1$ . Specified as: a fullword integer; inc2x > 0. If inc1x = 1, then  $inc2x \ge n1$ . See "On Return" on page 787. inc1y is the stride between the elements in array Y for the first dimension. If the array is stored in the normal form, inc1y = 1. If the array is stored in the transposed form, *inc1y* is the leading dimension of the array and  $inc1y \ge n2$ . Specified as: a fullword integer; inc1y > 0. If inc2y = 1, then  $inc1y \ge n2$ . inc2y is the stride between the elements in array Y for the second dimension. If the array is stored in the transposed form, inc2y = 1. If the array is stored in the normal form, inc2y is the leading dimension of the array and  $inc2y \ge n1$ . Specified as: a fullword integer; inc2y > 0. If inc1y = 1, then  $inc2y \ge n1$ . n1 is the length of the first dimension of the two-dimensional data in the array to be transformed. Specified as: a fullword integer; n1 ≤ 37748736 and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38. n2 is the length of the second dimension of the two-dimensional data in the array to be transformed. Specified as: a fullword integer; n2 ≤ 37748736 and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38. isign controls the direction of the transform, determining the sign Isign of the exponents of  $W_{n1}$  and  $W_{n2}$ , where: If isign = positive value, Isign = + (transforming time to frequency). If isign = negative value, Isign = - (transforming frequency to time). Specified as: a fullword integer; isign > 0 or isign < 0. scale is the scaling constant scale. See "Function" on page 789 for its usage.

Specified as: a number of the data type indicated in Table 131 on page 785,

where scale > 0.0 or scale < 0.0.

aux1

is the working storage for this subroutine, where:

If *init*  $\neq$  0, the working storage is computed.

If init = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in *aux1*. Specified as: a fullword integer; *naux1* ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31. *aux2* 

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCFT2 and DCFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, containing the elements resulting from the two-dimensional discrete Fourier transform of the data in X. Each element  $y_{k1,k2}$ , using zero-based indexing, is stored in Y(k1(inc1y)+k2(inc2y)) for k1 = 0, 1, ..., n1-1 and k2 = 0, 1, ..., n2-1.

Returned as: an array of (at least) length 1+(n1-1)inc1y+(n2-1)inc2y, containing numbers of the data type indicated in Table 131 on page 785. This array must be aligned on a doubleword boundary, and:

If inc1y = 1, the output array is stored in normal form, and  $inc2y \ge n1$ .

If inc2y = 1, the output array is stored in transposed form, and  $inc1y \ge n2$ .

See "Notes" on page 788 for more details.

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### **Notes**

- aux1 should **not** be used by the calling program between program calls to this subroutine with init ≠ 0 and init = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. If you specify the same array for X and Y, then *inc1x* must equal *inc1y*, and *inc2x* must equal *inc2y*. In this case, output overwrites input. If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. By appropriately specifying the *inc* arguments, this subroutine allows you to specify that it should use one of two forms of its arrays, the normal untransposed form or the transposed form. As a result, you **do not have to move any data**. Instead, the subroutine performs the adjustments for you. Also, either the input array or the output array can be in transposed form. The FFT computation is symmetrical with respect to *n1* and *n2*. They can be interchanged without the loss of generality. If they are interchanged, an array that is stored in the normal form appears as an array stored in the transposed form and vise versa. If, for performance reasons, the forms of the input and output arrays are different, then the input array should be specified in the normal form, and the output array should be specified in the transposed form. This can always be done by interchanging *n1* and *n2*.
- 4. Although the *inc* arguments for each array can be arbitrary, in most cases, one of the *inc* arguments is 1 for each array. If *inc1* = 1, the array is stored in normal form; that is, the first dimension of the array is along the columns. In this case, *inc2* is the leading dimension of the array and must be at least *n1*. Conversely, if *inc2* = 1, the array is stored in the transposed form; that is, the first dimension of the array is along the rows. In this case, *inc1* is the leading dimension of the array and must be at least *n2*. The rows of the arrays are accessed with a stride that equals the leading dimension of the array. To minimize cache interference in accessing a row, an optimal value should be used for the leading dimension of the array. You should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969 to determine this optimal value. Example 4 in the STRIDE subroutine description explains how it is used to find either *inc1* or *inc2*.

**Processor-Independent Formulas for SCFT2 for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on *n1* and *n2*.

```
NAUX1 Formulas
```

```
If \max(n1, n2) \le 8192, use naux1 = 40000.
If \max(n1, n2) > 8192, use naux1 = 40000+1.14(n1+n2).
```

#### NAUX2 Formulas

```
If \max(n1, n2) < 252, use naux2 = 20000.

If \max(n1, n2) \ge 252, use naux2 = 20000 + (r+256)(s+1.14), where r = \max(n1, n2) and s = \min(64, n1, n2).
```

**Processor-Independent Formulas for DCFT2 for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on *n1* and *n2*.

#### NAUX1 Formulas

```
If \max(n1, n2) \le 2048, use naux1 = 40000.
If \max(n1, n2) > 2048, use naux1 = 40000+2.28(n1+n2).
```

#### NAUX2 Formulas

```
If \max(n1, n2) < 252, use naux2 = 20000.

If \max(n1, n2) \ge 252, use naux2 = 20000 + (2r + 256)(s + 2.28), where r = \max(n1, n2) and s = \min(64, n1, n2).
```

**Function:** The two-dimensional discrete Fourier transform of complex data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(Isign)j1k1} W_{n2}^{(Isign)j2k2}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$ 

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$
  
 $W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$ 

and where:

 $x_{j1,j2}$  are elements of array X.  $y_{k1,k2}$  are elements of array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/((n1)(n2)) and isign being negative. See references [1], [4], and [20].

Two invocations of this subroutine are necessary:

1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.

2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n1 > 37748736
- 2. n2 > 37748736
- 3.  $inc1x|inc2x|inc1y|inc2y \le 0$
- 4. scale = 0.0
- 5. isign = 0
- 6. The subroutine has not been initialized with the present arguments.
- 7. The length of one of the transforms in *n1* or *n2* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 8. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 9. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to compute a two-dimensional transform where both input and output are stored in normal form (inc1x = inc1y = 1). Also, inc2x = inc2y so the same array can be used for both input and output. The arrays are declared as follows:

```
COMPLEX*8 X(6,8),Y(6,8)
REAL*8 AUX1(20000), AUX2(10000)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage: EQUIVALENCE (X,Y). First, initialize AUX1 using the calling sequence shown below with INIT  $\neq 0$ . Then use the same calling sequence with INIT = 0 to do the calculation.

#### Call Statement and Input

INIT = 1(for initialization)
INIT = 0(for computation)

SCALE = 1.0

X is an array with 6 rows and 8 columns with (1.0, 0.0) in all locations.

*Output:* Y is an array with 6 rows and 8 columns having (48.0, 0.0) in location Y(1,1) and (0.0, 0.0) in all others.

**Example 2:** This example shows how to compute a two-dimensional inverse Fourier transform. For this example, X is stored in normal untransposed form (inc1x = 1), and Y is stored in transposed form (inc2y = 1). The arrays are declared as follows:

```
COMPLEX*16 X(6,8),Y(8,6)
REAL*8 AUX1(20000), AUX2(10000)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input

Output: Y is an array with 8 rows and 6 columns with (1.0, 0.0) in all locations.

# SRCFT2 and DRCFT2—Real-to-Complex Fourier Transform in Two Dimensions

These subroutines compute the two-dimensional discrete Fourier transform of real data in a two-dimensional array.

Table 132. Data Types		
X, scale	Υ	Subroutine
Short-precision real	Short-precision complex	SRCFT2
Long-precision real	Long-precision complex	DRCFT2

Note: Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

# **Syntax**

Fortran	CALL SRCFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3)
	CALL DRCFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2)
C and C++	srcft2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	drcft2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SRCFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	CALL DRCFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);

# On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of xand y are not used or changed.

If *init* = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with init  $\neq$  0.

Specified as: a fullword integer. It can have any value.

is the array X, containing n1 rows and n2 columns of data to be transformed. The data in each column is stored with stride 1. Specified as: an inc2x by (at least) *n2* array, containing numbers of the data type indicated in Table 132. See "Notes" on page 794 for more details.

# inc2x

is the leading dimension (stride between columns) of array X. Specified as: a fullword integer;  $inc2x \ge n1$ .

V See "On Return" on page 794. inc2y

is the leading dimension (stride between columns) of array Y. Specified as: a fullword integer;  $inc2y \ge ((n1)/2)+1$ .

n1

is the number of rows of data—that is, the length of the columns in array X involved in the computation. The length of the columns in array Y are (n1)/2+1. Specified as: a fullword integer;  $n1 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n2

is the number of columns of data—that is, the length of the rows in arrays X and Y involved in the computation. Specified as: a fullword integer;  $n2 \le 37748736$  and must be one of the values listed in "Acceptable Lengths" for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

isign

controls the direction of the transform, determining the sign Isign of the exponents of  $W_{n1}$  and  $W_{n2}$ , where:

If isign = positive value, lsign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

scale

is the scaling constant scale. See "Function" on page 795 for its usage. Specified as: a number of the data type indicated in Table 132 on page 792, where scale > 0.0 or scale < 0.0.

aux1

is the working storage for this subroutine, where:

If *init*  $\neq$  0, the working storage is computed.

If *init* = 0, the working storage is used in the computation of the Fourier transforms.

Specified as: an area of storage, containing *naux1* long-precision real numbers. naux1

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer;  $naux1 \ge (minimum \ value \ required for$ successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31. aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SRCFT2 and DRCFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### aux3

this argument is provided for migration purposes only and is ignored.

Specified as: an area of storage containing *naux3* long-precision real numbers. *naux3* 

this argument is provided for migration purposes only and is ignored.

Specified as: a fullword integer.

#### On Return

У

has the following meaning, where:

If  $init \neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, containing the results of the complex discrete Fourier transform of X. The output consists of n2 columns of data. The data in each column is stored with stride 1. Due to complex conjugate symmetry, the output consists of only the first ((n1)/2)+1 rows of the array—that is,  $y_{k1,k2}$ , where k1 = 0, 1, ..., (n1)/2 and k2 = 0, 1, ..., n2-1.

Returned as: an *inc2y* by (at least) *n2* array, containing numbers of the data type indicated in Table 132 on page 792. This array must be aligned on a doubleword boundary.

### aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

# Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. If you specify the same array for X and Y, then *inc2x* must equal (2)(*inc2y*). In this case, output overwrites input. If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 3. For selecting optimal strides (or leading dimensions *inc2x* and *inc2y*) for your input and output arrays, you should use "STRIDE—Determine the Stride Value

for Optimal Performance in Specified Fourier Transform Subroutines" on page 969. Example 5 in the STRIDE subroutine description explains how it is used for these subroutines.

4. Be sure to align array X on a doubleword boundary, and specify an even number for *inc2x*, if possible.

**Processor-Independent Formulas for SRCFT2 for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on *n1* and *n2*.

#### NAUX1 Formulas

```
If \max(n1/2, n2) \le 8192, use naux1 = 45000.
If \max(n1/2, n2) > 8192, use naux1 = 40000 + 0.82n1 + 1.14n2.
```

### NAUX2 Formulas

```
If n1 \le 16384 and n2 < 252, use naux2 = 20000.

If n1 > 16384 and n2 < 252, use naux2 = 20000+0.57n1.

If n2 \ge 252, add the following to the above storage requirements: (n2+256)(1.14+s)

where s = \min(64, 1+n1/2).
```

**Processor-Independent Formulas for DRCFT2 for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on *n1* and *n2*.

#### NAUX1 Formulas

```
If n \le 2048, use naux1 = 42000.

If n > 2048, use naux1 = 40000+1.64n1+2.28n2, where n = \max(n1/2, n2).
```

# NAUX2 Formulas

```
If n1 \le 4096 and n2 < 252, use naux2 = 20000.

If n1 > 4096 and n2 < 252, use naux2 = 20000+1.14n1.

If n2 \ge 252, add the following to the above storage requirements: ((2)n2+256) (2.28+s) where s = \min(64, 1+n1/2).
```

**Function:** The two-dimensional complex conjugate even discrete Fourier transform of real data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(lsign)j1k1} W_{n2}^{(lsign)j2k2}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$ 

where:

$$W_{n1} = e^{-2\pi (\sqrt{-1})/n1}$$

$$W_{n2} = e^{-2\pi (\sqrt{-1})/n2}$$

and where:

 $x_{j1,j2}$  are elements of array X.  $y_{k1,k2}$  are elements of array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

The output in array Y is complex. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/((n1)(n2)) and isign being negative. See references [1], [4], [19], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

#### **Error Conditions**

*Resource Errors:* Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- $1. \ n1 > 37748736$
- 2. n2 > 37748736
- 3. inc2x < n1
- 4. inc2y < (n1)/2+1
- 5. scale = 0.0
- 6. isign = 0
- 7. The subroutine has not been initialized with the present arguments.
- 8. The length of one of the transforms in *n1* or *n2* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 9. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- Error 2015 is recoverable or naux2≠0, and naux2 is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to compute a two-dimensional transform. The arrays are declared as follows:

```
COMPLEX*8 Y(0:6,0:7)
REAL*4 X(0:11,0:7)
REAL*8 AUX1(1000), AUX2(1000), AUX3(1)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

INIT = 1(for initialization)
INIT = 0(for computation)
SCALE = 1.0

X is an array with 12 rows and 8 columns having 1.0 in location X(0,0) and 0.0 in all others.

Output: Y is an array with 7 rows and 8 columns with (1.0, 0.0) in all locations.

**Example 2:** This example shows another transform computation with different data using the same initialized array AUX1 in Example 1.

### Call Statement and Input

SCALE = 1.0

X is an array with 12 rows and 8 columns with 1.0 in all locations.

*Output:* Y is an array with 7 rows and 8 columns having (96.0, 0.0) in location Y(0,0) and (0.0, 0.0) in all others.

**Example 3:** This example shows the same array being used for input and output, where isign = -1 and scale = 1/((N1)(N2)). The arrays are declared as follows:

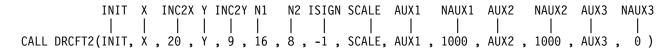
```
COMPLEX*16 Y(0:8,0:7)
REAL*8 X(0:19,0:7)
REAL*8 AUX1(1000), AUX2(1000), AUX3(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage.

```
EQUIVALENCE (X,Y)
```

This requires  $inc2x \ge 2(inc2y)$ . First, initialize AUX1 using the calling sequence shown below with INIT  $\ne 0$ . Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input



INIT = 1(for initialization)
INIT = 0(for computation)
SCALE = 1.0/128.0

```
2.0
                                      2.0 -2.0
                                                  -2.0
                2.0 -2.0 -2.0
                                  2.0
          2.0 -2.0 -2.0
                           2.0
                                 2.0 -2.0
                                            -2.0
                                                   2.0
         -2.0 -2.0
                     2.0
                            2.0
                                      -2.0
                                             2.0
                                -2.0
                                                   2.0
                2.0
         -2.0
                     2.0
                          -2.0
                                -2.0
                                       2.0
                                             2.0
                                                  -2.0
                2.0
                    -2.0
          2.0
                          -2.0
                                 2.0
                                       2.0
                                            -2.0
                                                  -2.0
          2.0 -2.0 -2.0
                           2.0
                                 2.0
                                      -2.0
                                            -2.0
                                                   2.0
         -2.0
               -2.0
                     2.0
                           2.0
                                -2.0
                                      -2.0
                                             2.0
                                                   2.0
         -2.0
                2.0
                      2.0
                          -2.0
                                 -2.0
                                       2.0
                                             2.0
                                                  -2.0
          2.0
                2.0
                    -2.0
                          -2.0
                                  2.0
                                       2.0
                                            -2.0
                                                  -2.0
                     -2.0
                           2.0
                                      -2.0
Χ
          2.0
               -2.0
                                 2.0
                                            -2.0
                                                   2.0
         -2.0
              -2.0
                     2.0
                           2.0 -2.0
                                      -2.0
                                             2.0
                                                   2.0
                2.0
                                       2.0
         -2.0
                      2.0
                          -2.0 -2.0
                                             2.0
                                                  -2.0
          2.0
                2.0
                    -2.0
                          -2.0
                                 2.0
                                       2.0
                                            -2.0
                                                  -2.0
                     -2.0
          2.0
               -2.0
                           2.0
                                 2.0
                                      -2.0
                                            -2.0
                                                   2.0
         -2.0 -2.0
                      2.0
                           2.0 -2.0
                                      -2.0
                                             2.0
                                                   2.0
         -2.0
                2.0
                      2.0 -2.0 -2.0
                                      2.0
                                             2.0 -2.0
```

*Output:* Y is an array with 9 rows and 8 columns having (1.0, 1.0) in location Y(4,2) and (0.0, 0.0) in all others.

# SCRFT2 and DCRFT2—Complex-to-Real Fourier Transform in Two Dimensions

These subroutines compute the two-dimensional discrete Fourier transform of complex conjugate even data in a two-dimensional array.

Table 133. Data Types		
Х	Y, scale	Subroutine
Short-precision complex	Short-precision real	SCRFT2
Long-precision complex	Long-precision real	DCRFT2

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

# Syntax

Fortran	CALL SCRFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3)
	CALL DCRFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2)
C and C++	scrft2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	dcrft2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);
PL/I	CALL SCRFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2, aux3, naux3);
	CALL DCRFT2 (init, x, inc2x, y, inc2y, n1, n2, isign, scale, aux1, naux1, aux2, naux2);

# On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the discrete Fourier transform of the given array is computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

X

is the array X, containing n2 columns of data to be transformed. Due to complex conjugate symmetry, the input consists of only the first ((n1)/2)+1 rows of the array—that is,  $x_{j1,j2}$ , j1 = 0, 1, ..., (n1)/2, j2 = 0, 1, ..., n2-1. The data in each column is stored with stride 1.

Specified as: an *inc2x* by (at least) *n2* array, containing numbers of the data type indicated in Table 133. This array must be aligned on a doubleword boundary.

# inc2x

is the leading dimension (stride between columns) of array X. Specified as: a fullword integer;  $inc2x \ge ((n1)/2)+1$ .

```
See "On Return" on page 801.
inc2v
    is the leading dimension (stride between the columns) of array Y. Specified as:
    a fullword integer; inc2y \ge n1+2.
n1
    is the number of rows of data—that is, the length of the columns in array Y
   involved in the computation. The length of the columns in array X are (n1)/2+1.
    Specified as: a fullword integer; n1 \le 37748736 and must be one of the values
   listed in "Acceptable Lengths for the Transforms" on page 739. For all other
   values specified less than 37748736, you have the option of having the next
   larger acceptable value returned in this argument. For details, see "Providing a
    Correct Transform Length to ESSL" on page 38.
n2
    is the number of columns of data—that is, the length of the rows in arrays X
   and Y involved in the computation. Specified as: a fullword integer;
   n2 ≤ 37748736 and must be one of the values listed in "Acceptable Lengths
   for the Transforms" on page 739. For all other values specified less than
    37748736, you have the option of having the next larger acceptable value
   returned in this argument. For details, see "Providing a Correct Transform
   Length to ESSL" on page 38.
isign
    controls the direction of the transform, determining the sign Isign of the
    exponents of W_{n1} and W_{n2}, where:
   If isign = positive value, Isign = + (transforming time to frequency).
   If isign = negative value, Isign = - (transforming frequency to time).
    Specified as: a fullword integer; isign > 0 or isign < 0.
scale
   is the scaling constant scale. See "Function" on page 802 for its usage.
    Specified as: a number of the data type indicated in Table 133 on page 799,
    where scale > 0.0 or scale < 0.0.
aux1
    is the working storage for this subroutine, where:
   If init \neq 0, the working storage is computed.
   If init = 0, the working storage is used in the computation of the Fourier
   transforms.
    Specified as: an area of storage, containing naux1 long-precision real numbers.
naux1
    is the number of doublewords in the working storage specified in aux. Specified
    as: a fullword integer: naux1 ≥ (minimum value required for successful
    processing). To determine a sufficient value, use the processor-independent
   formulas. For all other values specified less than the minimum value, you have
```

aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

see "Using Auxiliary Storage in ESSL" on page 31.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

the option of having the minimum value returned in this argument. For details,

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

#### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCRFT2 and DCRFT2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, *naux2* ≥ (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### aux3

this argument is provided for migration purposes only and is ignored.

Specified as: an area of storage, containing *naux3* long-precision real numbers. *naux3* 

this argument is provided for migration purposes only and is ignored.

Specified as: a fullword integer.

#### On Return

У

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is the array Y, containing n1 rows and n2 columns of results of the real discrete Fourier transform of X. The data in each column of Y is stored with stride 1.

Returned as: an *inc2y* by (at least) *n2* array, containing numbers of the data type indicated in Table 133 on page 799. See "Notes" for more details. *aux1* 

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

#### Notes

- aux1 should **not** be used by the calling program between program calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. If you specify the same array for X and Y, then (2)(inc2x) must equal inc2y. In this case, output overwrites input. If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- For selecting optimal strides (or leading dimensions inc2x and inc2y) for your input and output arrays, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on

page 969. Example 6 in the STRIDE subroutine description explains how it is used for these subroutines.

4. Be sure to align array Y on a doubleword boundary, and specify an even number for inc2y, if possible.

Processor-Independent Formulas for SCRFT2 for NAUX1 and NAUX2: The required values of naux1 and naux2 depend on n1 and n2.

# NAUX1 Formulas

```
If \max(n1/2, n2) \le 8192, use naux1 = 45000.
If \max(n1/2, n2) > 8192, use naux1 = 40000+0.82n1+1.14n2.
```

#### NAUX2 Formulas

```
If n1 \le 16384 and n2 < 252, use naux2 = 20000.
If n1 > 16384 and n2 < 252, use naux2 = 20000+0.57n1.
If n2 \ge 252, add the following to the above storage requirements:
    (n2+256)(1.14+s)
    where s = \min(64, 1+n1/2).
```

Processor-Independent Formulas for DCRFT2 for NAUX1 and NAUX2: The required values of naux1 and naux2 depend on n1 and n2.

# NAUX1 Formulas

```
If n \le 2048, use naux1 = 42000.
If n > 2048, use naux1 = 40000+1.64n1+2.28n2,
where n = \max(n1/2, n2).
```

#### NAUX2 Formulas

```
If n1 \le 4096 and n2 < 252, use naux2 = 20000.
If n1 > 4096 and n2 < 252, use naux2 = 20000+1.14n1.
If n2 \ge 252, add the following to the above storage requirements:
    ((2)n2+256) (2.28+s)
    where s = \min(64, 1+n1/2).
```

Function: The two-dimensional discrete Fourier transform of complex conjugate even data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2} = scale \sum_{j1=0}^{n1-1} \sum_{j2=0}^{n2-1} x_{j1,j2} W_{n1}^{(Isign)j1k1} W_{n2}^{(Isign)j2k2}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$ 

where:

$$W_{n1} = e^{-2\pi(\sqrt{-1})/n1}$$
  

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

and where:

 $x_{j1,j2}$  are elements of array X.  $y_{k1,k2}$  are elements of array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

Because of the complex conjugate symmetry, the output in array Y is real. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/((n1)(n2)) and isign being negative. See references [1], [4], and [20].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the Fourier transform.

#### **Error Conditions**

*Resource Errors:* Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. *n1* > 37748736
- 2. n2 > 37748736
- 3. inc2x < (n1)/2+1
- 4. inc2y < n1+2
- 5. scale = 0.0
- 6. isign = 0
- 7. The subroutine has not been initialized with the present arguments.
- 8. The length of one of the transforms in *n1* or *n2* is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 9. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- Error 2015 is recoverable or naux2≠0, and naux2 is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to compute a two-dimensional transform. The arrays are declared as follows:

```
REAL*4 Y(0:13,0:7)
COMPLEX*8 X(0:6,0:7)
REAL*8 AUX1(1000), AUX2(1000), AUX3(1)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

INIT = 1(for initialization)
INIT = 0(for computation)

SCALE = 1.0/96.0

X is an array with 7 rows and 8 columns with (1.0, 0.0) in all locations.

# Output

**Example 2:** This example shows another transform computation with different data using the same initialized array AUX1 in Example 1.

#### Call Statement and Input

SCALE = 1.0/96.0

X is an array with 7 rows and 8 columns having (96.0, 0.0) in location X(0,0) and (0.0, 0.0) in all others.

Output

```
1.0 1.0 1.0
         1.0 1.0 1.0
                      1.0 1.0 1.0
                                     1.0
                                          1.0
         1.0
                       1.0 1.0 1.0
                                1.0
                                          1.0
                       1.0
                           1.0
                                     1.0
                       1.0 1.0 1.0
             1.0
                  1.0
Υ
                                          1.0
         1.0
             1.0
                 1.0
                       1.0 1.0 1.0
                       1.0 1.0
         1.0
             1.0
                  1.0
                       1.0 1.0
                                1.0
                                     1.0
                  1.0
                       1.0
                           1.0
                                1.0
             1.0
                  1.0
                       1.0 1.0
                               1.0
                                     1.0
                                          1.0
                       1.0
                           1.0
                                1.0
                                     1.0
                                          1.0
```

**Example 3:** This example shows the same array being used for input and output. The arrays are declared as follows:

```
REAL*8 Y(0:17,0:7)
COMPLEX*16 X(0:8,0:7)
REAL*8 AUX1(1000), AUX2(1000), AUX3(1)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage.

```
EQUIVALENCE (X,Y)
```

This requires inc2y = 2(inc2x). First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

# Call Statement and Input

= 1.0

X is an array with 9 rows and 8 columns having (1.0, 1.0) in location X(4,2) and (0.0, 0.0) in all others.

# Output

SCALE

# **SCRFT2 and DCRFT2**

		Γ							-	1
		2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	İ
		2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	١
		-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	١
		-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	ĺ
		2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	İ
		2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	İ
		-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	İ
		-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	İ
Υ	=	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	İ
		2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	İ
		-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	İ
		-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	١
		2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	١
		2.0	-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	ĺ
		-2.0	-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	İ
		-2.0	2.0	2.0	-2.0	-2.0	2.0	2.0	-2.0	İ
						•			•	ĺ
			•	•	•	•	•	•	•	I
		L							-	

# SCFT3 and DCFT3—Complex Fourier Transform in Three Dimensions

These subroutines compute the three-dimensional discrete Fourier transform of complex data.

Table 134. Data Types		
X, Y	scale	Subroutine
Short-precision complex	Short-precision real	SCFT3
Long-precision complex	Long-precision real	DCFT3

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

# Syntax

Fortran	CALL SCFT3   DCFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux)
C and C++	scft3   dcft3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);
PL/I	CALL SCFT3   DCFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);

# On Entry

Χ

is the array X, containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in X(j1+j2(inc2x)+j3(inc3x)) for j1=0,1,...,n1-1,j2=0,1,...,n2-1, and j3=0,1,...,n3-1. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x(\ge n1)$ , and  $inc3x(\ge (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 134. This array must be aligned on a doubleword boundary. If the array is dimensioned X(LDA1,LDA2,LDA3), then LDA1 = inc2x, (LDA1)(LDA2) = inc3x, and  $LDA3 \ge n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes" on page 809.

inc2x

is the stride between the elements in array X for the second dimension. Specified as: a fullword integer;  $inc2x \ge n1$ .

inc3x

is the stride between the elements in array X for the third dimension. Specified as: a fullword integer;  $inc3x \ge (n2)(inc2x)$ .

See "On Return" on page 808.

inc2y

is the stride between the elements in array Y for the second dimension. Specified as: a fullword integer;  $inc2y \ge n1$ .

inc3v

is the stride between the elements in array Y for the third dimension. Specified as: a fullword integer;  $inc3y \ge (n2)(inc2y)$ .

n1

is the length of the first dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n1 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n2

is the length of the second dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n2 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n3

is the length of the third dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n3 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

isign

controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:

If isign = positive value, Isign = + (transforming time to frequency).

If isign = negative value, Isign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

scale

is the scaling constant scale. See "Function" on page 810 for its usage. Specified as: a number of the data type indicated in Table 134 on page 807, where scale > 0.0 or scale < 0.0.

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine.

Specified as: an area of storage, containing *naux* long-precision real numbers. On output, the contents are overwritten.

naux

is the number of doublewords in the working storage specified in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SCFT3 and DCFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

On Return

У

is the array Y, containing the elements resulting from the three-dimensional discrete Fourier transform of the data in X. Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in Y(k1+k2(inc2y)+k3(inc3y)) for k1=0,1,...,n1-1,k2=0,1,...,n2-1, and k3=0,1,...,n3-1. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y(\ge n1)$ , and  $inc3y(\ge (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 134 on page 807. This array must be aligned on a doubleword boundary. If the array is dimensioned Y(LDA1,LDA2,LDA3), then LDA1 = inc2y, (LDA1)(LDA2) = inc3y, and  $LDA3 \ge n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes."

#### Notes

1. If you specify the same array for X and Y, then *inc2x* must be greater than or equal to *inc2y*, and *inc3x* must be greater than or equal to *inc3y*. In this case, output overwrites input. When using the ESSL SMP library in a multithreaded environment, if *inc2x* > *inc2y* or *inc3x* > *inc3y*, these subroutines run on a single thread and issue an attention message.

If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

2. You should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969 to determine the optimal values for the strides *inc2y* and *inc3y* for your output array. The strides for your input array do not affect performance. Example 7 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

**Processor-Independent Formulas for SCFT3 for NAUX:** Use the following formulas for calculating *naux*:

```
1. If \max(n2, n3) < 252 and:

If n1 \le 8192, use naux = 60000.

If n1 > 8192, use naux = 60000+2.28n1.

2. If n2 \ge 252, n3 < 252, and:

If n1 \le 8192, use naux = 60000+\lambda.

If n1 > 8192, use naux = 60000+2.28n1+\lambda, where \lambda = (n2+256)(s+2.28) and s = \min(64, n1).

3. If n2 < 252, n3 \ge 252, and:

If n1 \le 8192, use naux = 60000+\psi.

If n1 > 8192, use naux = 60000+\psi.

If n1 > 8192, use naux = 60000+2.28n1+\psi, where \psi = (n3+256)(s+2.28) and s = \min(64, (n1)(n2)).
```

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

**Processor-Independent Formulas for DCFT3 for NAUX:** Use the following formulas for calculating *naux*:

1. If  $\max(n2, n3) < 252$  and:

If  $n1 \le 2048$ , use naux = 60000.

If n1 > 2048, use naux = 60000+4.56n1.

2. If  $n2 \ge 252$ , n3 < 252, and:

If  $n1 \le 2048$ , use  $naux = 60000+\lambda$ .

If n1 > 2048, use  $naux = 60000+4.56n1+\lambda$ , where  $\lambda = ((2)n2+256)(s+4.56)$  and  $s = \min(64, n1)$ .

3. If n2 < 252,  $n3 \ge 252$ , and:

If  $n1 \le 2048$ , use  $naux = 60000+\psi$ . If n1 > 2048, use  $naux = 60000+4.56n1+\psi$ , where  $\psi = ((2)n3+256)(s+4.56)$  and  $s = \min(64, (n1)(n2))$ .

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

**Function:** The three-dimensional discrete Fourier transform of complex data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2,k3} = scale \sum_{jl=0}^{nl-1} \sum_{j2=0}^{n2-1} \sum_{j3=0}^{n3-1} x_{jl,j2,j3} \ W_{nl}^{(lsign)j1kl} \ W_{n2}^{(lsign)j2k2} \ W_{n3}^{(lsign)j3k3}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$   
 $k3 = 0, 1, ..., n3-1$ 

where:

$$W_{nI} = e^{-2\pi(\sqrt{-1})/nI}$$

$$W_{n2} = e^{-2\pi(\sqrt{-1})/n2}$$

$$W_{n3} = e^{-2\pi(\sqrt{-1})/n3}$$

and where:

 $x_{j1,j2,j3}$  are elements of array X.  $y_{k1,k2,k3}$  are elements of array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/((n1)(n2)(n3)) and isign being negative. See references [1], [4], [5], [19], and [20].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. n1 > 37748736
- 2. *n2* > 37748736
- 3. n3 > 37748736
- 4. inc2x < n1
- 5. inc3x < (n2)(inc2x)
- 6. inc2y < n1
- 7. inc3y < (n2)(inc2y)
- 8. scale = 0.0
- 9. isign = 0
- 10. The length of one of the transforms in *n*1, *n*2, or *n*3 is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 11. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example shows how to compute a three-dimensional transform. In this example, INC2X ≥ INC2Y and INC3X ≥ INC3Y, so that the same array can be used for both input and output. The STRIDE subroutine is called to select good values for the INC2Y and INC3Y strides. (As explained below, STRIDE is not called for INC2X and INC3X.) Using the transform lengths (N1 = 32, N2 = 64, and N3 = 40) along with the output data type (short-precision complex: 'C'), STRIDE is called once for each stride needed. First, it is called for INC2Y:

```
CALL STRIDE (N2,N1,INC2Y,'C',0)
```

The output value returned for INC2Y is 32. Then STRIDE is called again for INC3Y:

```
CALL STRIDE (N3,N2*INC2Y,INC3Y,'C',0)
```

The output value returned for INC3Y is 2056. Because INC3Y is not a multiple of INC2Y, Y is not declared as a three-dimensional array. It is declared as a two-dimensional array, Y(INC3Y,N3).

To equivalence the X and Y arrays requires  $INC2X \ge INC2Y$  and  $INC3X \ge INC3Y$ . Therefore, INC2X is set equal to INC2Y(=32). Also, to declare the X array as a three-dimensional array, INC3X must be a multiple of INC2X. Therefore, its value is set as INC3X = (65)(INC2X) = 2080.

The arrays are declared as follows:

```
COMPLEX*8 X(32,65,40),Y(2056,40)
REAL*8 AUX(30000)
```

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

EQUIVALENCE (X,Y)

Call Statement and Input

```
X INC2X INC3X Y INC2Y INC3Y N1 N2
                                                                            N3 ISIGN SCALE
                                                                                                    AUX
                                                                                                            NAUX
CALL SCFT3( \dot{X} , 3\dot{2} , 20\dot{8}0 , \dot{Y} , 3\dot{2} , 20\dot{5}6 , 3\dot{2} , 6\dot{4} , 4\dot{0} , \dot{1} , SCALE , AUX , 30\dot{0}00)
```

SCALE = 1.0

X has (1.0,2.0) in location X(1,1,1) and (0.0,0.0) in all other locations.

Output: Y has (1.0,2.0) in locations Y(ij,k), where ij = 1, 2048 and j = 1, 40. It remains unchanged elsewhere.

# SRCFT3 and DRCFT3—Real-to-Complex Fourier Transform in Three Dimensions

These subroutines compute the three-dimensional discrete Fourier transform of real data in a three-dimensional array.

Table 135. Data Types		
X, scale	Υ	Subroutine
Short-precision real	Short-precision complex	SRCFT3
Long-precision real	Long-precision complex	DRCFT3

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

# Syntax

Fortran	CALL SRCFT3   DRCFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux)
C and C++	srcft3   drcft3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);
PL/I	CALL SRCFT3   DRCFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);

# On Entry

Χ

is the array X, containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in X(j1+j2(inc2x)+j3(inc3x)) for j1=0,1,...,n1-1,j2=0,1,...,n2-1, and j3=0,1,...,n3-1. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x(\ge n1)$ , and  $inc3x(\ge (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 135. If the array is dimensioned X(LDA1,LDA2,LDA3), then LDA1 = inc2x, (LDA1)(LDA2) = inc3x, and  $LDA3 \ge n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes" on page 815.

inc2x

is the stride between the elements in array X for the second dimension. Specified as: a fullword integer;  $inc2x \ge n1$ .

inc3x

is the stride between the elements in array X for the third dimension. Specified as: a fullword integer;  $inc3x \ge (n2)(inc2x)$ .

See "On Return" on page 814.

inc2y

is the stride between the elements in array Y for the second dimension. Specified as: a fullword integer;  $inc2y \ge n1/2+1$ .

inc3y

is the stride between the elements in array Y for the third dimension. Specified as: a fullword integer;  $inc3y \ge (n2)(inc2y)$ .

n1

is the length of the first dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n1 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n2

is the length of the second dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n2 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n3

is the length of the third dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n3 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

isign

controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:

If isign = positive value, Isign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

scale

is the scaling constant scale. See "Function" on page 816 for its usage. Specified as: a number of the data type indicated in Table 135 on page 813, where scale > 0.0 or scale < 0.0.

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine.

Specified as: an area of storage, containing *naux* long-precision real numbers. On output, the contents are overwritten.

naux

is the number of doublewords in the working storage specified in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SRCFT3 and DRCFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

On Return

V

is the array Y, containing the elements resulting from the three-dimensional discrete Fourier transform of the data in X. Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in Y(k1+k2(inc2y)+k3(inc3y)) for k1=0,1,...,n1/2, k2=0,1,...,n2-1, and k3=0,1,...,n3-1. Due to complex conjugate symmetry, the output consists of only the first n1/2+1 values along the first dimension of the array, for k1=0,1,...,n1/2. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y(\ge n1/2+1)$ , and  $inc3y(\ge (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 135 on page 813. This array must be aligned on a doubleword boundary. If the array is dimensioned Y(LDA1,LDA2,LDA3), then LDA1 = inc2y, (LDA1)(LDA2) = inc3y, and  $LDA3 \ge n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes."

#### Notes

- 1. If you specify the same array for X and Y, then inc2x must be greater than or equal to (2)(inc2y), and inc3x must be greater than or equal to (2)(inc3y). In this case, output overwrites input. When using the ESSL SMP library in a multithreaded environment, if inc2x > (2)(inc2y) or inc3x > (2)(inc3y), these subroutines run on a single thread and issue an attention message.
  - If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. To achieve the best performance, you should align array X on a doubleword boundary, and *inc2x* and *inc3x* should be even numbers. The strides for your input array do not affect performance as long as they are even numbers. In addition, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969 to determine the optimal values for the strides *inc2y* and *inc3y* for your output array. Example 8 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

**Processor-Independent Formulas for SRCFT3 for NAUX:** Use the following formulas for calculating *naux*:

```
1. If \max(n2, n3) < 252 and:
```

```
If n1 \le 16384, use naux = 65000.
If n1 > 16384, use naux = 60000+1.39n1.
```

2. If  $n2 \ge 252$ , n3 < 252, and:

```
If n1 \le 16384, use naux = 65000 + \lambda.

If n1 > 16384, use naux = 60000 + 1.39n1 + \lambda,

where \lambda = (n2 + 256)(s + 2.28) and s = \min(64, 1 + n1/2).
```

3. If n2 < 252,  $n3 \ge 252$ , and:

```
If n1 \le 16384, use naux = 65000+\psi.

If n1 > 16384, use naux = 60000+1.39n1+\psi,

where \psi = (n3+256)(s+2.28) and s = \min(64, (n2)(1+n1/2)).
```

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

If *inc2x* or *inc3x* is an odd number, or if array X is not aligned on a doubleword boundary, you should add the following amount to all the formulas given above:

$$n2(1+n1/2)$$

**Processor-Independent Formulas for DRCFT3 for NAUX:** Use the following formulas for calculating *naux*:

1. If  $\max(n2, n3) < 252$  and:

If 
$$n1 \le 4096$$
, use  $naux = 62000$ .  
If  $n1 > 4096$ , use  $naux = 60000+2.78n1$ .

2. If  $n2 \ge 252$ , n3 < 252, and:

If 
$$n1 \le 4096$$
, use  $naux = 62000 + \lambda$ .  
If  $n1 > 4096$ , use  $naux = 60000 + 2.78n1 + \lambda$ , where  $\lambda = ((2)n2 + 256)(s + 4.56)$  and  $s = \min(64, n1/2)$ .

3. If n2 < 252,  $n3 \ge 252$ , and:

If 
$$n1 \le 4096$$
, use  $naux = 62000+\psi$ .  
If  $n1 > 4096$ , use  $naux = 60000+2.78n1+\psi$ , where  $\psi = ((2)n3+256)(s+4.56)$  and  $s = \min(64, n2(1+n1/2))$ .

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

**Function:** The three-dimensional complex conjugate even discrete Fourier transform of real data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2,k3} = scale \sum_{jl=0}^{nl-1} \sum_{ij=0}^{n2-1} \sum_{j3=0}^{n3-1} x_{jl,j2,j3} W_{nl}^{(lsign)j1kl} W_{n2}^{(lsign)j2k2} W_{n3}^{(lsign)j3k3}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$   
 $k3 = 0, 1, ..., n3-1$ 

where:

$$W_{nI} = e^{-2\pi \left(\sqrt{-1}\right)/nI}$$

$$W_{n2} = e^{-2\pi \left(\sqrt{-1}\right)/n2}$$

$$W_{n3} = e^{-2\pi \left(\sqrt{-1}\right)/n3}$$

and where:

 $x_{j1,j2,j3}$  are elements of array X.  $y_{k1,k2,k3}$  are elements of array Y. Isign is + or – (determined by argument isign). scale is a scalar value.

The output in array Y is complex. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with scale = 1.0/((n1)(n2)(n3)) and isign being negative. See references [1], [4], [5], [19], and [20].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

# Input-Argument Errors

- 1. n1 > 37748736
- 2. n2 > 37748736
- 3. n3 > 37748736
- 4. inc2x < n1
- 5. inc3x < (n2)(inc2x)
- 6. inc2y < n1/2+1
- 7. inc3y < (n2)(inc2y)
- 8. scale = 0.0
- 9. isign = 0
- 10. The length of one of the transforms in *n*1, *n*2, or *n*3 is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 11. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example shows how to compute a three-dimensional transform. In this example, INC2X  $\geq$  (2)(INC2Y) and INC3X  $\geq$  (2)(INC3Y), so that the same array can be used for both input and output. The STRIDE subroutine is called to select good values for the INC2Y and INC3Y strides. Using the transform lengths (N1 = 32, N2 = 64, and N2 = 40) along with the output data type (short-precision complex: 'C'), STRIDE is called once for each stride needed. First, it is called for INC2Y:

```
CALL STRIDE (N2, N1/2+1, INC2Y, 'C', 0)
```

The output value returned for INC2Y is 17. (This value is equal to N1/2+1.) Then STRIDE is called again for INC3Y:

```
CALL STRIDE (N3, N2*INC2Y, INC3Y, 'C', 0)
```

The output value returned for INC3Y is 1088. Because INC3Y is a multiple of INC2Y—that is, INC3Y = (N2)(INC2Y)—Y is declared as a three-dimensional array, Y(17,64,40). (In general, for larger arrays, these types of values for INC2Y and INC3Y are not returned by STRIDE, and you are probably not able to declare Y as a three-dimensional array.)

To equivalence the X and Y arrays requires  $INC2X \ge (2)(INC2Y)$  and  $INC3X \ge (2)(INC3Y)$ . Therefore, the values INC2X = (2)(INC2Y) = 34 and INC3X = (2)(INC3Y) = 2176 are set, and X is declared as a three-dimensional array, X(34,64,40).

The arrays are declared as follows:

REAL\*4 X(34,64,40)COMPLEX\*8 Y(17,64,40) REAL\*8 AUX (32000)

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

EQUIVALENCE (X,Y)

# Call Statement and Input

SCALE = 1.0

X has 1.0 in location X(1,1,1) and 0.0 in all other locations.

Output: Y has (1.0,0.0) in all locations.

# SCRFT3 and DCRFT3—Complex-to-Real Fourier Transform in Three Dimensions

These subroutines compute the three-dimensional discrete Fourier transform of complex conjugate even data in a three-dimensional array.

Table 136. Data Types		
Х	Y, scale	Subroutine
Short-precision complex	Short-precision real	SCRFT2
Long-precision complex	Long-precision real	DCRFT2

**Note:** For each use, only one invocation of this subroutine is necessary. The initialization phase, preparing the working storage, is a relatively small part of the total computation, so it is performed on each invocation.

# Syntax

Fortran	CALL SCRFT3   DCRFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux)
C and C++	scrft3   dcrft3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);
PL/I	CALL SCRFT3   DCRFT3 (x, inc2x, inc3x, y, inc2y, inc3y, n1, n2, n3, isign, scale, aux, naux);

# On Entry

Χ

is the array X, containing the three-dimensional data to be transformed, where each element  $x_{j1,j2,j3}$ , using zero-based indexing, is stored in X(j1+j2(inc2x)+j3(inc3x)) for j1=0,1,...,n1/2,j2=0,1,...,n2-1, and j3=0,1,...,n3-1. Due to complex conjugate symmetry, the input consists of only the first n1/2+1 values along the first dimension of the array, for j1=0,1,...,n1/2. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2x(\ge n1/2+1)$ , and  $inc3x(\ge (n2)(inc2x))$ , respectively.

Specified as: an array, containing numbers of the data type indicated in Table 136. This array must be aligned on a doubleword boundary. If the array is dimensioned X(LDA1,LDA2,LDA3), then LDA1 = inc2x, (LDA1)(LDA2) = inc3x, and  $LDA3 \ge n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes" on page 821.

inc2x

is the stride between the elements in array X for the second dimension. Specified as: a fullword integer;  $inc2x \ge n1/2+1$ .

inc3x

is the stride between the elements in array X for the third dimension. Specified as: a fullword integer;  $inc3x \ge (n2)(inc2x)$ .

See "On Return" on page 820.

inc2y

is the stride between the elements in array Y for the second dimension. Specified as: a fullword integer;  $inc2y \ge n1+2$ .

inc3y

is the stride between the elements in array Y for the third dimension. Specified as: a fullword integer;  $inc3y \ge (n2)(inc2y)$ .

n1

is the length of the first dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n1 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n2

is the length of the second dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n2 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

n3

is the length of the third dimension of the three-dimensional data in the array to be transformed. Specified as: a fullword integer;  $n3 \le 37748736$  and must be one of the values listed in "Acceptable Lengths for the Transforms" on page 739. For all other values specified less than 37748736, you have the option of having the next larger acceptable value returned in this argument. For details, see "Providing a Correct Transform Length to ESSL" on page 38.

isign

controls the direction of the transform, determining the sign *Isign* of the exponents of  $W_{n1}$ ,  $W_{n2}$ , and  $W_{n3}$ , where:

If isign = positive value, Isign = + (transforming time to frequency).

If isign = negative value, lsign = - (transforming frequency to time).

Specified as: a fullword integer; isign > 0 or isign < 0.

scale

is the scaling constant scale. See "Function" on page 822 for its usage. Specified as: a number of the data type indicated in Table 136 on page 819, where scale > 0.0 or scale < 0.0.

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is a storage work area used by this subroutine. Specified as: an area of storage, containing *naux* long-precision real numbers. On output, the contents are overwritten.

naux

is the number of doublewords in the working storage specified in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SCRFT3 and DCRFT3 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

On Return

У

is the array Y, containing the elements resulting from the three-dimensional discrete Fourier transform of the data in X. Each element  $y_{k1,k2,k3}$ , using zero-based indexing, is stored in Y(k1+k2(inc2y)+k3(inc3y)) for k1=0,1,...,n1-1,k2=0,1,...,n2-1, and k3=0,1,...,n3-1. The strides for the elements in the first, second, and third dimensions are assumed to be 1,  $inc2y (\ge n1+2)$ , and  $inc3y (\ge (n2)(inc2y))$ , respectively.

Returned as: an array, containing numbers of the data type indicated in Table 136 on page 819. If the array is dimensioned Y(LDA1,LDA2,LDA3), then LDA1 = inc2y, (LDA1)(LDA2) = inc3y, and LDA3  $\geq n3$ . For information on how to set up this array, see "Setting Up Your Data" on page 742. For more details, see "Notes."

#### Notes

- If you specify the same array for X and Y, then inc2y must equal (2)(inc2x) and inc3y must equal (2)(inc3x). In this case, output overwrites input. If you specify different arrays X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. To achieve the best performance, you should align array Y on a doubleword boundary, and *inc2y* and *inc3y* should be even numbers. In addition, you should use "STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines" on page 969 to determine the optimal values for the strides *inc2y* and *inc3y* for your output array. To obtain the best performance, you should use *inc2x* = *inc2y*/2 and *inc3x* = *inc3y*/2. Example 9 in the STRIDE subroutine description explains how it is used for these subroutines. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

**Processor-Independent Formulas for SCRFT3 for Calculating NAUX:** Use the following formulas for calculating *naux*:

```
1. If \max(n2, n3) < 252 and:

If n1 \le 16384, use naux = 65000.

If n1 > 16384, use naux = 60000+1.39n1.

2. If n2 \ge 252, n3 < 252, and:

If n1 \le 16384, use naux = 65000+\lambda.

If n1 > 16384, use naux = 60000+1.39n1+\lambda, where \lambda = (n2+256)(s+2.28) and s = \min(64, 1+n1/2).

3. If n2 < 252, n3 \ge 252, and:

If n1 \le 16384, use naux = 65000+\psi.

If n1 > 16384, use naux = 60000+1.39n1+\psi, where \psi = (n3+256)(s+2.28) and s = \min(64, (n2)(1+n1/2)).
```

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

If *inc2y* or *inc3y* is an odd number, or if array Y is not aligned on a doubleword boundary, you should add the following amount to all the formulas given above:

```
(1+n1/2)(\max(n2, n3))
```

Processor-Independent Formulas for DCRFT3 for NAUX: Use the following formulas for calculating naux:

1. If  $\max(n2, n3) < 252$  and: If  $n1 \le 4096$ , use naux = 62000. If n1 > 4096, use naux = 60000+2.78n1. 2. If  $n2 \ge 252$ , n3 < 252, and: If  $n1 \le 4096$ , use  $naux = 62000 + \lambda$ . If n1 > 4096, use  $naux = 60000+2.78n1+\lambda$ , where  $\lambda = ((2)n2+256)(s+4.56)$ and  $s = \min(64, n1/2)$ . 3. If n2 < 252,  $n3 \ge 252$ , and:

> If  $n1 \le 4096$ , use  $naux = 62000 + \psi$ . If n1 > 4096, use  $naux = 60000+2.78n1+\psi$ , where  $\psi = ((2)n3+256)(s+4.56)$ and  $s = \min(64, n2(1+n1/2))$ .

4. If  $n2 \ge 252$  and  $n3 \ge 252$ , use the larger of the values calculated for cases 2 and 3 above.

Function: The three-dimensional discrete Fourier transform of complex conjugate even data in array X, with results going into array Y, is expressed as follows:

$$y_{k1,k2,k3} = scale \sum_{jl=0}^{nl-1} \sum_{i2=0}^{n2-1} \sum_{j3=0}^{n3-1} x_{jl,j2,j3} \ W_{nl}^{(lsign)j1kl} \ W_{n2}^{(lsign)j2k2} \ W_{n3}^{(lsign)j3k3}$$

for:

$$k1 = 0, 1, ..., n1-1$$
  
 $k2 = 0, 1, ..., n2-1$   
 $k3 = 0, 1, ..., n3-1$ 

where:

$$W_{nI} = e^{-2\pi \left(\sqrt{-1}\right)/nI}$$

$$W_{n2} = e^{-2\pi \left(\sqrt{-1}\right)/n2}$$

$$W_{n3} = e^{-2\pi \left(\sqrt{-1}\right)/n3}$$

and where:

 $x_{i1.i2.i3}$  are elements of array X.  $y_{k1,k2,k3}$  are elements of array Y. Isign is + or - (determined by argument isign). scale is a scalar value.

Because of the complex conjugate symmetry, the output in array Y is real. For scale = 1.0 and isign being positive, you obtain the discrete Fourier transform, a function of frequency. The inverse Fourier transform is obtained with

scale = 1.0/((n1)(n2)(n3)) and isign being negative. See references [1], [4], [5], [19], and [20].

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

### Input-Argument Errors

- 1. *n1* > 37748736
- 2. n2 > 37748736
- 3. n3 > 37748736
- 4. inc2x < n1/2+1
- 5. inc3x < (n2)(inc2x)
- 6. inc2y < n1+2
- 7. inc3y < (n2)(inc2y)
- 8. scale = 0.0
- 9. isign = 0
- 10. The length of one of the transforms in *n*1, *n*2, or *n*3 is not an allowable value. Return code 1 is returned if error 2030 is recoverable.
- 11. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example:** This example shows how to compute a three-dimensional transform. In this example, INC2Y = (2)(INC2X) and INC3Y = (2)(INC3X), so that the same array can be used for both input and output. The STRIDE subroutine is called to select good values for the INC2Y and INC3Y strides. (As explained below, STRIDE is not called for INC2X and INC3X.) Using the transform lengths (N1 = 32, N2 = 64, and N3 = 40) along with the output data type (short-precision real: 'S'), STRIDE is called once for each stride needed. First, it is called for INC2Y:

```
CALL STRIDE (N2, N1+2, INC2Y, 'S', 0)
```

The output value returned for INC2Y is 34. (This value is equal to N1+2.) Then STRIDE is called again for INC3Y:

```
CALL STRIDE (N3,N2*INC2Y,INC3Y,'S',0)
```

The output value returned for INC3Y is 2176. Because INC3Y is a multiple of INC2Y—that is, INC3Y = (N2)(INC2Y)—Y is declared as a three-dimensional array, Y(34,64,40). (In general, for larger arrays, these types of values for INC2Y and INC3Y are not returned by STRIDE, and you are probably not able to declare Y as a three-dimensional array.)

A good stride value for INC2X is INC2Y/2, and a good stride value for INC3X is INC3Y/2. Also, to equivalence the X and Y arrays requires INC2Y = (2)(INC2X) and INC3Y = (2)(INC3X). Therefore, the values INC2X = INC2Y/2 = 17 and INC3X = INC3Y/2 = 1088 are set, and X is declared as a three-dimensional array, X(17,64,40).

The arrays are declared as follows:

COMPLEX\*8 X(17,64,40) REAL\*4 Y(34,64,40)REAL\*8 AUX (32000)

Arrays X and Y are made equivalent by the following statement, making them occupy the same storage:

EQUIVALENCE (X,Y)

Call Statement and Input

X INC2X INC3X Y INC2Y INC3Y N1 N2 N3 ISIGN SCALE AUX NAUX CALL SCRFT3(  $\dot{X}$  ,  $\dot{17}$  ,  $\dot{1088}$  ,  $\dot{Y}$  ,  $\dot{34}$  ,  $\dot{2176}$  ,  $\dot{32}$  ,  $\dot{64}$  ,  $\dot{40}$  ,  $\dot{1}$  , SCALE , AUX , 32000)

> SCALE = 1.0

X has (1.0,0.0) in location X(1,1,1) and (0.0,0.0) in all other locations.

Output: Y has 1.0 in all locations.

# **Convolution and Correlation Subroutines**

This section contains the convolution and correlation subroutine descriptions.

# SCON and SCOR—Convolution or Correlation of One Sequence with One or More Sequences

These subroutines compute the convolutions and correlations of a sequence with one or more sequences using a direct method. The input and output sequences contain short-precision real numbers.

**Note:** These subroutines are considered obsolete. They are provided in ESSL only for compatibility with earlier releases. You should use SCOND, SCORD, SDCON, SDCOR, SCONF, and SCORF instead, because they provide **better performance**. For further details, see "Convolution and Correlation Considerations" on page 743.

# Syntax

Fortran	CALL SCON   SCOR (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2)
C and C++	scon   scor (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2);
PL/I	CALL SCON   SCOR (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2);

# On Entry

init

is a flag, where:

If  $init \neq 0$ , no computation is performed, error checking is performed, and the subroutine exits back to the calling program.

If init = 0, the convolutions or correlations of the sequence in h with the sequences in x are computed.

Specified as: a fullword integer. It can have any value.

h

is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequences in array X. Specified as: an array of (at least) length  $1+(N_h-1)|inc1h|$ , containing short-precision real numbers.

inc1h

is the stride between the elements within the sequence in array H. Specified as: a fullword integer; inc1h > 0.

Х

is the array X, consisting of m input sequences of length  $N_x$ , each to be convolved or correlated with the sequence in array H. Specified as: an array of (at least) length  $1 + (m-1)inc2x + (N_x-1)inc1x$ , containing short-precision real numbers.

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. Specified as: a fullword integer; inc2x > 0.

y See "On Return" on page 827.

inc1y

is the stride between the elements within each sequence in output array Y. Specified as: a fullword integer; inc1y > 0.

inc2y

is the stride between the first elements of each sequence in output array Y. Specified as: a fullword integer; inc2y > 0.

nh

is the number of elements,  $N_h$ , in the sequence in array H. Specified as: a fullword integer;  $N_h > 0$ .

nx

is the number of elements,  $N_x$ , in each sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

m

is the number of sequences in array X to be convolved or correlated. Specified as: a fullword integer; m > 0.

iy0

is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y. Specified as: a fullword integer. It can have any value.

ny

is the number of elements,  $N_y$ , in each sequence in array Y. Specified as: a fullword integer;  $N_y > 0$  for SCON and  $N_y \ge -N_h + 1$  for SCOR.

aux1

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

### naux1

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

aux2

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

naux2

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

### On Return

У

is array Y, consisting of m output sequences of length  $N_y$  that are the result of the convolutions or correlations of the sequence in array H with the sequences in array X. Returned as: an array of (at least) length  $1 + (m-1)inc2y + (N_v-1)inc1y$ , containing short-precision real numbers.

### Notes

- 1. Output should not overwrite input; that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. Auxiliary storage is not needed, but the arguments *aux1*, *naux1*, *aux2*, and *naux2* must still be specified. You can assign any values to these arguments.

**Function:** The convolutions and correlations of a sequence in array H with one or more sequences in array X are expressed as follows:

Convolutions for SCON:

$$y_{ki} = \sum_{j=\max(0,k-N_x+1)}^{\min(N_h-1,k)} h_j x_{k-j,i}$$

Correlations for SCOR:

$$y_{ki} = \sum_{j=\max(0,-k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j,i}$$

for:

$$k = iy0, iy0+1, ..., iy0+N_y-1$$
  
 $i = 1, 2, ..., m$ 

where:

 $y_{ki}$  are elements of the m sequences of length  $N_v$  in array Y.

 $x_{ki}$  are elements of the *m* sequences of length  $N_x$  in array X.

 $h_i$  are elements of the sequence of length  $N_h$  in array H.

 $i\dot{y}0$  is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y.

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See references [17] and [78].

Only one invocation of this subroutine is needed:

- 1. You do not need to invoke the subroutine with *init* ≠ 0. If you do, however, the subroutine performs error checking, exits back to the calling program, and no computation is performed.
- 2. With *init* = 0, the subroutine performs the calculation of the convolutions or correlations.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. nh, nx, ny, or  $m \le 0$
- 2. inc1h, inc1x, inc2x, inc1y, or  $inc2y \le 0$

**Example 1:** This example shows how to compute a convolution of a sequence in H, which is a ramp function, and three sequences in X, a triangular function and its cyclic translates. It computes the full range of nonzero values of the convolution plus two extra points, which are set to 0. The arrays are declared as follows:

```
REAL*4 H(0:4999), X(0:49999), Y(0:49999)
REAL*8 AUX1, AUX2
```

### Call Statement and Input

INIT = 0(for computation) H = (1.0, 2.0, 3.0, 4.0)

X contains the following three sequences:

```
1.0 2.0 3.0
2.0 1.0 2.0
3.0 2.0 1.0
4.0 3.0 2.0
5.0 4.0 3.0
6.0 5.0 4.0
5.0 6.0 5.0
4.0 5.0 6.0
3.0 4.0 5.0
2.0 3.0 4.0
```

Output: Y contains the following three sequences:

```
2.0
1.0
           3.0
4.0
     5.0
           8.0
10.0 10.0 14.0
20.0 18.0 22.0
30.0 20.0 18.0
40.0 30.0 20.0
48.0 40.0 30.0
52.0 48.0 40.0
50.0 52.0 48.0
40.0 50.0 52.0
29.0 38.0 47.0
18.0 25.0 32.0
8.0 12.0 16.0
0.0 0.0 0.0
0.0
      0.0
           0.0
```

**Example 2:** This example shows how the output from Example 1 differs when the values for NY and *inc2y* are 10 rather than 15. The output is the same except that it consists of only the first 10 values produced in Example 1.

Output: Y contains the following three sequences:

```
    1.0
    2.0
    3.0

    4.0
    5.0
    8.0

    10.0
    10.0
    14.0

    20.0
    18.0
    22.0

    30.0
    20.0
    18.0

    40.0
    30.0
    20.0

    48.0
    40.0
    30.0

    52.0
    48.0
    40.0

    50.0
    52.0
    48.0

    40.0
    50.0
    52.0
```

**Example 3:** This example shows how the output from Example 2 differs if the value for IY0 is 3 rather than 0. The output is the same except it starts at element 3 of the convolution sequences rather than element 0.

Output: Y contains the following three sequences:

```
    20.0
    18.0
    22.0

    30.0
    20.0
    18.0

    40.0
    30.0
    20.0

    48.0
    40.0
    30.0

    52.0
    48.0
    40.0

    50.0
    52.0
    48.0

    40.0
    50.0
    52.0

    29.0
    38.0
    47.0

    18.0
    25.0
    32.0

    8.0
    12.0
    16.0
```

**Example 4:** This example shows how to compute a correlation of a sequence in H, which is a ramp function, and three sequences in X, a triangular function and its cyclic translates. It computes the full range of nonzero values of the correlation plus two extra points, which are set to 0. The arrays are declared as follows:

```
REAL*4 H(0:4999), X(0:49999), Y(0:49999)
REAL*8 AUX1, AUX2
```

Call Statement and Input

```
INIT = 0(for computation)
H = (1.0, 2.0, 3.0, 4.0)
```

X contains the following three sequences:

```
1.0 2.0 3.0
2.0 1.0 2.0
3.0 2.0 1.0
4.0 3.0 2.0
5.0 4.0 3.0
6.0 5.0 4.0
5.0 6.0 5.0
4.0 5.0 6.0
3.0 4.0 5.0
2.0 3.0 4.0
```

Output: Y contains the following three sequences:

```
4.0
     8.0 12.0
11.0 10.0 17.0
20.0 15.0 16.0
30.0 22.0 18.0
40.0 30.0 22.0
50.0 40.0 30.0
52.0 50.0 40.0
48.0 52.0 50.0
40.0 48.0 52.0
30.0 40.0 48.0
16.0 22.0 28.0
7.0 10.0 13.0
2.0
     3.0 4.0
0.0
      0.0
           0.0
0.0
      0.0
           0.0
```

**Example 5:** This example shows how the output from Example 4 differs when the values for NY and INC2Y are 10 rather than 15. The output is the same except that it consists of only the first 10 values produced in Example 4.

Output: Y contains the following three sequences:

```
4.08.012.011.010.017.020.015.016.030.022.018.040.030.022.050.040.030.052.050.040.048.052.050.040.048.052.030.040.048.0
```

**Example 6:** This example shows how the output from Example 5 differs if the value for IY0 is 0 rather than -3. The output is the same except it starts at element 0 of the correlation sequences rather than element -3.

*Output:* Y contains the following three sequences:

```
    30.0
    22.0
    18.0

    40.0
    30.0
    22.0

    50.0
    40.0
    30.0

    52.0
    50.0
    40.0

    48.0
    52.0
    50.0

    40.0
    48.0
    52.0

    30.0
    40.0
    48.0

    16.0
    22.0
    28.0

    7.0
    10.0
    13.0

    2.0
    3.0
    4.0
```

### SCOND and SCORD—Convolution or Correlation of One Sequence with Another Sequence Using a Direct Method

These subroutines compute the convolution and correlation of a sequence with another sequence using a direct method. The input and output sequences contain short-precision real numbers.

### Notes:

- These subroutines compute the convolution and correlation using direct methods. In most cases, these subroutines provide **better performance** than using SCON or SCOR, if you determine that SCON or SCOR would have used a direct method for its computation. For information on how to make this determination, see reference [4].
- 2. For long-precision data, you should use DDCON or DDCOR with the decimation rate, *id*, equal to 1.

### Syntax

Fortran	CALL SCOND   SCORD (h, inch, x, incx, y, incy, nh, nx, iy0, ny)
C and C++	scond   scord (h, inch, x, incx, y, incy, nh, nx, iy0, ny);
PL/I	CALL SCOND   SCORD (h, inch, x, incx, y, incy, nh, nx, iy0, ny);

### On Entry

h

is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequence in array X. Specified as: an array of (at least) length  $1+(N_h-1)|inch|$ , containing short-precision real numbers.

inch

is the stride between the elements within the sequence in array H. Specified as: a fullword integer; inch > 0 or inch < 0.

Χ

is the array X, consisting of the input sequence of length  $N_x$ , to be convolved or correlated with the sequence in array H. Specified as: an array of (at least) length  $1+(N_x-1)|incx|$ , containing short-precision real numbers.

incx

is the stride between the elements within the sequence in array X. Specified as: a fullword integer; incx > 0 or incx < 0.

У

See "On Return" on page 833.

incy

is the stride between the elements within the sequence in output array Y. Specified as: a fullword integer; incy > 0 or incy < 0.

nh

is the number of elements,  $N_h$ , in the sequence in array H. Specified as: a fullword integer;  $N_h > 0$ .

nx

is the number of elements,  $N_x$ , in the sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

iy0

is the convolution or correlation index of the element to be stored in the first position of the sequence in array Y. Specified as: a fullword integer. It can have any value.

ny

is the number of elements,  $N_y$ , in the sequence in array Y. Specified as: a fullword integer;  $N_y > 0$ .

### On Return

V

is the array Y of length  $N_y$ , consisting of the output sequence that is the result of the convolution or correlation of the sequence in array H with the sequence in array X. Returned as: an array of (at least) length  $1+(N_y-1)|incy|$ , containing short-precision real numbers.

### Notes

- 1. Output should not overwrite input—that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. If iy0 and ny are such that output outside the basic range is needed, where the basic range is  $0 \le k \le (nh+nx-2)$  for SCOND and  $(-nh+1) \le k \le (nx-1)$  for SCORD, the subroutine stores zeros using scalar code. It is not efficient to store many zeros in this manner. It is more efficient to set iy0 and ny so that the output is produced within the above range of k values.

**Function:** The convolution and correlation of a sequence in array H with a sequence in array X are expressed as follows:

Convolution for SCOND:

$$y_k = \sum_{j=\max(0,k-N_x+1)}^{\min(N_h-1,k)} h_j x_{k-j}$$

Correlation for SCORD:

$$y_k = \sum_{j=\max(0,-k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j}$$

for 
$$k = iy0$$
,  $iy0+1$ , ...,  $iy0+N_v-1$ 

where:

 $y_k$  are elements of the sequence of length  $N_v$  in array Y.

 $x_k$  are elements of the sequence of length  $N_x$  in array X.

 $h_i$  are elements of the sequence of length  $N_h$  in array H.

*iy0* is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y.

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See reference [4].

**Special Usage:** SCORD can also perform the functions of SCON and SACOR; that is, it can compute convolutions and autocorrelations. To compute a convolution, you must specify a negative stride for H (see Example 9). To compute the autocorrelation, you must specify the two input sequences to be the same (see Example 10). In fact, you can also compute the autoconvolution by using both of these techniques together, letting the two input sequences be the same, and specifying a negative stride for the first input sequence.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. nh, nx, or  $ny \le 0$ 2. inch, incx, or incy = 0
- **Example 1:** This example shows how to compute a convolution of a sequence in H with a sequence in X, where both sequences are ramp functions.

Call Statement and Input

**Example 2:** This example shows how the output from Example 1 differs when the value for IY0 is -2 rather than 0, and NY is 15 rather than 11. The output has two zeros at the beginning and end of the sequence, for points outside the range of nonzero output.

Call Statement and Input

```
H INCH X INCX Y INCY NH NX IYO NY

| | | | | | | | | | | | | | | |

CALL SCOND(H, 1, X, 1, Y, 1, 4, 8, -2, 15)

H = (1.0, 2.0, 3.0, 4.0)

X = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0)

Output

Y = (0.0, 0.0, 11.0, 34.0, 70.0, 120.0, 130.0, 140.0, 150.0, 160.0, 151.0, 122.0, 72.0, 0.0, 0.0)
```

**Example 3:** This example shows how the same output as Example 1 can be obtained when H and X are interchanged, because the convolution is symmetric in H and X. (The arguments are switched in the calling sequence.)

Call Statement and Input

**Example 4:** This example shows how the output from Example 1 differs when a negative stride is specified for the sequence in H. By reversing the H sequence, the correlation is computed.

Call Statement and Input

**Example 5:** This example shows how to compute the autoconvolution of a sequence by letting the two input sequences for H and X be the same. (X is specified for both arguments in the calling sequence.)

Call Statement and Input

**Example 6:** This example shows how to compute a correlation of a sequence in H with a sequence in X, where both sequences are ramp functions.

Output

**Example 7:** This example shows how the output from Example 6 differs when the value for IY0 is -5 rather than -3 and NY is 15 rather than 11. The output has two zeros at the beginning and end of the sequence, for points outside the range of nonzero output.

Call Statement and Input

**Example 8:** This example shows how the output from Example 6 differs when H and X are interchanged (in the calling sequence). The output sequence is the reverse of that in Example 6. To get the full range of output, IY0 is set to –NX+1.

Call Statement and Input

**Example 9:** This example shows how the output from Example 6 differs when a negative stride is specified for the sequence in H. By reversing the H sequence, the convolution is computed.

**Example 10:** This example shows how to compute the autocorrelation of a sequence by letting the two input sequences for H and X be the same. (X is specified for both arguments in the calling sequence.)

# SCONF and SCORF—Convolution or Correlation of One Sequence with One or More Sequences Using the Mixed-Radix Fourier Method

These subroutines compute the convolutions and correlations, respectively, of a sequence with one or more sequences using the mixed-radix Fourier method. The input and output sequences contain short-precision real numbers.

**Note:** Two invocations of these subroutines are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### **Syntax**

Fortran	CALL SCONF   SCORF (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2)
C and C++	sconf   scorf (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2);
PL/I	CALL SCONF   SCORF (init, h, inc1h, x, inc1x, inc2x, y, inc1y, inc2y, nh, nx, m, iy0, ny, aux1, naux1, aux2, naux2);

### On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions, the transform of the sequence in h, and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the convolutions or correlations of the sequence that was in h at initialization with the sequences in x are computed. h is not used or changed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

h

is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequences in array X. Specified as: an array of (at least) length  $1+(N_h-1)|inc1h|$ , containing short-precision real numbers.

### inc1h

is the stride between the elements within the sequence in array H. Specified as: a fullword integer; inc1h > 0.

Χ

is the array X, consisting of m input sequences of length  $N_x$ , each to be convolved or correlated with the sequence in array H. Specified as: an array of (at least) length  $1+(N_x-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.

### inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

### inc2x

is the stride between the first elements of the sequences in array X. Specified as: a fullword integer; inc2x > 0.

y
See "On Return" on page 840.

inc1v

is the stride between the elements within each sequence in output array Y. Specified as: a fullword integer; inc1y > 0.

inc2v

is the stride between the first elements of each sequence in output array Y. Specified as: a fullword integer; inc2y > 0.

nh

is the number of elements,  $N_h$ , in the sequence in array H. Specified as: a fullword integer;  $N_h > 0$ .

nx

is the number of elements,  $N_x$ , in each sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

m

is the number of sequences in array X to be convolved or correlated. Specified as: a fullword integer; m > 0.

iy0

is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y. Specified as: a fullword integer. It can have any value.

ny

is the number of elements,  $N_y$ , in each sequence in array Y. Specified as: a fullword integer;  $N_v > 0$ .

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , the working storage is computed.

If init = 0, the working storage is used in the computation of the convolutions.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer; naux1 > 23 and  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 23 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SCONF and SCORF dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

### On Return

V

has the following meaning, where:

If init  $\neq 0$ , this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of m output sequences of length  $N_y$  that are the result of the convolutions or correlations of the sequence in array H with the sequences in array X.

Returned as: an array of (at least) length  $1+(N_y-1)inc1y+(m-1)inc2y$ , containing short-precision real numbers.

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

### **Notes**

- aux1 should **not** be used by the calling program between calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. If you specify the same array for X and Y, then *inc1x* and *inc1y* must be equal, and *inc2x* and *inc2y* must be equal. In this case, output overwrites input.
- 3. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 4. If *iy0* and *ny* are such that output outside the basic range is needed, the subroutine stores zeros. These ranges are:  $0 \le k \le N_x + N_h 2$  for SCONF and  $1 N_h \le k \le N_x 1$  for SCORF.

**Formulas for the Length of the Fourier Transform:** Before calculating the necessary sizes of *naux1* and *naux2*, you must determine the length *n* of the Fourier transform. The value of *n* is based on *nf*. You can use one of two techniques to determine *nf*:

- Use the simple overestimate of nf = nx+nh-1. (If iy0 = 0 and ny > nh+nx, this is the actual value, not an overestimate.)
- Use the values of the arguments iy0, nh, nx, and ny inserted into the following formulas to get a value for the variable nf:

```
iy0p = max(iy0, 0)

ix0 = max((iy0p+1)-nh, 0)

ih0 = max((iy0p+1)-nx, 0)

nd = ix0+ih0

n1 = iy0+ny
```

```
nxx = min(n1, nx)-ix0

nhh = min(n1, nh)-ih0

ntt = nxx+nhh-1

nn1 = n1-nd

iyy0 = iy0p-nd

nzleft = max(0, nhh-iyy0-1)

nzrt = min(nn1, ntt)-nxx

nf = max(12, nxx+max(nzleft, nzrt))
```

After calculating the value for *nf*, using one of these two techniques, refer to the formula or table of allowable values of *n* in "Acceptable Lengths for the Transforms" on page 739, selecting the value equal to or greater than *nf*.

**Processor-Independent Formulas for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on the value determined for *n* in "Formulas for the Length of the Fourier Transform" on page 840.

### NAUX1 Formulas

```
If n \le 16384, use naux1 = 58000.
If n > 16384, use naux1 = 40000+2.14n.
```

### NAUX2 Formulas

```
If n \le 16384, use naux2 = 30000.
If n > 16384, use naux2 = 20000+1.07n.
```

**Function:** The convolutions and correlations of a sequence in array H with one or more sequences in array X are expressed as follows.

Convolutions for SCONF:

$$y_{ki} = \sum_{j=\max(0,k-N_x+1)}^{\min(N_h-1,k)} h_j x_{k-j,i}$$

Correlations for SCORF:

$$y_{ki} = \sum_{j=\max(0,-k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j,i}$$

for:

$$k = iy0, iy0+1, ..., iy0+N_y-1$$
  
 $i = 1, 2, ..., m$ 

### where:

 $y_{ki}$  are elements of the m sequences of length  $N_y$  in array Y.  $x_{ki}$  are elements of the m sequences of length  $N_x$  in array X.  $h_j$  are elements of the sequence of length  $N_h$  in array H. iy0 is the convolution or correlation index of the element to be stored in the first position of each sequence in array Y.

min and max select the minimum and maximum values, respectively.

These subroutines use a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application. The length of the transform, n, that you must calculate to determine the correct sizes for naux1 and naux2 is the same length used by the Fourier transform subroutines called by this subroutine. It is assumed that elements outside the range of definition are zero. See references [17] and [78].

Two invocations of this subroutine are necessary:

- 1. With *init*  $\neq$  0, the subroutine tests and initializes arguments of the program, setting up the aux1 working storage.
- 2. With init = 0, the subroutine checks that the initialization arguments in the aux1 working storage correspond to the present arguments, and if so, performs the calculation of the convolutions.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

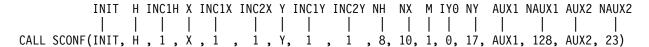
### Input-Argument Errors

- 1. nh, nx, ny, or  $m \le 0$
- 2. inc1h, inc1x, inc2x, inc1y, or  $inc2y \le 0$
- 3. The resulting internal Fourier transform length n, is too large. See "Convolutions and Correlations by Fourier Methods" on page 745.
- 4. The subroutine has not been initialized with the present arguments.
- 5. naux1 ≤ 23
- 6. naux1 is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 7. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

Example 1: This example shows how to compute a convolution of a sequence in H, where H and X are ramp functions. It calculates all nonzero values of the convolution of the sequences in H and X. The arrays are declared as follows:

REAL\*4 
$$H(8)$$
,  $X(10,1)$ ,  $Y(17)$ 

Because this convolution is symmetric in H and X, you can interchange the H and X sequences, leaving all other arguments the same, and you get the same output shown below. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.



```
INIT = 1(for initialization)

INIT = 0(for computation)

H = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0)

X = (11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0, 19.0, 20.0)

Output

Y = (11.0, 34.0, 70.0, 120.0, 185.0, 266.0, 364.0, 480.0, 516.0, 552.0, 567.0, 560.0, 530.0, 476.0, 397.0, 292.0, 160.0)
```

**Example 2:** This example shows how the output from Example 1 differs when the value for NY is 21 rather than 17, and the value for IY0 is -2 rather than 0. This yields two zeros on each end of the convolution.

### Output

```
Y = (0.0, 0.0, 11.0, 34.0, 70.0, 120.0, 185.0, 266.0, 364.0, 480.0, 516.0, 552.0, 567.0, 560.0, 530.0, 476.0, 397.0, 292.0, 160.0, 0.0, 0.0)
```

**Example 3:** This example shows how to compute the autoconvolution by letting the two input sequences be the same for Example 2. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input

**Example 4:** This example shows how to compute all nonzero values of the convolution of the sequence in H with the two sequences in X. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input

X contains the following two sequences:

```
11.0 12.0
12.0 13.0
13.0 14.0
14.0 15.0
15.0 16.0
16.0 17.0
17.0 18.0
18.0 19.0
19.0 20.0
20.0 11.0
```

### Output: Y contains the following two sequences:

```
11.0
       12.0
34.0
       37.0
70.0
       76.0
120.0 130.0
185.0 200.0
266.0 287.0
364.0 392.0
480.0 516.0
516.0 552.0
552.0 578.0
567.0 582.0
560.0 563.0
530.0 520.0
476.0 452.0
397.0 358.0
292.0 237.0
160.0
      88.0
```

**Example 5:** This example shows how to compute a correlation of a sequence in H, where H and X are ramp functions. It calculates all nonzero values of the correlation of the sequences in H and X. The arrays are declared as follows:

```
REAL*4 H(8), X(10,1)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

```
INIT H INC1H X INC1X INC2X Y INC1Y INC2Y NH NX M IYO NY AUX1 NAUX1 AUX2 NAUX2
                                CALL SCORF(INIT, H , 1 , X, 1 , 1 , Y, 1 , 1 , 8, 10, 1, -7, 17, AUX1, 128, AUX2, 23)
                   INIT
                           = 1(for initialization)
                   INIT
                            = 0(for computation)
                   Н
                            =(same as input H in Example 1)
                   Χ
                            =(same as input X in Example 1)
                   Output
                   Υ
                            = (88.0, 173.0, 254.0, 330.0, 400.0, 463.0, 518.0, 564.0,
                                600.0, 636.0, 504.0, 385.0, 280.0, 190.0, 116.0,
                                59.0, 20.0)
```

**Example 6:** This example shows how the output from Example 5 differs when the value for NY is 21 rather than 17, and the value for IY0 is -9 rather than 0. This yields two zeros on each end of the correlation.

Output

```
Y = (0.0, 0.0, 88.0, 173.0, 254.0, 330.0, 400.0, 463.0, 518.0, 564.0, 600.0, 636.0, 504.0, 385.0, 280.0, 190.0, 116.0, 59.0, 20.0, 0.0, 0.0)
```

**Example 7:** This example shows the effect of interchanging H and X. It uses the same input as Example 5, with H and X switched in the calling sequence, and with IY0 with a value of -9. Unlike convolution, as noted in Example 1, the correlation is not symmetric in H and X. First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

Call Statement and Input

**Example 8:** This example shows how to compute the autocorrelation by letting the two input sequences be the same. First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation. Because there is only one H input sequence, only one autocorrelation can be computed. Furthermore, this usage does not take advantage of the fact that the output is symmetric. Therefore, you should use SACORF to compute autocorrelations, because it does not have either of these problems.

Call Statement and Input

88.0)

Example 9: This example shows how to compute all nonzero values of the correlation of the sequence in H with the two sequences in X. First, initialize AUX1 using the calling sequence shown below with INIT ≠ 0. Then use the same calling sequence with INIT = 0 to do the calculation.

### Call Statement and Input

```
INIT H INC1H X INC1X INC2X Y INC1Y INC2Y NH NX M IYO NY AUX1 NAUX1 AUX2 NAUX2
CALL SCONF(INIT, H , 1 , X, 1 , 10 , Y, 1 , 17 , 8, 10, 2, -7, 17, AUX1, 148, AUX2, 43)
                    INIT
                              = 1(for initialization)
                    INIT
                                 0(for computation)
                              =(same as input H in Example 4)
                    Χ
                              =(same as input X in Example 4)
```

### Output: Y contains the following two sequences:

```
88.0
       96.0
173.0 188.0
254.0
      275.0
330.0 356.0
400.0 430.0
463.0 496.0
518.0 553.0
564.0 600.0
600.0 636.0
636.0 592.0
504.0 462.0
385.0 346.0
280.0 245.0
190.0 160.0
116.0
      92.0
59.0
       42.0
20.0
       11.0
```

## SDCON, DDCON, SDCOR, and DDCOR—Convolution or Correlation with Decimated Output Using a Direct Method

These subroutines compute the convolution and correlation of a sequence with another sequence, with decimated output, using a direct method.

Table 137. Data Types	
h, x, y	Subroutine
Short-precision real	SDCON
Long-precision real	DDCON
Short-precision real	SDCOR
Long-precision real	DDCOR

**Note:** These subroutines are the short- and long-precision equivalents of SCOND and SCORD when the decimation interval id is equal to 1. Because there is no long-precision version of SCOND and SCORD, you can use DDCON and DDCOR, respectively, with decimation interval id = 1 to perform the same function.

### Syntax

Fortran	CALL SDCON   DDCON   SDCOR   DDCOR (h, inch, x, incx, y, incy, nh, nx, iy0, ny, id)
C and C++	sdcon   ddcon   sdcor   ddcor (h, inch, x, incx, y, incy, nh, nx, iy0, ny, id);
PL/I	CALL SDCON   DDCON   SDCOR   DDCOR (h, inch, x, incx, y, incy, nh, nx, iy0, ny, id);

### On Entry

h

is the array H, consisting of the sequence of length  $N_h$  to be convolved or correlated with the sequence in array X. Specified as: an array of (at least) length  $1+(N_h-1)|inch|$ , containing numbers of the data type indicated in Table 137.

inch

is the stride between the elements within the sequence in array H. Specified as: a fullword integer; inch > 0 or inch < 0.

Χ

is the array X, consisting of the input sequence of length  $N_x$ , to be convolved or correlated with the sequence in array H. Specified as: an array of (at least) length  $1+(N_x-1)|incx|$ , containing numbers of the data type indicated in Table 137.

incx

is the stride between the elements within the sequence in array X. Specified as: a fullword integer; incx > 0 or incx < 0.

У

See "On Return" on page 848.

incy

is the stride between the elements within the sequence in output array Y. Specified as: a fullword integer; incy > 0 or incy < 0.

nh

is the number of elements,  $N_h$ , in the sequence in array H. Specified as: a fullword integer;  $N_h > 0$ .

### SDCON, DDCON, SDCOR, and DDCOR

nx

is the number of elements,  $N_x$ , in the sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

iy0

is the convolution or correlation index of the element to be stored in the first position of the sequence in array Y. Specified as: a fullword integer. It can have any value.

ny

is the number of elements,  $N_y$ , in the sequence in array Y. Specified as: a fullword integer;  $N_y > 0$ .

id

is the decimation interval id for the output sequence in array Y; that is, every id-th value of the convolution or correlation is produced. Specified as: a fullword integer; id > 0.

### On Return

У

is the array Y of length  $N_y$ , consisting of the output sequence that is the result of the convolution or correlation of the sequence in array H with the sequence in array X, given for every *id*-th value in the convolution or correlation.

Returned as: an array of (at least) length  $1+(N_y-1)|incy|$ , containing numbers of the data type indicated in Table 137 on page 847.

#### **Notes**

- 1. If you specify the same array for X and Y, the following conditions must be true: incx = incy, incx > 0, incy > 0, id = 1, and iy0 ≥ N<sub>h</sub>-1 for \_DCON and iy0 ≥ 0 for \_DCOR. In this case, output overwrites input. In all other cases, output should not overwrite input; that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. If iy0 and ny are such that output outside the basic range is needed, where the basic range is  $0 \le k \le (nh+nx-2)$  for SDCON and DDCON and is  $(-nh+1) \le k \le (nx-1)$  for SDCOR and DDCOR, the subroutine stores zeros using scalar code. It is not efficient to store many zeros in this manner. If you anticipate that this will happen, you may want to adjust iy0 and ny, so the subroutine computes only for k in the above range, or use the ESSL subroutine SSCAL or DSCAL to store the zeros, so you achieve better performance.

**Function:** The convolution and correlation of a sequence in array H with a sequence in array X, with decimated output, are expressed as follows:

Convolution for SDCON and DDCON:

$$y_k = \sum_{j=\max(0,k-N_x+1)}^{\min(N_h-1,k)} h_j x_{k-j}$$

Correlation for SDCOR and DDCOR:

$$y_k = \sum_{j=\max(0,-k)}^{\min(N_h-1, N_x-1-k)} h_j x_{k+j}$$

for k = iy0, iy0+id, iy0+(2)id, ...,  $iy0+(N_v-1)id$ 

where:

 $y_k$  are elements of the sequence of length  $N_v$  in array Y.

 $x_k$  are elements of the sequence of length  $N_x$  in array X.

 $h_i$  are elements of the sequence of length  $N_h$  in array H.

*iy0* is the convolution or correlation index of the element to be stored in the first position of the sequence in array Y.

min and max select the minimum and maximum values, respectively.

It is assumed that elements outside the range of definition are zero. See reference [4].

**Special Usage:** SDCON and DDCON can also perform a correlation, autoconvolution, or autocorrelation. To compute a correlation, you must specify a negative stride for H. To compute the autoconvolution, you must specify the two input sequences to be the same. You can also compute the autocorrelation by using both of these techniques together, letting the two input sequences be the same, and specifying a negative stride for the first input sequence. For examples of this, see the examples for SCOND on page 834. Because SCOND and SDCON are functionally the same, their results are the same as long as the decimation interval id = 1 for SDCON.

SDCOR and DDCOR can also perform a convolution, autocorrelation, or autoconvolution. To compute a convolution, you must specify a negative stride for H. To compute the autocorrelation, you must specify the two input sequences to be the same. You can also compute the autoconvolution by using both of these techniques together, letting the two input sequences be the same and specifying a negative stride for the first input sequence. For examples of these, see the examples for SCORD on page 835. Because SCORD and SDCOR are functionally the same, their results are the same as long as the decimation interval id = 1 for SDCOR.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. nh, nx, or  $ny \le 0$
- 2. inch, incx, or incy = 0
- 3.  $id \leq 0$

**Example 1:** This example shows how to compute a convolution of a sequence in X, where both sequences are ramp functions. It shows how a decimated output can be obtained, using the same input as "Example 1" on page 834 for SCOND and using a decimation interval ID = 2.

**Note:** For further examples of use, see the examples for SCOND on page 834. Because SCOND and SDCON are functionally the same, their results are the same as long as the decimation interval ID = 1 for SDCON.

Call Statement and Input

**Example 2:** This example shows how to compute a correlation of a sequence in  $\mathbb{R}$  with a sequence in  $\mathbb{X}$ , where both sequences are ramp functions. It shows how a decimated output can be obtained, using the same input as "Example 6" on page 835 for SCORD and using a decimation interval  $\mathbb{R}$  ID = 2.

**Note:** For further examples of use, see the examples for SCORD on page 835. Because SCORD and SDCOR are functionally the same, their results are the same as long as the decimation interval ID = 1 for SDCOR.

Call Statement and Input

**Example 3:** This example shows how to compute the same function as computed in "Example 1" on page 834 for SCOND. The input sequences and arguments are the same as that example, except a decimation interval ID = 1 is specified here for SDCON.

### SACOR—Autocorrelation of One or More Sequences

This subroutine computes the autocorrelations of one or more sequences using a direct method. The input and output sequences contain short-precision real numbers.

**Note:** This subroutine is considered obsolete. It is provided in ESSL only for compatibility with earlier releases. You should use SCORD, SDCOR, SCORF and SACORF instead, because they provide **better performance**. For further details, see reference [4].

### Syntax

Fortran	CALL SACOR (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2)
C and C++	sacor (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2);
PL/I	CALL SACOR (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2);

### On Entry

init

is a flag, where:

If  $init \neq 0$ , no computation is performed, error checking is performed, and the subroutine exits back to the calling program.

If init = 0, the autocorrelations of the sequence in x are computed.

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m input sequences of length  $N_x$ , to be autocorrelated. Specified as: an array of (at least) length  $1+(N_v-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. Specified as: a fullword integer; inc2x > 0.

V

See "On Return" on page 852.

inc1y

is the stride between the elements within each sequence in output array Y. Specified as: a fullword integer; inc1y > 0.

inc2v

is the stride between the first elements of each sequence in output array Y. Specified as: a fullword integer; inc2y > 0.

nx

is the number of elements,  $N_x$ , in each sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

m

is the number of sequences in array X to be correlated. Specified as: a fullword integer; m > 0.

ny

is the number of elements,  $N_y$ , in each sequence in array Y. Specified as: a fullword integer;  $N_y > 0$ .

aux1

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

naux1

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

aux2

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

naux2

is no longer used in the computation, but must still be specified as a dummy argument (for migration purposes from Version 1 of ESSL). It can have any value.

On Return

У

is array Y, consisting of m output sequences of length  $N_y$  that are the autocorrelation functions of the sequences in array X. Returned as: an array of (at least) length  $1 + (N_y-1)inc1y + (m-1)inc2y$ , containing short-precision real numbers.

### Notes

- 1. Output should not overwrite input; that is, input arrays X and H must have no common elements with output array Y. Otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. Auxiliary storage is not needed, but the arguments *aux1*, *naux1*, *aux2*, and *naux2* must still be specified. You can assign any values to these arguments.

**Function:** The autocorrelations of the sequences in array X are expressed as follows:

$$y_{ki} = \sum_{j=0}^{N_x - 1 - k} x_{ji} x_{j+k,i}$$

for:

$$k = 0, 1, ..., N_y-1$$
  
 $i = 1, 2, ..., m$ 

where:

 $y_{ki}$  are elements of the m sequences of length  $N_y$  in array Y.  $x_{ii}$  and  $x_{i+k,i}$  are elements of the m sequences of length  $N_x$  in array X.

See references [17] and [78].

Only one invocation of this subroutine is needed:

- 1. You do not need to invoke the subroutine with *init* ≠ 0. If you do, however, the subroutine performs error checking, exits back to the calling program, and no computation is performed.
- 2. With *init* = 0, the subroutine performs the calculation of the convolutions or correlations.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. nx, ny, or  $m \le 0$
- 2. inc1x, inc2x, inc1y, or  $inc2y \le 0$  (or incompatible)

**Example 1:** This example shows how to compute an autocorrelation for three short sequences in array X, where the input sequence length NX is equal to the output sequence length NY. This gives all nonzero autocorrelation values.

The arrays are declared as follows:

Call Statement and Input

INIT = 0(for computation)

X contains the following three sequences:

- 1.0 2.0 3.0
- 2.0 1.0 2.0
- 3.0 2.0 1.0
- 4.0 3.0 2.0
- 4.0 4.0 3.0
- 3.0 4.0 4.0
- 2.0 3.0 4.0

Output: Y contains the following three sequences:

- 59.0 59.0 59.0
- 54.0 50.0 44.0
- 43.0 39.0 30.0
- 29.0 27.0 24.0
- 16.0 18.0 21.0
- 7.0 11.0 20.0
- 2.0 6.0 12.0

**Example 2:** This example shows how the output from Example 1 differs when the values for NY and INC2Y are 9 rather than 7. This shows that when NY is greater than NX, the output array is longer, and that part is filled with zeros.

Output: Y contains the following three sequences:

```
59.0 59.0 59.0
54.0 50.0 44.0
43.0 39.0 30.0
29.0 27.0 24.0
16.0 18.0 21.0
7.0 11.0 20.0
2.0
     6.0 12.0
0.0 0.0 0.0
0.0
     0.0
           0.0
```

Example 3: This example shows how the output from Example 1 differs when the value for NY is 5 rather than 7. Also, the values for INC1X and INC1Y are 3, and the values for INC2X and INC2Y are 1 rather than 7. This shows that when NY is less than NX, the output array is shortened.

*Output:* Y contains the following three sequences:

```
59.0 59.0 59.0
54.0 50.0 44.0
43.0 39.0 30.0
29.0 27.0 24.0
16.0 18.0 21.0
```

### SACORF—Autocorrelation of One or More Sequences Using the Mixed-Radix Fourier Method

This subroutine computes the autocorrelations of one or more sequences using the mixed-radix Fourier method. The input and output sequences contain short-precision real numbers.

**Note:** Two invocations of this subroutine are necessary: one to prepare the working storage for the subroutine, and the other to perform the computations.

### Syntax

Fortran	CALL SACORF (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2)
C and C++	sacorf (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2);
PL/I	CALL SACORF (init, x, inc1x, inc2x, y, inc1y, inc2y, nx, m, ny, aux1, naux1, aux2, naux2);

### On Entry

init

is a flag, where:

If  $init \neq 0$ , trigonometric functions and other parameters, depending on arguments other than x, are computed and saved in aux1. The contents of x and y are not used or changed.

If init = 0, the autocorrelations of the sequence in x are computed. The only arguments that may change after initialization are x, y, and aux2. All scalar arguments must be the same as when the subroutine was called for initialization with  $init \neq 0$ .

Specified as: a fullword integer. It can have any value.

Χ

is the array X, consisting of m input sequences of length  $N_{\rm x}$ , to be autocorrelated. Specified as: an array of (at least) length

 $1+(N_x-1)inc1x+(m-1)inc2x$ , containing short-precision real numbers.

inc1x

is the stride between the elements within each sequence in array X. Specified as: a fullword integer; inc1x > 0.

inc2x

is the stride between the first elements of the sequences in array X. Specified as: a fullword integer; inc2x > 0.

У

See "On Return" on page 856.

inc1v

is the stride between the elements within each sequence in output array Y. Specified as: a fullword integer; inc1y > 0.

inc2y

is the stride between the first elements of each sequence in output array Y. Specified as: a fullword integer; inc2y > 0.

nx

is the number of elements,  $N_x$ , in each sequence in array X. Specified as: a fullword integer;  $N_x > 0$ .

m

is the number of sequences in array X to be correlated. Specified as: a fullword integer; m > 0.

ny

is the number of elements,  $N_y$ , in each sequence in array Y. Specified as: a fullword integer;  $N_v > 0$ .

### aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , the working storage is computed.

If init = 0, the working storage is used in the computation of the autocorrelations.

Specified as: an area of storage, containing *naux1* long-precision real numbers. *naux1* 

is the number of doublewords in the working storage specified in aux1. Specified as: a fullword integer; naux1 > 21 and  $naux1 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For values between 21 and the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

#### aux2

has the following meaning:

If naux2 = 0 and error 2015 is unrecoverable, aux2 is ignored.

Otherwise, it is the working storage used by this subroutine, which is available for use by the calling program between calls to this subroutine.

Specified as: an area of storage, containing *naux2* long-precision real numbers. On output, the contents are overwritten.

### naux2

is the number of doublewords in the working storage specified in *aux2*. Specified as: a fullword integer, where:

If naux2 = 0 and error 2015 is unrecoverable, SACORF dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux2 \ge$  (minimum value required for successful processing). To determine a sufficient value, use the processor-independent formulas. For all other values specified less than the minimum value, you have the option of having the minimum value returned in this argument. For details, see "Using Auxiliary Storage in ESSL" on page 31.

### On Return

У

has the following meaning, where:

If *init* ≠ 0, this argument is not used, and its contents remain unchanged.

If init = 0, this is array Y, consisting of m output sequences of length  $N_y$  that are the autocorrelation functions of the sequences in array X.

Returned as: an array of (at least) length  $1+(N_y-1)inc1y+(m-1)inc2y$ , containing short-precision real numbers.

aux1

is the working storage for this subroutine, where:

If  $init \neq 0$ , it contains information ready to be passed in a subsequent invocation of this subroutine.

If init = 0, its contents are unchanged.

Returned as: the contents are not relevant.

### Notes

- aux1 should **not** be used by the calling program between calls to this subroutine with *init* ≠ 0 and *init* = 0. However, it can be reused after intervening calls to this subroutine with different arguments.
- 2. If you specify the same array for X and Y, then *inc1x* and *inc1y* must be equal and *inc2x* and *inc2y* must be equal. In this case, output overwrites input.
- 3. If you specify different arrays for X and Y, they must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.
- 4. If ny is such that output outside the basic range is needed, the subroutine stores zeros. This range is:  $0 \le k \le nx-1$ .

Formula for Calculating the Length of the Fourier Transform: Before calculating the necessary sizes of *naux1* and *naux2*, you must determine the length *n* of the Fourier transform. To do this, you use the values of the arguments *nx* and *ny*, inserted into the following formula, to get a value for the variable *nf*. After calculating *nf*, reference the formula or table of allowable values of *n* in "Acceptable Lengths for the Transforms" on page 739, selecting the value equal to or greater than *nf*. Following is the formula for determining *nf*:

$$nf = \min(ny, nx) + nx + 1$$

**Processor-Independent Formulas for NAUX1 and NAUX2:** The required values of *naux1* and *naux2* depend on the value determined for *n* in "Formula for Calculating the Length of the Fourier Transform" and the argument *m*.

NAUX1 Formulas

```
If n \le 16384, use naux1 = 55000.
If n > 16384, use naux1 = 40000+1.89n.
```

NAUX2 Formulas

If 
$$n \le 16384$$
, use  $naux2 = 50000$ .  
If  $n > 16384$ , use  $naux2 = 40000+1.64n$ .

**Function:** The autocorrelations of the sequences in array X are expressed as follows:

$$y_{ki} = \sum_{j=0}^{N_x - 1 - k} x_{ji} x_{j+k,i}$$

for:

$$k = 0, 1, ..., N_v-1$$

$$i = 1, 2, ..., m$$

where:

 $y_{ki}$  are elements of the m sequences of length  $N_y$  in array Y.  $x_{ii}$  and  $x_{i+k,i}$  are elements of the m sequences of length  $N_x$  in array X.

This subroutine uses a Fourier transform method with a mixed-radix capability. This provides maximum performance for your application. The length of the transform, n, that you must calculate to determine the correct sizes for naux1 and naux2 is the same length used by the Fourier transform subroutines called by this subroutine. See references [17] and [78].

Two invocations of this subroutine are necessary:

- 1. With *init* ≠ 0, the subroutine tests and initializes arguments of the program, setting up the *aux1* working storage.
- 2. With *init* = 0, the subroutine checks that the initialization arguments in the *aux1* working storage correspond to the present arguments, and if so, performs the calculation of the autocorrelations.

#### **Error Conditions**

*Resource Errors:* Error 2015 is unrecoverable, naux2 = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. nx, ny, or  $m \le 0$
- 2. inc1x, inc2x, inc1y, or  $inc2y \le 0$  (or incompatible)
- 3. The resulting correlation is too long.
- 4. The subroutine has not been initialized with the present arguments.
- 5.  $naux1 \le 21$
- 6. *naux1* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.
- 7. Error 2015 is recoverable or *naux2*≠0, and *naux2* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to compute an autocorrelation for three short sequences in array X, where the input sequence length NX is equal to the output sequence length NY. This gives all nonzero autocorrelation values. The arrays are declared as follows:

```
REAL*4 X(0:49999), Y(0:49999)
REAL*8 AUX1(30788), AUX2(17105)
```

First, initialize AUX1 using the calling sequence shown below with INIT  $\neq$  0. Then use the same calling sequence with INIT = 0 to do the calculation.

INIT = 1(for initialization)
INIT = 0(for computation)

X contains the following three sequences:

1.0 2.0 3.0 2.0 1.0 2.0 3.0 2.0 1.0 4.0 3.0 2.0 4.0 4.0 3.0 3.0 4.0 4.0 2.0 3.0 4.0

Output: Y contains the following three sequences:

59.0 59.0 59.0 54.0 50.0 44.0 43.0 39.0 30.0 29.0 27.0 24.0 16.0 18.0 21.0 7.0 11.0 20.0 2.0 6.0 12.0

**Example 2:** This example shows how the output from Example 1 differs when the value for NY and INC2Y are 9 rather than 7. This shows that when NY is greater than NX, the output array is longer and that part is filled with zeros.

Output: Y contains the following three sequences:

 59.0
 59.0
 59.0

 54.0
 50.0
 44.0

 43.0
 39.0
 30.0

 29.0
 27.0
 24.0

 16.0
 18.0
 21.0

 7.0
 11.0
 20.0

 2.0
 6.0
 12.0

 0.0
 0.0
 0.0

 0.0
 0.0
 0.0

**Example 3:** This example shows how the output from Example 1 differs when the value for NY is 5 rather than 7. Also, the values for INC1X and INC1Y are 3 rather than 1, and the values for INC2X and INC2Y are 1 rather than 7. This shows that when NY is less than NX, the output array is shortened.

Output: Y contains the following three sequences:

59.0 59.0 59.0 54.0 50.0 44.0 43.0 39.0 30.0 29.0 27.0 24.0 16.0 18.0 21.0

### **Related-Computation Subroutines**

This section contains the related-computation subroutine descriptions.

### **SPOLY and DPOLY—Polynomial Evaluation**

These subroutines evaluate a polynomial of degree k, using coefficient vector  $\mathbf{u}$ , input vector  $\mathbf{x}$ , and output vector  $\mathbf{y}$ :

$$y_i = u_0 + u_1 x_i + u_2 x_i^2 + \ldots + u_k x_i^k$$
 for  $i = 1, 2, ..., n$ 

where  $u_k$ ,  $x_i$ , and  $y_i$  are elements of  $\boldsymbol{u}$ ,  $\boldsymbol{x}$ , and  $\boldsymbol{y}$ , respectively.

Table 138. Data Types	
u, x, y	Subroutine
Short-precision real	SPOLY
Long-precision real	DPOLY

### Syntax

Fortran	CALL SPOLY   DPOLY (u, incu, k, x, incx, y, incy, n)
C and C++	spoly   dpoly (u, incu, k, x, incx, y, incy, n);
PL/I	CALL SPOLY   DPOLY (u, incu, k, x, incx, y, incy, n);

### On Entry

и

is the coefficient vector  $\mathbf{u}$  of length k+1. It contains elements  $u_0$ ,  $u_1$ ,  $u_0$ ,  $u_1$ ,  $u_2$ , ...,  $u_k$ , which are stored in this order. Specified as: a one-dimensional array of (at least) length 1+k|incu|, containing numbers of the data type indicated in Table 138.

incu

is the stride for vector **u**. Specified as: a fullword integer. It can have any value.

k

is the degree k of the polynomial. Specified as: a fullword integer;  $k \ge 0$ .

is the input vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 138.

incx

is the stride for vector **x**. Specified as: a fullword integer. It can have any value.

y See "On Return."

incy

is the stride for the output vector y. Specified as: a fullword integer. It can have any value.

*n* is the number of elements in input vector  $\mathbf{x}$  and the number of resulting elements in output vector  $\mathbf{y}$ . Specified as: a fullword integer;  $n \ge 0$ .

### On Return

is the output vector  $\mathbf{y}$  of length n, containing the results of the polynomial evaluation. Returned as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 138.

**Note:** Vectors **u**, **x**, and **y** must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

**Function:** The evaluation of the polynomial:

$$y_i = u_0 + u_1 x_i + u_2 x_i^2 + ... + u_k x_i^k$$
 for  $i = 1, 2, ..., n$ 

is expressed as follows:

$$y_i = u_0 + x_i (u_1 + x_i (u_2 + ... + x_i (u_{k-1} + x_i u_k) ...)$$
 for  $i = 1, 2, ..., n$ 

See reference [75] for Horner's Rule. If n is 0, no computation is performed. For SPOLY, intermediate results are accumulated in long precision.

SPOLY provides the same function as the IBM 3838 function POLY, with restrictions removed. DPOLY provides a long-precision computation that is not included in the IBM 3838 functions. See the IBM 3838 Array Processor Functional Characteristics manual.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. 
$$k < 0$$

2. n < 0

Example 1: This example shows a polynomial evaluation with the degree, K, equal to 0.

Call Statement and Input

Output

$$Y = (4.0, 4.0, 4.0)$$

Example 2: This example shows a polynomial evaluation, using a negative stride INCU for vector  $\mathbf{u}$ . For  $\mathbf{u}$ , processing begins at element U(4) which is 1.0.

**Example 3:** This example shows a polynomial evaluation, using a stride INCX of 0 for input vector  $\mathbf{x}$ .

Call Statement and Input

**Example 4:** This example shows a polynomial evaluation, using a stride INCX greater than 1 for input vector  $\mathbf{x}$ , and a negative stride INCY for output vector  $\mathbf{y}$ . For  $\mathbf{y}$ , results are stored beginning at element Y(5).

# SIZC and DIZC—I-th Zero Crossing

These subroutines find the position of the *i*-th zero crossing in vector **x**. This is the *i*-th transition between positive and negative or negative and positive, where 0 is considered a positive value. It returns the position of the element in vector **x** where the *i*-th zero crossing is detected. The direction of the scan is either from the first element to the last or from the last element to the first, depending on the value you specify for the scan direction argument.

Table 139. Data Types	
x	Subroutine
Short-precision real	SIZC
Long-precision real	DIZC

#### Syntax

Fortran	CALL SIZC   DIZC (x, idrx, n, i, ky)	
C and C++	sizc   dizc (x, idrx, n, i, ky);	
PL/I CALL SIZC   DIZC (x, idrx, n, i, ky);		

#### On Entry

Х

is the target vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 139. idrx

indicates the scan direction. If it is positive or 0, x is scanned from the first element to the last (1, n). If it is negative, x is scanned from the last element to the first (n, 1). Specified as: a fullword integer. It can have any value.

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer; n > 1.

is the number of the zero crossing to be identified. Specified as: a fullword integer; i > 0.

ky See "On Return."

#### On Return

ky

is the integer vector  $\mathbf{k}\mathbf{y}$  of length 2, containing elements  $ky_1$  and  $ky_2$ , where:

If the *i*-th zero crossing is found:

- $ky_1 = j$ , where j is the position of the element  $x_j$  at the point that the i-th zero crossing is found. The position is always relative to the beginning of the vector regardless of the scan direction.
- $ky_2 = i$

If the i-th zero crossing is not found:

- $ky_1 = 0$
- $ky_2$  = the total number of zero crossings encountered in the scan.

Returned as: an array of (at least) length 2, containing fullword integers.

**Note:** The *aux* and *naux* arguments, required in some earlier releases of ESSL, are no longer required by these subroutines. If your program still includes them, you do not have to change your program; it continues to run normally. It ignores these arguments. However, if you did any program checking for error code 2015, you may want to remove it, because this error no longer occurs. (You must not code these arguments in your C program.)

**Function:** The *i*-th zero crossing in vector  $\mathbf{x}$  is found by scanning vector  $\mathbf{x}$  for i occurrences of TRUE for the following logical expressions. A zero crossing is defined here as a crossing either from a positive value to a negative value or from a negative value to a positive value, where 0 is considered a positive value. If the i-th zero crossing is found, the value of j at that point is returned in  $ky_1$  as the position of the i-th zero crossing, and i is returned in  $ky_2$ .

If  $idrx \ge 0$ :

TRUE = 
$$(x_{j-1} < 0 \text{ and } x_j \ge 0) \text{ or } (x_{j-1} \ge 0 \text{ and } x_j < 0) \text{ for } j = 2, n$$

If idrx < 0:

TRUE = 
$$(x_{j+1} < 0 \text{ and } x_j \ge 0)$$
 or  $(x_{j+1} \ge 0 \text{ and } x_j < 0)$  for  $j = n-1, 1$ 

If the position of the *i*-th zero crossing is not found, 0 is returned in  $y_1$  and the number of zero crossings encountered in the scan is returned in  $y_2$ .

SIZC provides the same functions as the IBM 3838 functions NZCP and NZCN, with restrictions removed. It combines these functions into one ESSL subroutine. DIZC provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. 
$$n \le 1$$
  
2.  $i \le 0$ 

**Example 1:** This example shows a scan of a vector **x** from the first element to the last. It is looking for the fifth zero crossing, which is encountered at position 9.

**Example 2:** This example shows a scan of a vector  $\mathbf{x}$  from the last element to the first. It is looking for the seventh zero crossing, which is encountered at position 3. Because IDRX is negative, X is scanned from the last element, X(12), to the first element, X(1).

Call Statement and Input

**Example 3:** This example shows a scan of a vector  $\mathbf{x}$  when the i-th zero crossing is not found. It encounters seven zero crossings and returns this value in KY(2).

## STREC and DTREC—Time-Varying Recursive Filter

These subroutines implement the first-order time-varying recursive equation, using initial value s, target vectors u and x, and output vector y.

Table 140. Data Types		
s, u, x, y	Subroutine	
Short-precision real	STREC	
Long-precision real	DTREC	

#### Syntax

Fortran	CALL STREC   DTREC (s, u, incu, x, incx, y, incy, n, iopt)	
C and C++	strec   dtrec (s, u, incu, x, incx, y, incy, n, iopt);	
PL/I	CALL STREC   DTREC (s, u, incu, x, incx, y, incy, n, iopt);	

#### On Entry

s

is the scalar s used in the initial computation for  $y_1$ . Specified as: a number of the data type indicated in Table 140.

и

is the target vector  $\mathbf{u}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incu|, containing numbers of the data type indicated in Table 140.

incu

is the stride for target vector u. Specified as: a fullword integer. It can have any value.

Х

is the target vector  $\mathbf{x}$  of length n. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 140.

incx

is the stride for target vector **x**. Specified as: a fullword integer. It can have any value.

У

See "On Return."

incy

is the stride for output vector y. Specified as: a fullword integer; incy > 0 or incy < 0.

n

is the number of elements in vectors u and x and the number of resulting elements in output vector y. Specified as: a fullword integer;  $n \ge 0$ .

iopt

this argument has no effect on the performance of the computation, but still must be specified as: a fullword integer; iopt = 0 or 1.

#### On Return

У

is the vector y of length n, containing the results of the implementation of the first-order time-varying recursive equation. Returned as: a one-dimensional

array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 140.

**Note:** Vectors u, x, and y must have no common elements; otherwise, results are unpredictable. See "Concepts" on page 55.

Function: The first-order time-varying recursive equation is expressed as follows:

STREC provides the same function as the IBM 3838 function REC, with restrictions removed. DTREC provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. *incy* = 0 2. *n* < 0
- 3.  $iopt \neq 0$  or 1

**Example 1:** This example shows all strides INCU, INCX, and INCY equal to 1 for vectors  $\mathbf{u}$ ,  $\mathbf{x}$ , and  $\mathbf{y}$ , respectively.

Call Statement and Input

**Example 2:** This example shows a stride, INCU, that is greater than 1 for vector  $\mathbf{u}$ . The strides INCX and INCY for vectors  $\mathbf{x}$  and  $\mathbf{y}$ , respectively, are 1.

Output

$$Y = (4.0, 14.0, 29.0, 30.0)$$

**Example 3:** This example shows a stride, INCU, of 1 for vector  $\mathbf{u}$ , a stride, INCX, that is greater than 1 for vector  $\mathbf{x}$ , and a negative stride, INCY, for vector  $\mathbf{y}$ . For  $\mathbf{y}$ , results are stored beginning at element Y(4).

## **SQINT** and **DQINT—Quadratic** Interpolation

These subroutines perform a quadratic interpolation at specified points in the vector  $\mathbf{x}$ , using initial linear displacement in the samples  $\mathbf{s}$ , sample interval  $\mathbf{g}$ , output scaling parameter  $\Omega$ , and sample reflection times in vector  $\mathbf{t}$ . The result is returned in vector  $\mathbf{y}$ .

Table 141. Data Types	
$x$ , $s$ , $g$ , $\Omega$ , $t$ , $y$	Subroutine
Short-precision real	SQINT
Long-precision real	DQINT

#### **Syntax**

Fortran	CALL SQINT   DQINT (s, g, omega, x, incx, n, t, inct, y, incy, m)	
C and C++	C and C++ sqint   dqint (s, g, omega, x, incx, n, t, inct, y, incy, m);	
PL/I	CALL SQINT   DQINT (s, g, omega, x, incx, n, t, inct, y, incy, m);	

#### On Entry

s

is the scalar *s*, containing the initial linear displacement in samples. Specified as: a number of the data type indicated in Table 141.

g

is the scalar g, containing the sample interval. Specified as: a number of the data type indicated in Table 141; g > 0.0.

#### omega

is the output scaling parameter  $\Omega$ . Specified as: a number of the data type indicated in Table 141.

X

is the vector  $\mathbf{x}$  of length n, containing the trace data. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 141.

#### incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0 or incx < 0.

n

is the number of elements in vector  $\mathbf{x}$ . Specified as: a fullword integer;  $n \ge 3$ .

t

is the vector t of length m, containing the sample reflection times to be processed. Specified as: a one-dimensional array of (at least) length 1+(m-1)|inct|, containing numbers of the data type indicated in Table 141.

inct

is the stride for vector t. Specified as: a fullword integer; inct > 0 or inct < 0.

See "On Return" on page 871.

incy

is the stride for output vector y. Specified as: a fullword integer; incy > 0 or incy < 0.

m

is the number of elements in vector t and the number of elements in output vector y. Specified as: a fullword integer;  $m \ge 0$ .

On Return

У

is the vector  $\mathbf{y}$  of length m, containing the results of the quadratic interpolation. Returned as: a one-dimensional array of (at least) length 1+(m-1)|incy|, containing numbers of the data type indicated in Table 141 on page 870.

**Function:** The quadratic interpolation, which is expressed as follows:

$$y_i = \Omega \left( trace_{k_i} (f_i^2 - f_i) + 2 \ trace_{k_i+1} (1 - f_i^2) + trace_{k_i+2} (f_i^2 + f_i) \right)$$

for 
$$i = 1, 2, ..., m$$

uses the following values:

**x** is the vector containing the specified points.

s is the initial linear displacement in the samples.

g is a sample interval.

 $\Omega$  is the output scaling parameter.

t is the vector containing the sample reflection times.

and where trace, k, f, and w are four working vectors, and so is a working scalar defined as:

```
trace_1 = 3x_1 - 3x_2 + x_3

trace_{i+1} = x_i for i = 1, 2, ..., n

so = s+2.0

w_i = so+t_i / g for i = 1, 2, ..., m

f_i = fraction part of w_i

k_i+1 = integer part of w_i
```

**Note:** Allowing  $k_i+1$  to have a value of 2 results in performance degradation. If possible, avoid specifying a point at which this occurs.

If *n* or *m* is 0, no computation is performed.

SQINT provides the same function as the IBM 3838 function INT, with restrictions removed. DQINT provides a long-precision computation that is not included in the IBM 3838 functions. See the *IBM 3838 Array Processor Functional Characteristics* manual.

#### **Error Conditions**

Computational Errors: The condition  $(k_i+1 > n)$  or  $(k_i+1 \le 2)$  has occurred, where n is the number of elements in vector  $\mathbf{x}$ . See "Function" for how to calculate  $k_i$ .

- The lower range *l* and the upper range *j* of the vector are identified in the computational error message.
- The return code is set to 1.
- The ranges I and j of the vector can be determined at run time by using the ESSL error-handling facilities. To obtain this information, you must use ERRSET to change the number of allowable errors for error code 2100 in the ESSL error option table; otherwise, the default value causes your program to terminate when this error occurs. For details, see "What Can You Do about ESSL Computational Errors?" on page 48.

Input-Argument Errors

1. 
$$n < 3$$

2. 
$$m < 0$$

$$3. q \leq 0$$

4. 
$$incx = 0$$

5. 
$$inct = 0$$

6. 
$$incy = 0$$

**Example 1:** This example shows a quadratic interpolation, using vectors with strides of 1.

Call Statement and Input

$$Y = (9.0, 11.0, 13.0, 15.0)$$

**Example 2:** This example shows a quadratic interpolation, using vectors with a positive stride of 1 and negative strides of -1.

Call Statement and Input

#### Output

$$Y = (3.0, 5.0, 7.0, 9.0)$$

Example 3: This example shows a quadratic interpolation, using vectors with a positive stride greater than 1 and negative strides less than -1.

Call Statement and Input

**Example 4:** This example shows a quadratic interpolation, using vectors with positive strides and larger values for S and G than shown in the previous examples.

# SWLEV, DWLEV, CWLEV, and ZWLEV—Wiener-Levinson Filter Coefficients

These subroutines compute the coefficients of an n-point Wiener-Levinson filter, using vector  $\mathbf{x}$ , the trace for which the filter is to be designed, and vector  $\mathbf{u}$ , the right-hand side of the system, chosen to remove reverberations or sharpen the wavelet. The result is returned in vector  $\mathbf{y}$ .

Table 142. Data Types		
x, u, y	aux	Subroutine
Short-precision real	Long-precision real	SWLEV
Long-precision real	Long-precision real	DWLEV
Short-precision complex	Long-precision complex	CWLEV
Long-precision complex	Long-precision complex	ZWLEV

#### Syntax

Fortran	CALL SWLEV   DWLEV   CWLEV   ZWLEV   (x, incx, u, incu, y, incy, n, aux, naux)	
C and C++	and C++ swlev   dwlev   cwlev   zwlev (x, incx, u, incu, y, incy, n, aux, naux);	
PL/I CALL SWLEV   DWLEV   CWLEV   ZWLEV (x, incx, u, incu, y, incy, n, aux, naux);		

#### On Entry

Х

is the vector  $\mathbf{x}$  of length n, containing the trace data for which the filter is to be designed.

For SWLEV and DWLEV, *x* represents the first row (or the first column) of a positive definite or negative definite symmetric Toeplitz matrix, which is the autocorrelation matrix for which the filter is designed.

For CWLEV and ZWLEV, *x* represents the first row of a positive definite or negative definite complex Hermitian Toeplitz matrix, which is the autocorrelation matrix for which the filter is designed.

Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 142.

incx

is the stride for vector  $\mathbf{x}$ . Specified as: a fullword integer; incx > 0.

и

is the vector  $\mathbf{u}$  of length n, containing the right-hand side of the system to be solved. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incu|, containing numbers of the data type indicated in Table 142.

incu

is the stride for vector **u**. Specified as: a fullword integer. It can have any value.

y See "On Return" on page 875.

incy

is the stride for vector  $\mathbf{y}$ . Specified as: a fullword integer; incy > 0 or incy < 0.

n

is the number of elements in vectors x, u, and y. Specified as: a fullword integer;  $n \ge 0$ .

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by these subroutines.

Specified as: an area of storage of length *naux*, containing numbers of the data type indicated in Table 142 on page 874.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SWLEV, DWLEV, CWLEV, and ZWLEV dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge 3n$ .

You cannot use dynamic allocation if you need the information returned in AUX(1).

#### On Return

V

is the vector  $\mathbf{y}$  of length n, containing the solution vector—that is, the coefficients of the n-point Wiener-Levinson filter. Returned as: a one-dimensional array of (at least) length 1+(n-1)|incy|, containing numbers of the data type indicated in Table 142 on page 874.

aux

is the storage work area used by these subroutines, where if  $naux \neq 0$ :

If AUX(1) = 0.0, the input Toeplitz matrix is positive definite or negative definite.

If AUX(1) > 0.0, the input Toeplitz matrix is indefinite (that is, it is not positive definite and it is not negative definite). The value returned in AUX(1) is the order of the first submatrix of  $\boldsymbol{A}$  that is indefinite. The subroutine continues processing. See reference [59] for information about under what circumstances your solution vector  $\boldsymbol{y}$  would be valid.

All other values in *aux* are overwritten and are not significant.

Returned as: an area of storage of length naux, containing numbers of the data type indicated in Table 142 on page 874, where AUX(1) $\geq$ 0.0.

#### Notes

- 1. For a description of a positive definite or negative definite symmetric Toeplitz matrix, see "Positive Definite or Negative Definite Symmetric Toeplitz Matrix" on page 71.
- 2. For a description of a positive definite or negative definite complex Hermitian Toeplitz matrix, see "Positive Definite or Negative Definite Complex Hermitian Toeplitz Matrix" on page 72.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The computation of the coefficients of an n-point Wiener-Levinson filter in vector **y** is expressed as solving the following system:

$$Ay = u$$

#### where:

- For SWLEV and DWLEV, matrix A is a real symmetric Toeplitz matrix whose first row (or first column) is represented by vector x.
  - For CWLEV and ZWLEV, matrix  $\boldsymbol{A}$  is a complex Hermitian Toeplitz matrix whose first row is represented by vector  $\boldsymbol{x}$ .
- *u* is the vector specifying the right side of the system, chosen to remove reverberations or to sharpen the wavelet.
- y is the solution vector.

See reference [59], [27], and the *IBM 3838 Array Processor Functional Characteristics*.

If *n* is 0, no computation is performed. For SWLEV and CWLEV, intermediate results are accumulated in long precision.

SWLEV provides the same function as the IBM 3838 function WLEV, with restrictions removed. See the *IBM 3838 Array Processor Functional Characteristics* manual.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2.  $incx \le 0$
- 3. incy = 0
- 4. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to compute filter coefficients in vector y by solving the system Ay = u. Matrix A is:

This input Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

**Example 2:** This example shows how to compute filter coefficients in vector y by solving the system Ay = u. Matrix A is:

This input Toeplitz matrix is not positive definite, as indicated by the zero value in AUX(1) on output.

Call Statement and Input

**Example 3:** This example shows a vector  $\mathbf{x}$  with a stride greater than 1, a vector  $\mathbf{u}$  with a negative stride, and a vector  $\mathbf{y}$  with a stride of 1. It uses the same input Toeplitz matrix as in Example 2, which is not positive definite.

**Example 4:** This example shows how to compute filter coefficients in vector y by solving the system Ay = u. Matrix A is:

This input complex Hermitian Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

#### Call Statement and Input

**Example 5:** This example shows a vector  $\mathbf{x}$  with a stride greater than 1, a vector  $\mathbf{u}$  with a negative stride, and a vector  $\mathbf{y}$  with a stride of 1. It uses the same input complex Hermitian Toeplitz matrix as in Example 4.

This input complex Hermitian Toeplitz matrix is positive definite, as indicated by the zero value in AUX(1) on output.

# Chapter 13. Sorting and Searching

The sorting and searching subroutines are described in this chapter.

## Overview of the Sorting and Searching Subroutines

The sorting and searching subroutines operate on three types of data: integer, short-precision real, and long-precision-real (Table 143). The sorting subroutines perform sorts with or without index designations. The searching subroutines perform either a binary or sequential search.

Table 143. List of Sorting and Searching Subroutines				
Descriptive Name	Integer Subroutine	Short- Precision Subroutine	Long- Precision Subroutine	Page
Sort the Elements of a Sequence	ISORT	SSORT	DSORT	882
Sort the Elements of a Sequence and Note the Original Element Positions	ISORTX	SSORTX	DSORTX	884
Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions	ISORTS	SSORTS	DSORTS	887
Binary Search for Elements of a Sequence X in a Sorted Sequence Y	IBSRCH	SBSRCH	DBSRCH	890
Sequential Search for Elements of a Sequence X in the Sequence Y	ISSRCH	SSSRCH	DSSRCH	894

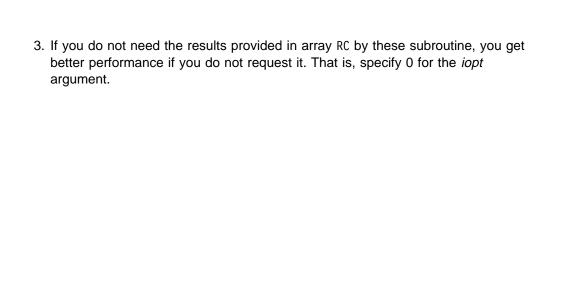
#### **Use Considerations**

It is important to understand the concept of stride for sequences when using these subroutines. For example, in the sort subroutines, a negative stride causes a sequence to be sorted into descending order in an array. In the search subroutines, a negative stride reverses the direction of the search. See "How Stride Is Used for Vectors" on page 58.

# **Performance and Accuracy Considerations**

- 1. The binary search subroutines provide better performance than the sequential search subroutines because of the nature of the searching algorithms. However, the binary search subroutines require that, before the subroutine is called, the sequence to be searched is sorted into ascending order. Therefore, if your data is already sorted, a binary search subroutine is faster. On the other hand, if your data is in random order and the number of elements being searched for is small, a sequential search subroutine is faster than doing a sort and binary search.
- 2. When doing multiple invocations of the binary search subroutines, you get better overall performance from the searching algorithms by doing fewer invocations and specifying larger search element arrays for argument *x*.

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# **Sorting and Searching Subroutines**

This section contains the sorting and searching subroutine descriptions.

## ISORT, SSORT, and DSORT—Sort the Elements of a Sequence

These subroutines sort the elements of sequence x.

Table 144. Data Types		
x	Subroutine	
Integer	ISORT	
Short-precision real	SSORT	
Long-precision real	DSORT	

#### **Syntax**

Fortran	CALL ISORT   SSORT   DSORT (x, incx, n)	
C and C++	isort   ssort   dsort $(x, incx, n)$ ;	
PL/I	CALL ISORT   SSORT   DSORT (x, incx, n);	

#### On Entry

is the sequence x of length n, to be sorted. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 144.

#### incx

is the stride for both the input sequence x and the output sequence x. If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.

Specified as: a fullword integer. It can have any value.

is the number of elements in sequence x. Specified as: a fullword integer;  $n \ge 0$ .

#### On Return

is the sequence x of length n, with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 144.

**Function:** The elements of input sequence **x** are sorted into ascending order, in place and using a partition sort. The elements of output sequence x can be expressed as follows:

$$X_1 \leq X_2 \leq X_3 \leq \cdots \leq X_n$$

By specifying a negative stride for sequence x, the elements of sequence x are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array. If *n* is 0 or 1 or if *incx* is 0, no sort is performed. See reference [69].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows a sequence **x** with a positive stride.

Call Statement and Input

**Example 2:** This example shows a sequence **x** with a negative stride.

# ISORTX, SSORTX, and DSORTX—Sort the Elements of a Sequence and Note the Original Element Positions

These subroutines sort the elements of sequence x. The original positions of the elements in sequence x are returned in the indices array, INDX. Where equal elements occur in the input sequence, they do not necessarily remain in the same relative order in the output sequence.

**Note:** If you need a stable sort, you should use ISORTS, SSORTS, or DSORTS rather than these subroutines.

Table 145. Data Types		
x	Subroutine	
Integer	ISORTX	
Short-precision real	SSORTX	
Long-precision real	DSORTX	

#### Syntax

Fortran	CALL ISORTX   SSORTX   DSORTX (x, incx, n, indx)	
C and C++	isortx   ssortx   dsortx (x, incx, n, indx);	
PL/I	CALL ISORTX   SSORTX   DSORTX (x, incx, n, indx);	

#### On Entry

Χ

is the sequence x of length n, to be sorted. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx| elements, containing numbers of the data type indicated in Table 145.

incx

is the stride for both the input sequence x and the output sequence x. If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.

Specified as: a fullword integer. It can have any value.

n

is the number of elements in sequence x. Specified as: a fullword integer;  $n \ge 0$ .

indx

See "On Return."

#### On Return

Χ

is the sequence x of length n, with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 145.

indx

is the array, referred to as INDX, containing the n indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence x.

**Note:** It is important to remember that when you specify a negative stride, ESSL assumes that the order of the input and output sequence elements in the X array is reversed; however, the elements in INDX are not reversed. See "Function" on page 885.

Returned as: a one-dimensional array of length n, containing fullword integers;  $1 \le (INDX \text{ elements}) \le n$ .

**Function:** The elements of input sequence x are sorted into ascending order, in place and using a partition sort. The elements of output sequence x can be expressed as follows:

$$X_1 \leq X_2 \leq X_3 \leq \dots \leq X_n$$

Where equal elements occur in the input sequence, they do not necessarily remain in the same relative order in the output sequence.

By specifying a negative stride for  $\mathbf{x}$ , the elements of input sequence  $\mathbf{x}$  are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array.

In addition, the INDX array contains the n indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence x. (These are not the positions in the array, but rather the positions in the sequence.) For each element  $x_j$  in the input sequence, becoming element  $xx_k$  in the output sequence, the elements in INDX are defined as follows:

$$INDX(k) = j$$
 for  $j = 1$ ,  $n$  and  $k = 1$ ,  $n$  where  $xx_k = x_j$ 

To understand INDX when you specify a negative stride, you should remember that both the input and output sequences, x, are assumed to be in reverse order in array X, but INDX is not affected by stride. The sequence elements of x are assumed to be stored in your input array as follows:

$$X = (x_n, x_{n-1}, ..., x_1)$$

The sequence elements of x are stored in your output array by ESSL as follows:

$$X = (xx_n, xx_{n-1}, \dots, xx_1)$$

where the elements  $xx_k$  are the elements  $x_j$ , sorted into descending order in X. As an example of how INDX is calculated, if  $xx_1 = x_{n-1}$ , then INDX(1) = n-1.

If *n* is 0, no computation is performed. See reference [69].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows how to sort a sequence **x** into ascending order by specifying a positive stride.

Call Statement and Input

**Example 2:** This example shows how to sort a sequence x into descending order by specifying a negative stride. Therefore, both the input and output sequences are assumed to be reversed in the array X. The input sequence is assumed to be stored as follows:

$$X = (x_5, x_4, x_3, x_2, x_1) = (2, -1, 5, 1, -2)$$

The output sequence is stored by ESSL as follows:

$$X = (xx_5, xx_4, xx_3, xx_2, xx_1) = (5, 2, 1, -1, -2)$$

As a result, INDX is defined as follows:

INDX = 
$$(indx_1, indx_2, indx_3, indx_4, indx_5) = (1, 4, 2, 5, 3)$$

For example, because output sequence element  $xx_4 = 2$  is input sequence element  $x_5$ , then INDX(4) = 5.

Call Statement and Input

Output

$$X = (5, 2, 1, -1, -2)$$
  
INDX = (1, 4, 2, 5, 3)

# ISORTS, SSORTS, and DSORTS—Sort the Elements of a Sequence Using a Stable Sort and Note the Original Element Positions

These subroutines sort the elements of sequence x using a stable sort; that is, where equal elements occur in the input sequence, they remain in the same relative order in the output sequence. The original positions of the elements in sequence x are returned in the indices array INDX.

**Note:** If you need a stable sort, then you should use these subroutines rather than ISORTX, SSORTX, or DSORTX.

Table 146. Data Types	
<b>x</b> , work	Subroutine
Integer	ISORTS
Short-precision real	SSORTS
Long-precision real	DSORTS

#### Syntax

Fortran	CALL ISORTS   SSORTS   DSORTS (x, incx, n, indx, work, lwork)	
C and C++	isorts   ssorts   dsorts (x, incx, n, indx, work, lwork);	
PL/I	CALL ISORTS   SSORTS   DSORTS (x, incx, n, indx, work, lwork);	

#### On Entry

Χ

is the sequence x of length n, to be sorted. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx| elements, containing numbers of the data type indicated in Table 146.

#### incx

is the stride for both the input sequence x and the output sequence x. If it is positive, elements are sorted into ascending order in the array, and if it is negative, elements are sorted into descending order in the array.

Specified as: a fullword integer. It can have any value.

n

is the number of elements in sequence x. Specified as: a fullword integer;  $n \ge 0$ .

#### indx

See "On Return" on page 888.

#### work

is the storage work area used by this subroutine. Its size is specified by *Iwork*. Specified as: an area of storage, containing numbers of the data type indicated in Table 146.

#### **Iwork**

is the size of the work area specified by *work*— that is, the number of elements in *work*. Specified as: a fullword integer;  $lwork \ge n/2$ .

**Note:** This is the value to achieve optimal performance. The sort is performed regardless of the value you specify for *lwork*, but you may receive an attention message.

On Return

Χ

is the sequence x of length n, with its elements sorted into designated order in the array. Returned as: a one-dimensional array, containing numbers of the data type indicated in Table 146 on page 887.

indx

is the array, referred to as INDX, containing the n indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence x.

**Note:** It is important to remember that when you specify a negative stride, ESSL assumes that the order of the input and output sequence elements in the X array is reversed; however, the elements in INDX are not reversed. See "Function."

Returned as: a one-dimensional array of length n, containing fullword integers;  $1 \le (INDX \text{ elements}) \le n$ .

**Function:** The elements of input sequence x are sorted into ascending order using a partition sort. The sorting is stable; that is, where equal elements occur in the input sequence, they remain in the same relative order in the output sequence. The elements of output sequence x can be expressed as follows:

$$X_1 \le X_2 \le X_3 \le \dots \le X_n$$

By specifying a negative stride for  $\mathbf{x}$ , the elements of input sequence  $\mathbf{x}$  are assumed to be reversed in the array,  $(x_n, x_{n-1}, \dots, x_1)$ , thus producing a sort into descending order within the array.

In addition, the INDX array contains the n indices that indicate, for the elements in the sorted output sequence, the original positions of those elements in input sequence x. (These are not the positions in the array, but rather the positions in the sequence.) For each element  $x_j$  in the input sequence, becoming element  $xx_k$  in the output sequence, the elements in INDX are defined as follows:

$$INDX(k) = j$$
 for  $j = 1$ ,  $n$  and  $k = 1$ ,  $n$   
where  $xx_k = x_j$ 

To understand INDX when you specify a negative stride, you should remember that both the input and output sequences,  $\mathbf{x}$ , are assumed to be in reverse order in array X, but INDX is not affected by stride. The sequence elements of  $\mathbf{x}$  are assumed to be stored in your input array as follows:

$$X = (x_0, x_{0-1}, ..., x_1)$$

The sequence elements of x are stored in your output array by ESSL as follows:

$$X = (xx_n, xx_{n-1}, \dots, xx_1)$$

where the elements  $xx_k$  are the elements  $x_j$ , sorted into descending order in X. As an example of how INDX is calculated, if  $xx_1 = x_{n-1}$ , then INDX(1) = n-1.

If *n* is 0, no computation is performed. See references [28] and [69].

#### **Error Conditions**

Resource Errors: Unable to allocate internal work area.

Computational Errors: None

Input-Argument Errors: n < 0

**Example 1:** This example shows how to sort a sequence x into ascending order by specifying a positive stride. Because this is a stable sort, the -1 elements remain in the same relative order in the output sequence, indicated by INDX(2) = 2 and INDX(3) = 4.

#### Call Statement and Input

**Example 2:** This example shows how to sort a sequence x into descending order by specifying a negative stride. Therefore, both the input and output sequences are assumed to be reversed in the array X. The input sequence is assumed to be stored as follows:

$$X = (x_5, x_4, x_3, x_2, x_1) = (2, -1, 5, -1, -2)$$

The output sequence is stored by ESSL as follows:

$$X = (xx_5, xx_4, xx_2, xx_2, xx_4) = (5, 2, -1, -1, -2)$$

As a result, INDX is defined as follows:

INDX = 
$$(indx_1, indx_2, indx_3, indx_4, indx_5) = (1, 2, 4, 5, 3)$$

For example, because output sequence element  $xx_4 = 2$  is input sequence element  $x_5$ , then INDX(4) = 5. Also, because this is a stable sort, the -1 elements remain in the same relative order in the output sequence, indicated by INDX(2) = 2 and INDX(3) = 4.

#### Call Statement and Input

#### Output

$$X = (5, 2, -1, -1, -2)$$
  
INDX = (1, 2, 4, 5, 3)

# IBSRCH, SBSRCH, and DBSRCH—Binary Search for Elements of a Sequence X in a Sorted Sequence Y

These subroutines perform a binary search for the locations of the elements of sequence  $\mathbf{x}$  in another sequence  $\mathbf{y}$ , where  $\mathbf{y}$  has been sorted into ascending order. The first occurrence of each element is found. When an exact match is not found, the position of the next larger element in  $\mathbf{y}$  is indicated. The locations are returned in the indices array INDX, and, optionally, return codes indicating whether the exact elements were found are returned in array RC.

Table 147. Data Types	
<i>x</i> , <i>y</i>	Subroutine
Integer	IBSRCH
Short-precision real	SBSRCH
Long-precision real	DBSRCH

#### Syntax

Fortran	CALL IBSRCH   SBSRCH   DBSRCH (x, incx, n, y, incy, m, indx, rc, iopt)
C and C++	ibsrch   sbsrch   dbsrch (x, incx, n, y, incy, m, indx, rc, iopt);
PL/I	CALL IBSRCH   SBSRCH   DBSRCH (x, incx, n, y, incy, m, indx, rc, iopt);

#### On Entry

Х

is the sequence  $\mathbf{x}$  of length n, containing the elements for which sequence  $\mathbf{y}$  is searched. Specified as: a one-dimensional array, containing numbers of the data type indicated in Table 147. It must have at least 1+(n-1)|incx| elements.

incx

is the stride for sequence x. Specified as: a fullword integer. It can have any value.

n

is the number of elements in sequence x and arrays INDX and RC. Specified as: a fullword integer;  $n \ge 0$ .

У

is the sequence y of length m, to be searched, where y must be sorted into ascending order.

**Note:** Be careful in specifying the stride for sequence *y*. A negative stride reverses the direction of the search, because the order of the sequence elements is reversed in the array.

Specified as: a one-dimensional array of (at least) length 1+(m-1)|incy|, containing numbers of the data type indicated in Table 147.

incy

is the stride for sequence y. Specified as: a fullword integer. It can have any value

m

is the number of elements in sequence y. Specified as: a fullword integer;  $m \ge 0$ .

indx

See "On Return" on page 891.

rc

See "On Return" on page 891.

iopt

has the following meaning, where:

If iopt = 0, the rc argument is not used in the computation.

If iopt = 1, the rc argument is used in the computation.

Specified as: a fullword integer; iopt = 0 or 1.

#### On Return

indx

is the array, referred to as INDX, containing the n indices that indicate the positions of the elements of sequence  $\mathbf{x}$  in sequence  $\mathbf{y}$ . The first occurrence of the element found in sequence  $\mathbf{y}$  is indicated in array INDX. When an exact match between an element of sequence  $\mathbf{x}$  and an element of sequence  $\mathbf{y}$  is not found, the position of the next larger element in sequence  $\mathbf{y}$  is indicated. When the element in sequence  $\mathbf{x}$  is larger than all the elements in sequence  $\mathbf{y}$ , then m+1 is indicated in array INDX.

Returned as: a one-dimensional array of length n, containing fullword integers;  $1 \le (INDX \text{ elements}) \le m+1$ .

rc

has the following meaning, where:

If iopt = 0, then rc is not used, and its contents remain unchanged.

If iopt = 1, it is the array, referred to as RC, containing the n return codes that indicate whether the elements in sequence  $\mathbf{x}$  were found in sequence  $\mathbf{y}$ . For i = 1, n, elements RC(i) = 0 if  $x_i$  matches an element in sequence  $\mathbf{y}$ , and RC(i) = 1 if an exact match is not found in sequence  $\mathbf{y}$ .

Returned as: a one-dimensional array of length n, containing fullword integers; RC(i) = 0 or 1.

#### **Notes**

- The elements of y must be sorted into ascending order; otherwise, results are unpredictable. For details on how to do this, see "ISORT, SSORT, and DSORT—Sort the Elements of a Sequence" on page 882.
- 2. If you do not need the results provided in array RC by these subroutines, you get better performance if you do not request it. That is, specify 0 for the *iopt* argument.

**Function:** These subroutines perform a binary search for the first occurrence (or last occurrence, using negative stride) of the locations of the elements of sequence x in another sequence y, where y must be sorted into ascending order before calling this subroutine. The first occurrence of each element is found. Two arrays are returned, containing the results of the binary searches:

• INDX, the indices array, contains the positions of the elements of sequence x in sequence y. When an exact match between values of elements in sequences x and y is not found, the location of the next larger element in sequence y is indicated in array INDX.

• RC, the return codes array, indicates for each element in sequence x whether the exact element was found in sequence y. If you do not need these results, you get better performance if you set iopt = 0.

The results returned for the INDX and RC arrays are expressed as follows:

```
For i = 1, n
    for all y_i \ge x_i, j = 1, m, INDX(i) = min(j)
    if all y_i < x_i, j = 1, m, INDX(i) = m+1
And for i = 1, n
    if x_i = y_{INDX(i)}, RC(i) = 0
    if x_i \neq y_{INDX(i)}, RC(i) = 1
```

#### where:

 $\boldsymbol{x}$  is a sequence of length n, containing the search elements.

y is a sequence of length m to be searched. It must be sorted into ascending order.

INDX is the array of length *n* of indices.

RC is the array of length n of return codes.

See reference [69]. If *n* is 0, no search is performed. If *m* is 0, then:

$$INDX(i) = 1$$
 and  $RC(i) = 1$  for  $i = 1$ ,  $n$ 

It is important to note that a negative stride for sequence y reverses the direction of the search, because the order of the sequence elements is reversed in the array. For more details on sorting sequences, see "Function" on page 882.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2. m < 0
- 3.  $iopt \neq 0$  or 1

**Example 1:** This example shows a search where sequences x and y have positive strides, and where the optional return codes are returned as part of the output.

**Example 2:** This example shows the same calling sequence as in Example 1, except that it includes the IOPT argument, specified as 1. This is equivalent to using the calling sequence in Example 1 and gives the same results.

Call Statement and Input

**Example 3:** This example shows a search where sequence x has a negative stride, and sequence y has a positive stride. The optional return codes are not requested, because IOPT is specified as 0.

Call Statement and Input

**Example 4:** This example shows a search where sequence x has a positive stride, and sequence y has a negative stride. As shown below, elements of y are in descending order in array Y. The optional return codes are not requested, because IOPT is specified as 0.

# ISSRCH, SSSRCH, and DSSRCH—Sequential Search for Elements of a Sequence X in the Sequence Y

These subroutines perform a sequential search for the locations of the elements of sequence  $\mathbf{x}$  in another sequence  $\mathbf{y}$ . Depending on the sign of the *idir* argument, the search direction indicator, the location of either the first or last occurrence of each element is indicated in the resulting indices array INDX. When an exact match between elements is not found, the position is indicated as 0.

Table 148. Data Types		
<i>x</i> , <i>y</i>	Subroutine	
Integer	ISSRCH	
Short-precision real	SSSRCH	
Long-precision real	DSSRCH	

#### Syntax

Fortran	CALL ISSRCH   SSSRCH   DSSRCH (x, incx, n, y, incy, m, idir, indx)	
C and C++	issrch   sssrch   dssrch (x, incx, n, y, incy, m, idir, indx);	
PL/I	CALL ISSRCH   SSSRCH   DSSRCH (x, incx, n, y, incy, m, idir, indx);	

#### On Entry

Х

is the sequence x of length n, containing the elements for which sequence y is searched. Specified as: a one-dimensional array of (at least) length 1+(n-1)|incx|, containing numbers of the data type indicated in Table 148.

incx

is the stride for sequence x. Specified as: a fullword integer. It can have any value.

n

is the number of elements in sequence  $\boldsymbol{x}$  and array INDX. Specified as: a fullword integer;  $n \ge 0$ .

У

is the sequence y of length m to be searched.

**Note:** Be careful in specifying the stride for sequence **y**. A negative stride reverses the direction of the search, because the order of the sequence elements is reversed in the array.

Specified as: a one-dimensional array of (at least) length 1+(m-1)|incy|, containing numbers of the data type indicated in Table 148.

incy

is the stride for sequence y. Specified as: a fullword integer. It can have any value.

m

is the number of elements in sequence y. Specified as: a fullword integer;  $m \ge 0$ .

idir

indicates the search direction, where:

If  $idir \ge 0$ , sequence y is searched from the first element to the last (1, n), thus finding the first occurrence of the element in the sequence.

If idir < 0, sequence y is searched from the last element to the first (n, 1), thus finding the last occurrence of the element in the sequence.

Specified as: a fullword integer. It can have any value.

indx

See On Return.

#### On Return

#### indx

is the array, referred to as INDX, containing the n indices that indicate the positions of the elements of sequence  $\mathbf{x}$  in sequence  $\mathbf{y}$ , where:

If  $idir \ge 0$ , the first occurrence of the element found in sequence y is indicated in array INDX.

If idir < 0, the last occurrence of the element found in sequence y is indicated in array INDX.

In all cases, if no match is found, 0 is indicated in array INDX.

Returned as: a one-dimensional array of length n, containing fullword integers;  $0 \le (INDX \text{ elements}) \le m$ .

**Function:** These subroutines perform a sequential search for the first occurrence (or last occurrence, using a negative *idir*) of the locations of the elements of sequence  $\mathbf{x}$  in another sequence  $\mathbf{y}$ . The results of the sequential searches are returned in the indices array INDX, indicating the positions of the elements of sequence  $\mathbf{x}$  in sequence  $\mathbf{y}$ . The positions indicated in array INDX are calculated relative to the first sequence element position—that is, the position of  $y_1$ . When an exact match between values of elements in sequences  $\mathbf{x}$  and  $\mathbf{y}$  is not found, 0 is indicated in array INDX for that position.

The results returned in array INDX are expressed as follows:

```
For i = 1, n

for all y_j = x_i, j = 1, m

INDX(i) = min(j), if idir \ge 0

INDX(i) = max(j), if idir < 0

if all y_j \ne x_i, j = 1, m

INDX(i) = 0
```

#### where:

 $\boldsymbol{x}$  is a sequence of length n, containing the search elements.  $\boldsymbol{y}$  is a sequence of length m to be searched. INDX is the array of length n of indices.

See reference [69]. If *n* is 0, no search is performed.

It is important to note that a negative stride for sequence y reverses the direction of the search, because the order of the sequence elements is reversed in the array.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. 
$$n < 0$$
 2.  $m < 0$ 

**Example 1:** This example shows a search where sequences **x** and **y** have positive strides, and the search direction indicator, *idir*, is positive.

Call Statement and Input

**Example 2:** This example shows a search where sequences **x** and **y** have positive strides, and the search direction indicator, *idir*, is negative.

Call Statement and Input

**Example 3:** This example shows a search where sequences **x** and **y** have negative strides, and the search direction indicator, *idir*, is positive.

Call Statement and Input

**Example 4:** This example shows a search where sequences **x** and **y** have negative strides, and the search direction indicator, *idir*, is negative.

## ISSRCH, SSSRCH, and DSSRCH

# **Chapter 14. Interpolation**

The interpolation subroutines are described in this chapter.

# **Overview of the Interpolation Subroutines**

The interpolation subroutines provide the capabilities of doing polynomial interpolation, local polynomial interpolation, and one- and two-dimensional cubic spline interpolation (Table 149).

Table 149. List of Interpolation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Polynomial Interpolation	SPINT	DPINT	901
Local Polynomial Interpolation	STPINT	DTPINT	906
Cubic Spline Interpolation	SCSINT	DCSINT	909
Two-Dimensional Cubic Spline Interpolation	SCSIN2	DCSIN2	915

### **Use Considerations**

Polynomial interpolation (SPINT and DPINT) is a global scheme. As the number of data points increases, the degree of the interpolating polynomial is raised; therefore, the graph of the interpolating polynomial tends to be oscillatory.

Local polynomial interpolation (STPINT and DTPINT) is a local scheme. The data generated is affected only by locally grouped data points. The degree of the local interpolating polynomial is usually lower than a global interpolating polynomial.

# **Performance and Accuracy Considerations**

- 1. Doing extrapolation with SPINT and DPINT is not encouraged unless you know the consequences of doing polynomial extrapolation.
- If performance is the overriding consideration, you should investigate using the general signal processing subroutines, DQINT and SQINT.
- 3. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

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# **Interpolation Subroutines**

This section contains the interpolation subroutine descriptions.

## **SPINT and DPINT—Polynomial Interpolation**

These subroutines compute the Newton divided difference coefficients and perform a polynomial interpolation through a set of data points at specified abscissas.

Table 150. Data Types	
x, y, c, t, s	Subroutine
Short-precision real	SPINT
Long-precision real	DPINT

### Syntax

Fortran	CALL SPINT   DPINT (x, y, n, c, ninit, t, s, m)
C and C++	spint   dpint $(x, y, n, c, ninit, t, s, m)$ ;
PL/I	CALL SPINT   DPINT $(x, y, n, c, ninit, t, s, m)$ ;

### On Entry

Х

is the vector  $\mathbf{x}$  of length n, containing the abscissas of the data points used in the interpolations. The elements of  $\mathbf{x}$  must be distinct. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 150.

У

is the vector  $\mathbf{y}$  of length n, containing the ordinates of the data points used in the interpolations. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 150.

n

is the number of elements in vectors x, y, and c—that is, the number of data points. Specified as: a fullword integer;  $n \ge 0$ .

С

is the vector  $\mathbf{c}$  of length n, where:

If  $ninit \le 0$ , all elements of c are undefined on entry.

If ninit > 0, c contains the Newton divided difference coefficients,  $c_j$  for j = 1, ninit, for the interpolating polynomial through the data points  $(x_j, y_j)$  for j = 1, ninit. If ninit < n, the values of  $c_j$  for j = ninit+1, n are undefined.

Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 150.

### ninit

indicates the following:

If  $ninit \le 0$ , this is the first call to this subroutine with the data in x and y; therefore, none of the Newton divided difference coefficients in c have been initialized.

If ninit > 0, a previous call to this subroutine was made with the data points  $(x_j, y_i)$  for j = 1, ninit, where:

 If ninit = n, all the Newton divided difference coefficients in c were computed for the data points. No additional coefficients are computed on this entry. • If ninit < n, the first ninit Newton divided difference coefficients in c were computed for the data points  $(x_j, y_j)$  for j = 1, ninit. The coefficients are updated for the additional data points  $(x_j, y_j)$  for j = ninit+1, n on this entry.

Specified as: a fullword integer;  $ninit \le n$ .

t

is the vector t of length m, containing the abscissas at which interpolation is to be done. Specified as: a one-dimensional array of (at least) length m, containing numbers of the data type indicated in Table 150 on page 901.

See "On Return."

m

is the number of elements in vectors t and s—that is, the number of interpolations to be performed. Specified as: a fullword integer;  $m \ge 0$ .

### On Return

С

is the vector  $\mathbf{c}$  of length n, containing the coefficients of the Newton divided difference form of the interpolating polynomial through the data points  $(x_j, y_j)$  for j = 1, n. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 150 on page 901.

#### ninit

is the number of coefficients, n, in output vector c. (If you call this subroutine again with the same data, this value should be specified for *ninit*.) Returned as: a fullword integer; ninit = n.

s

is the vector  $\mathbf{s}$  of length m, containing the resulting interpolated values; that is, each  $s_i$  is the value of the interpolating polynomial evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length m, containing numbers of the data type indicated in Table 150 on page 901.

#### Notes

- 1. In your C program, argument *ninit* must be passed by reference.
- Vectors x, y, and t must have no common elements with vectors c and s, and vector c must have no common element with vector s; otherwise, results are unpredictable.
- 3. The elements of vector **x** must be distinct; that is,  $x_i \neq x_j$  if  $i \neq j$  for i, j = 1, n.

**Function:** Polynomial interpolation is performed at specified abscissas,  $t_i$  for i = 1, m, in vector t, using the method of Newton divided differences through the data points:

$$(x_i, y_i)$$
 for  $j = 1$ ,  $n$ 

### where:

```
x_j are elements of vector \mathbf{x}. y_i are elements of vector \mathbf{y}.
```

The interpolated value at each  $t_i$  is returned in  $s_i$  for i = 1, m. See references [15] and [51]. The interpolating values returned in s are computed using the Newton divided difference coefficients, as defined in the following section.

The divided difference coefficients,  $c_j$  for j=1, n, are returned in vector  $\mathbf{c}$ . These coefficients can then be reused on subsequent calls to this subroutine, using the same data points  $(x_j, y_j)$ , but with new values of  $t_j$ . If the number of data points is increased from one call this subroutine to the next, the new coefficients are computed, and the existing coefficients are updated (not recomputed). This feature can be used to test for the convergence of the interpolations through a sequence of an increasingly larger set of points.

The values specified for *ninit* and m indicate which combination of functions are performed by this subroutine: computing the coefficients, performing the interpolation, or both. If m=0, only the divided difference coefficients are computed. No interpolation is performed. If n=0, no computation or interpolation is performed.

For SPINT, the Newton divided differences and interpolating values are accumulated in long precision.

Newton Divided Differences and Interpolating Values: The Newton divided differences of the following data points:

$$(x_j, y_j)$$
 for  $j = 1, n$   
where  $x_j \neq x_l$  if  $j \neq l$  for  $j, l = 1, n$ 

are denoted by  $\delta_k y_j$  for k = 0, 1, 2, ..., n-1 and j = 1, 2, ..., n-k, and are defined as follows:

For 
$$k=0$$
 and 1: 
$$\delta_0 y_j = y_j \quad \text{for } j=1,\,2,\,...,\,n$$
 
$$\delta_1 y_j = (y_{j+1}-y_j) \,/\, (x_{j+1}-x_j) \quad \text{for } j=1,\,2,\,...,\,n-1$$
 For  $k=2,\,3,\,...,\,n-1$ : 
$$\delta_k y_j = (\delta_{k-1}\,y_{j+1}-\delta_{k-1}y_j) \,/\, (x_{j+k}-x_j) \quad \text{for } j=1,\,2,\,...,\,n-k$$

The value s of the Newton divided difference form of the interpolating polynomial evaluated at an abscissa t is given by:

$$\begin{split} s &= y_n + (t - x_n) \ \delta_1 y_{n-1} \\ &+ (t - x_{n-1}) \ (t - x_n) \ \delta_2 y_{n-2} \\ &+ \ldots + (t - x_2) \ (t - x_3) \ \ldots \ (t - x_n) \ \delta_{n-1} y_1 \end{split}$$

Therefore, on output, the coefficients in vector *c* are as follows:

I

Also, the interpolating values in  $\mathbf{s}$ , in terms of  $\mathbf{c}$ , are as follows for i = 1, m:

$$\begin{split} S_i &= C_n + (t_i - X_n) \ C_{n-1} \\ &+ (t_i - X_{n-1}) \ (t_i - X_n) \ C_{n-2} \\ &+ \dots \\ &+ (t_i - X_2) \ (t_i - X_3) \ \dots \ (t_i - X_n) \ C_1 \end{split}$$

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

```
1. n < 0
2. ninit > n
3. m < 0
```

**Example 1:** This example shows a quadratic polynomial interpolation on the initial call with the specified data points; that is, NINIT = 0, and C contains all undefined values. On output, NINIT and C are updated with new values.

### Call Statement and Input

**Example 2:** This example shows a quadratic polynomial interpolation on a subsequent call with the same data points specified in Example 1, but using a different set of abscissas in T. In this case, NINIT = N = 3, and C contains the values defined on output in Example 1. On output here, the values in NINIT and C are unchanged.

### Call Statement and Input

**Example 3:** This example is the same as Example 2 except that it specifies additional data points on the subsequent call to the subroutine. In this case, 0 < NINIT < N. On output here, the values in NINIT and C are updated. The interpolating polynomial is a degree of 4.

Call Statement and Input

## STPINT and DTPINT—Local Polynomial Interpolation

These subroutines perform a polynomial interpolation at specified abscissas, using data points selected from a table of data.

Table 151. Data Types	
x, y, t, s, aux	Subroutine
Short-precision real	STPINT
Long-precision real	DTPINT

### Syntax

Fortran	CALL STPINT   DTPINT (x, y, n, nint, t, s, m, aux, naux)
C and C++	stpint   dtpint (x, y, n, nint, t, s, m, aux, naux);
PL/I	CALL STPINT   DTPINT (x, y, n, nint, t, s, m, aux, naux);

### On Entry

х

is the vector  $\mathbf{x}$  of length n, containing the abscissas of the data points used in the interpolations. The elements of  $\mathbf{x}$  must be distinct and sorted into ascending order. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 151.

is the vector **y** of length *n*, containing the ordinates of the data points used in the interpolations. Specified as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 151.

*n* is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ —that is, the number of data points. Specified as: a fullword integer;  $n \ge 0$ .

nint

is the number of data points to be used in the interpolation at any given point. Specified as: a fullword integer;  $0 \le nint \le n$ .

is the vector **t** of length *m*, containing the abscissas at which interpolation is to be done. For optimal performance, **t** should be sorted into ascending order. Specified as: a one-dimensional array of (at least) length *m*, containing numbers of the data type indicated in Table 151.

s See "On Return" on page 907.

is the number of elements in vectors t and s—that is, the number of interpolations to be performed. Specified as: a fullword integer;  $m \ge 0$ . aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 151. On output, the contents are overwritten.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, STPINT and DTPINT dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise, naux ≥ nint+m.

### On Return

s

is the vector  $\mathbf{s}$  of length m, containing the resulting interpolated values; that is, each  $s_i$  is the value of the interpolating polynomial evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length m, containing numbers of the data type indicated in Table 151 on page 906.

#### Notes

- 1. Vectors **x**, **y**, and **t** must have no common elements with vector **s** or work area *aux*; otherwise, results are unpredictable. See "Concepts" on page 55.
- 2. The elements of vector  $\mathbf{x}$  must be distinct and must be sorted into ascending order; that is,  $x_1 < x_2 < ... < x_n$ . Otherwise, results are unpredictable. For details on how to do this, see "ISORT, SSORT, and DSORT—Sort the Elements of a Sequence" on page 882.
- 3. The elements of vector t should be sorted into ascending order; that is,  $t_1 \le t_2 \le t_3 \le \dots \le t_m$ . Otherwise, performance is affected.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** Polynomial interpolation is performed at specified abscissas,  $t_i$  for i = 1, m, in vector t, using *nint* points selected from the following data:

$$(x_i, y_i)$$
 for  $j = 1$ ,  $n$ 

where:

$$x_1 < x_2 < x_3 < ... < x_n$$
  
 $x_j$  are elements of vector  $\mathbf{x}$ .  $y_i$  are elements of vector  $\mathbf{y}$ .

The points  $(x_j, y_j)$ , used in the interpolation at a given abscissa  $t_i$ , are chosen as follows, where k = nint/2:

```
For t_i \le x_{k+1}, the first nint points are used.
For t_i > x_{n-nint+k}, the last nint points are used.
Otherwise, points h through h+nint-1 are used, where:
x_{h+k-1} < t_i \le x_{h+k}
```

The interpolated value at each  $t_i$  is returned in  $s_i$  for i = 1, m. See references [15] and [51]. If n, nint, or m is 0, no computation is performed. For a definition of the polynomial interpolation function performed through a set of data points, see "Function" on page 902.

For STPINT, the Newton divided differences and interpolating values are accumulated in long precision.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2. nint < 0 or nint > n
- 3. m < 0
- 4. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows interpolation using two data points—that is, linear interpolation—at each  $t_i$  value.

Call Statement and Input

**Example 2:** This example shows interpolation using three data points—that is, quadratic interpolation—at each  $t_i$  value.

Call Statement and Input

## SCSINT and DCSINT—Cubic Spline Interpolation

These subroutines compute the coefficients of the cubic spline through a set of data points and evaluate the spline at specified abscissas.

Table 152. Data Types	
x, y, C, t, s	Subroutine
Short-precision real	SCSINT
Long-precision real	DCSINT

### Syntax

Fortran	CALL SCSINT   DCSINT (x, y, c, n, init, t, s, m)
C and C++	scsint   dcsint (x, y, c, n, init, t, s, m);
PL/I	CALL SCSINT   DCSINT (x, y, c, n, init, t, s, m);

### On Entry

Х

is the vector  $\mathbf{x}$  of length n, containing the abscissas of the data points that define the spline. The elements of  $\mathbf{x}$  must be distinct and sorted into ascending order. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 152.

У

is the vector  $\mathbf{y}$  of length n, containing the ordinates of the data points that define the spline. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 152.

С

is the matrix C with elements  $c_{jk}$  for j=1, n and k=1, 4 that contain the following:

If *init*  $\leq$  0, all elements of  $\boldsymbol{c}$  are undefined on entry.

If *init* = 1,  $c_{11}$  contains the spline derivative at  $x_1$ .

If *init* = 2,  $c_{21}$  contains the spline derivative at  $x_n$ .

If init = 3,  $c_{11}$  contains the spline derivative at  $x_1$ , and  $c_{21}$  contains the spline derivative at  $x_n$ .

If init > 3, **c** contains the coefficients of the spline computed for the data points  $(x_i, y_i)$  for j = 1, n on a previous call to this subroutine.

Specified as: an *n* by (at least) 4 array, containing numbers of the data type indicated in Table 152.

n

is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$  and the number of rows in matrix  $\mathbf{C}$ —that is, the number of data points. Specified as: a fullword integer;  $n \ge 0$ .

init

indicates the following, where in those cases for uninitialized coefficients, this is the first call to this subroutine with the data in x and y:

If  $init \le 0$ , the coefficients are uninitialized. The second derivatives of the spline at  $x_1$  and  $x_n$  are set to zero. (These are free end conditions, also called natural boundary conditions.)

If init = 1, the coefficients are uninitialized. The value in  $c_{11}$  is used as the spline derivative at  $x_1$ .

If init = 2, the coefficients are uninitialized. The value in  $c_{21}$  is used as the spline derivative at  $x_0$ .

If init = 3, the coefficients are uninitialized. The value in  $c_{11}$  is used as the spline derivative at  $x_1$  and the value in  $c_{21}$  is used as the spline derivative at  $x_n$ .

If *init* > 3, the coefficients in c were computed for data points  $(x_j, y_j)$  for j = 1, n on a previous call to this subroutine.

Specified as: a fullword integer. It can have any value.

t

is the vector t of length m, containing the abscissas at which the spline is evaluated. Specified as: a one-dimensional array of (at least) length m, containing numbers of the data type indicated in Table 152 on page 909.

See "On Return."

m

is the number of elements in vectors t and s—that is, the number of points at which the spline interpolation is evaluated. Specified as: a fullword integer;  $m \ge 0$ .

#### On Return

С

is the matrix C, containing the coefficients of the spline through the data points  $(x_j, y_j)$  for j = 1, n. Returned as: an n by (at least) 4 array, containing numbers of the data type indicated in Table 152 on page 909.

init

is an indicator that is set to indicate that the coefficients have been initialized. (If you call this subroutine again with the same data, this value should be specified for *init*.) Returned as: a fullword integer; init = 4.

s

is the vector  $\mathbf{s}$  of length m, containing the resulting values of the spline; that is, each  $s_i$  is the value of the spline evaluated at  $t_i$ . Returned as: a one-dimensional array of (at least) length m, containing numbers of the data type indicated in Table 152 on page 909.

### Notes

- 1. In your C program, argument *init* must be passed by reference.
- 2. Vectors **x**, **y**, and **t** must have no common elements with matrix **C** and vector **s**, and matrix **C** must have no common elements with vector **s**; otherwise, results are unpredictable.
- 3. The elements of vector  $\mathbf{x}$  must be distinct and must be sorted into ascending order; that is,  $x_1 < x_2 < ... < x_n$ . Otherwise, results are unpredictable. For details on how to do this, see "ISORT, SSORT, and DSORT—Sort the Elements of a Sequence" on page 882.

**Function:** Interpolation is performed at specified abscissas,  $t_i$  for i = 1, m, in vector t, using the cubic spline passing through the data points:

$$(x_i, y_i)$$
 for  $j = 1$ ,  $n$ 

where:

The value of the cubic spline at each  $t_i$  is returned in  $s_i$  for i=1, m. See references [15] and [51]. The coefficients of the spline,  $c_{jk}$  for j=1, n and k=1, 4, are returned in matrix c. These coefficients can then be reused on subsequent calls to this subroutine, using the same data points  $(x_j, y_j)$ , but with new values of  $t_i$ . The cubic spline values returned in s are computed using the coefficients as follows:

$$s_i = c_{i1} + c_{i2} (x_{i} t_i) + c_{i3} (x_{i} t_i)^2 + c_{i4} (x_{i} t_i)^3$$
 for  $i = 1$ ,  $m$ 

where:

$$j = 1$$
 for  $t_i \le x_1$   
 $j = k$  for  $x_1 < t_i \le x_n$ , such that  $x_{k-1} < t_i \le x_k$   
 $j = n$  for  $x_n < t_i$ 

The values specified for *m* and *init* indicate which combination of functions are performed by this subroutine:

- If m = 0 and init > 3, no computation is performed.
- If m = 0 and  $init \le 3$ , only the coefficients are computed, and no interpolation is performed.
- If *m* ≠ 0 and *init* > 3, the coefficients are not computed, and the interpolation is performed.
- If  $m \neq 0$  and  $init \leq 3$ , the coefficients are computed, and the interpolation is performed.

In addition, if n = 0, no computation is performed.

The values specified for *n* and *init* determine the type of spline function:

- If n = 1, the constructed spline is a constant function.
- If n = 2 and init = 0, the constructed spline is a line through the points.
- If n = 2 and init = 1, the constructed spline is a cubic function through the points whose derivative at  $x_1$  is  $c_{11}$ .
- If n = 2 and init = 2, the constructed spline is a cubic function through the points whose derivative at  $x_n$  is  $c_{21}$ .
- If n = 2 and init = 3, the constructed spline is a cubic function through the points whose derivative at  $x_1$  is  $c_{11}$  and at  $x_n$  is  $c_{21}$ .

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

**Example 1:** This example computes the spline coefficients through a set of data points with no derivative value specified. It also evaluates the spline at the abscissas specified in T. On output, INIT and C are updated with new values.

Call Statement and Input

**Example 2:** This example computes the spline coefficients through a set of data points with a derivative value specified at the right endpoint. It also evaluates the spline at the abscissas specified in T. On output, INIT and C are updated with new values.

### Call Statement and Input

Output

**Example 3:** This example computes the spline coefficients through a set of data points with a derivative value specified at both endpoints. It does not evaluate the spline at any points. On output, INIT and C are updated with new values. Because arrays are not needed for arguments t and s, the value 0 is specified in their place.

### Call Statement and Input

### Output

$$C = \begin{bmatrix} 0.000 & 1.000 & 3.230 & 1.230 \\ 1.000 & -1.770 & -0.460 & 1.230 \\ 2.000 & 0.079 & -1.389 & 0.310 \\ 1.100 & 1.152 & 0.316 & -0.568 \\ 0.000 & 1.312 & -0.476 & 0.264 \\ -1.000 & -0.100 & 1.888 & -0.788 \end{bmatrix}$$

INIT = 4

**Example 4:** This example evaluates the spline at a set of points, using the coefficients obtained in Example 3.

### Call Statement and Input

### **SCSINT and DCSINT**

```
С
         =(same as output C in Example 3)
Τ
         = (-1.000, 2.500, 4.000, 7.000)
Output
С
         =(same as output C in Example 3)
         = (24.762, 1.731, 1.100, 1.776)
INIT
```

# SCSIN2 and DCSIN2—Two-Dimensional Cubic Spline Interpolation

These subroutines compute the interpolation values at a specified set of points, using data defined on a rectangular mesh in the x-y plane.

Table 153. Data Types	
x, y, Z, t, u, aux, S	Subroutine
Short-precision real	SCSIN2
Long-precision real	DCSIN2

### Syntax

Fortran	CALL SCSIN2   DCSIN2 (x, y, z, n1, n2, ldz, t, u, m1, m2, s, lds, aux, naux)
C and C++	scsin2   dcsin2 (x, y, z, n1, n2, ldz, t, u, m1, m2, s, lds, aux, naux);
PL/I	CALL SCSIN2   DCSIN2 (x, y, z, n1, n2, ldz, t, u, m1, m2, s, lds, aux, naux);

### On Entry

Χ

n2

ldz

t

is the vector  $\mathbf{x}$  of length n1, containing the x-coordinates of the data points that define the spline. The elements of  $\mathbf{x}$  must be distinct and sorted into ascending order. Specified as: a one-dimensional array of (at least) length n1, containing numbers of the data type indicated in Table 153.

is the vector  $\mathbf{y}$  of length n2, containing the y-coordinates of the data points that define the spline. The elements of  $\mathbf{y}$  must be distinct and sorted into ascending order. Specified as: a one-dimensional array of (at least) length n2, containing numbers of the data type indicated in Table 153.

is the matrix Z, containing the data at  $(x_i, y_j)$  for i = 1, n1 and j = 1, n2 that defines the spline. Specified as: an Idz by (at least) n2 array, containing numbers of the data type indicated in Table 153.

n1 is the number of elements in vector  $\mathbf{x}$  and the number of rows in matrix  $\mathbf{Z}$ —that is, the number of x-coordinates at which the spline is defined. Specified as: a fullword integer;  $n1 \ge 0$ .

is the number of elements in vector  $\mathbf{y}$  and the number of columns in matrix  $\mathbf{Z}$ —that is, the number of y-coordinates at which the spline is defined. Specified as: a fullword integer;  $n2 \ge 0$ .

is the leading dimension of the array specified for z. Specified as: a fullword integer; Idz > 0 and  $Idz \ge n1$ .

is the vector t of length m1, containing the x-coordinates at which the spline is evaluated. Specified as: a one-dimensional array of (at least) length m1, containing numbers of the data type indicated in Table 153.

is the vector  $\mathbf{u}$  of length m2, containing the y-coordinates at which the spline is evaluated. Specified as: a one-dimensional array of (at least) length m2, containing numbers of the data type indicated in Table 153.

m1

is the number of elements in vector t—that is, the number of x-coordinates at which the spline interpolation is evaluated. Specified as: a fullword integer;  $m1 \ge 0$ .

m2

is the number of elements in vector  $\mathbf{u}$ —that is, the number of y-coordinates at which the spline interpolation is evaluated. Specified as: a fullword integer;  $m2 \ge 0$ .

S

See "On Return."

lds

is the leading dimension of the array specified for s. Specified as: a fullword integer; lds > 0 and  $lds \ge m1$ .

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing numbers of the data type indicated in Table 151 on page 906. On output, the contents are overwritten.

naux

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If *naux* = 0 and error 2015 is unrecoverable, SCSIN2 and DCSIN2 dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge (10)(max(n1, n2)) + (n2+1)(m1) + 2(m2)$ .

### On Return

s

is the matrix S with elements  $s_{kh}$  that contain the interpolation values at  $(t_k, u_h)$  for k = 1, m1 and k = 1, m2. Returned as: an lds by (at least) m2 array, containing numbers of the data type indicated in Table 153 on page 915.

### Notes

- The cyclic reduction method used to solve the equations in this subroutine can generate underflows on well-scaled problems. This does not affect accuracy, but it may decrease performance. For this reason, you may want to disable underflow before calling this subroutine.
- 2. Vectors **x**, **y**, **t**, and **u**, matrix **Z**, and the *aux* work area must have no common elements with matrix **S**; otherwise, results are unpredictable.
- 3. The elements within vectors  $\mathbf{x}$  and  $\mathbf{y}$  must be distinct. In addition, the elements in the vectors must be sorted into ascending order; that is,  $x_1 < x_2 < ... < x_{n1}$  and  $y_1 < y_2 < ... < y_{n2}$ . Otherwise, results are unpredictable. For details on how to do this, see "ISORT, SSORT, and DSORT—Sort the Elements of a Sequence" on page 882.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

Function: Interpolation is performed at a specified set of points:

$$(t_k, u_h)$$
 for  $k = 1, m1$  and  $h = 1, m2$ 

by fitting bicubic spline functions with natural boundary conditions, using the following set of data, defined on a rectangular grid,  $(x_i, y_j)$  for i = 1, n1 and j = 1, n2:

$$z_{ii}$$
 for  $i = 1$ ,  $n1$  and  $j = 1$ ,  $n2$ 

where  $t_k$ ,  $u_h$ ,  $x_i$ ,  $y_j$ , and  $z_{ij}$  are elements of vectors  $\mathbf{t}$ ,  $\mathbf{u}$ ,  $\mathbf{x}$ , and  $\mathbf{y}$  and matrix  $\mathbf{z}$ , respectively. In vectors  $\mathbf{x}$  and  $\mathbf{y}$ , elements are assumed to be sorted into ascending order.

The interpolation involves two steps:

1. For each *j* from 1 to *n2*, the single variable cubic spline:

$$s_{y_i}(x)$$

with natural boundary conditions, is constructed using the data points:

$$(x_i, z_{ii})$$
 for  $i = 1, n1$ 

The following interpolation values are then computed:

$$s_{y_i}(t_k)$$
 for  $k = 1, m1$ 

2. For each k from 1 to m1, the single variable cubic spline:

$$s_{t_k}(y)$$
,

with natural boundary conditions, is constructed using the data points:

$$(y_j, s_{y_j}(t_k))$$
 for  $j = 1, n2$ 

The following interpolation values are then computed:

$$s_{kh} = s_{t_k}(u_h) \qquad \text{for } l = 1, m2$$

See references [51] and [57]. Because natural boundary conditions (zero second derivatives at the end of the ranges) are used for the splines, unless the underlying function has these properties, interpolated values near the boundaries may be less satisfactory than elsewhere. If n1, n2, m1, or m2 is 0, no computation is performed.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

### Input-Argument Errors

- 1. n1 < 0 or n1 > Idz
- 2. n2 < 0
- 3. m1 < 0 or m1 > lds
- 4. m2 < 0
- 5. Idz < 0
- 6. lds < 0
- 7. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value specified in the syntax for this argument. Return code 1 is returned if error 2015 is recoverable.

Example: This example computes the interpolated values at a specified set of points, given by T and U, from a set of data points defined on a rectangular mesh in the x-y plane, using X, Y, and Z.

### Call Statement and Input

### Output

# **Chapter 15. Numerical Quadrature**

The numerical quadrature subroutines are described in this chapter.

### **Overview of the Numerical Quadrature Subroutines**

The numerical quadrature subroutines provide Gaussian quadrature methods for integrating a tabulated function and a user-supplied function over a finite, semi-infinite, or infinite region of integration (Table 154).

Table 154. List of Numerical Quadrature Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Numerical Quadrature Performed on a Set of Points	SPTNQ	DPTNQ	923
Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature	SGLNQ†	DGLNQ†	926
Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature	SGLNQ2†	DGLNQ2†	929
Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature	SGLGQ†	DGLGQ†	935
Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature	SGRAQ†	DGRAQ†	938
Numerical Quadrature Performed on a Function Using Gauss-Hermite Quadrature	SGHMQ†	DGHMQ†	942
† This subprogram is invoked as a function in a Fortran program.		•	•

### **Use Considerations**

This section contains some key points about using the numerical quadrature subroutines.

# **Choosing the Method**

The theoretical aspects of choosing the method to use for integration can be found in the references [26], [58], and [86].

# **Performance and Accuracy Considerations**

- 1. There are *n* function evaluations for a method of order *n*. Because function evaluations are expensive in terms of computing time, you should weigh the considerations for computing time and accuracy in choosing a value for *n*.
- 2. To achieve optimal performance in the \_GLNQ2 subroutines, specify the first variable integrated to be the variable having more points. This allows both the subroutine and the function evaluation to achieve optimal performance. Details on how to do this are given in "Notes" on page 930.

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3. There are some ESSL-specific rules that apply to the results of computations on the workstation processors using the ANSI/IEEE standards. For details, see "What Data Type Standards Are Used by ESSL, and What Exceptions Should You Know About?" on page 45.

# **Programming Considerations for the SUBF Subroutine**

This section describes how to design and code the *subf* subroutine for use by the numerical quadrature subrutines.

# **Designing SUBF**

For the Gaussian quadrature subroutines, you must supply a separate subroutine that is callable by ESSL. You specify the name of the subroutine in the *subf* argument. This subroutine name is selected by you. You should design the *subf* subroutine so it receives, as input, a tabulated set of points at which the integrand is evaluated, and it returns, as output, the values of the integrand evaluated at these points.

Depending on the numerical quadrature subroutine that you use, the *subf* subroutine is defined in one of the two following ways:

- For \_GLNQ, \_GLGQ, \_GRAQ, and \_GHMQ, you define the *subf* subroutine with three arguments: *t*, *y*, and *n*, where:
  - t is an input array, referred to as T, of tabulated Gaussian quadrature abscissas, containing n real numbers,  $t_i$ , where  $t_i$  is automatically provided by the ESSL subroutine and is determined by n and the Gaussian quadrature method chosen.
  - y is an output array, referred to as Y, containing n real numbers, where for the integrand, the following is true:  $y_i = f(t_i)$  for i = 1, n.
  - *n* is a positive integer indicating the number of elements in T and Y.
- For \_GLNQ2, you define the *subf* subroutine with six arguments: *s*, *n*1, *t*, *n*2, *z*, and *ldz*, where:
  - s is an input array, referred to as S, of tabulated Gaussian quadrature abscissas, containing n1 real numbers,  $s_i$ , where  $s_i$  is automatically provided by the ESSL subroutine and is determined by n1 and the Gaussian quadrature method.
  - n1 is a positive integer indicating the number of elements in S and the number of rows to be used in array **Z**.
  - is an input array, referred to as T, of tabulated Gaussian quadrature abscissas, containing n2 real numbers,  $t_i$ , where  $t_i$  is automatically provided by the ESSL subroutine and is determined by n2 and the Gaussian quadrature method.
  - *n2* is a positive integer indicating the number of elements in T and the number of columns to be used in array **Z**.
  - z is an Idz by (at least) n2 output array, referred to as Z, of real numbers, where for the integrand, the following is true:  $z_{ij} = f(s_i, t_j)$  for i = 1, n1 and j = 1, n2.
  - *Idz* is a positive integer indicating the size of the leading dimension of the array **Z**.

# Coding and Setting Up SUBF in Your Program

Examples of coding a *subf* subroutine in Fortran are provided for each subroutine in this chapter. Examples of coding a *subf* subroutine in C, C++, and PL/I are provided in "Example 1" on page 931.

Depending on the programming language you use for your program that calls the numerical quadrature subroutines, you have a choice of one or more languages that you can use for writing *subf*. These rules and other language-related coding rules for setting up *subf* in your program are described in the following sections:

- "Setting Up a User-Supplied Subroutine for ESSL in Fortran" on page 111
- "Setting Up a User-Supplied Subroutine for ESSL in C" on page 131
- "Setting Up a User-Supplied Subroutine for ESSL in C++" on page 147

# **Numerical Quadrature Subroutines**

This section contains the numerical quadrature subroutine descriptions.

# SPTNQ and DPTNQ—Numerical Quadrature Performed on a Set of Points

These subroutines approximate the integral of a real valued function specified in tabular form,  $(x_i, y_i)$  for i = 1, n. For more than four points, an error estimate is returned along with the resulting value.

Table 155. Data Types	
x, y, xyint, eest	Subroutine
Short-precision real	SPTNQ
Long-precision real	DPTNQ

### Syntax

Fortran	CALL SPTNQ   DPTNQ (x, y, n, xyint, eest)
C and C++	sptnq   dptnq (x, y, n, xyint, eest);
PL/I	CALL SPTNQ   DPTNQ (x, y, n, xyint, eest);

### On Entry

Χ

is the vector  $\mathbf{x}$  of length n, containing the abscissas of the data points to be integrated. The elements of  $\mathbf{x}$  must be distinct and sorted into ascending or descending order. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 155.

У

is the vector  $\mathbf{y}$  of length n, containing the ordinates of the data points to be integrated. Specified as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 155.

n

is the number of elements in vectors  $\mathbf{x}$  and  $\mathbf{y}$ —that is, the number of data points. The value of n determines the algorithm used by this subroutine. For details, see "Function" on page 924. Specified as: a fullword integer;  $n \ge 2$ .

xyint

See "On Return."

eest

See "On Return."

### On Return

xyint

is the approximation *xyint* of the integral. Returned as: a number of the data type indicated in Table 155.

eest

has the following meaning, where:

If n < 5, it is undefined and is set to 0.

If  $n \ge 5$ , it is an estimate, *eest*, of the error in the integral, where *xyint*+*eest* tends to give a better approximation to the integral than *xyint*. For details, see references [26] and [58].

Returned as: a number of the data type indicated in Table 155.

### **Notes**

- 1. In your C program, arguments xyint and eest must be passed by reference.
- 2. The elements of vector  $\mathbf{x}$  must be distinct—that is,  $x_i \neq x_j$  for  $i \neq j$ ,—and they must be sorted into ascending or descending order; otherwise, results are unpredictable. For how to do this, see "ISORT, SSORT, and DSORT—Sort the Elements of a Sequence" on page 882.

**Function:** The integral is approximated for a real valued function specified in tabular form,  $(x_i, y_j)$  for i = 1, n, where  $x_i$  are distinct and sorted into ascending or descending order, and  $n \ge 2$ . If  $y_i = f(x_i)$  for i = 1, n, then on output, xyint is an approximation to the integral of the following form:

$$\int_{x_1}^{x_n} f(x) dx$$

The algorithm used by this subroutine is based on the number of data points used in the computation, where:

- If n = 2, the trapezoid rule is used to do the integration.
- If n = 3, the parabola through the three points is integrated.
- If  $n \ge 4$ , the method of Gill and Miller is used to do the integration.

For  $n \ge 5$ , an estimate of the error *eest* is returned. For the method of Gill and Miller, it is shown that adding the estimate of the error *eest* to the result *xyint* often gives a better approximation to the integral than the result *xyint* by itself. For n < 5, an estimate of the error is not returned. In this case, a value of 0 is returned for *eest*. See references [58] and [26].

### **Error Conditions**

Computational Errors: None

Input-Argument Errors: n < 2

**Example 1:** This example shows the result of an integration, where the abscissas in X are sorted into ascending order.

Call Statement and Input

XYINT = 15.137 EEST = -0.003

**Example 2:** This example shows the result of an integration, where the abscissas in X are sorted into descending order.

### Call Statement and Input

$$X$$
 = (4.3, 3.9, 3.4, 3.0, 2.6, 2.1, 1.5, 1.0, 0.4, 0.0)  
 $Y$  = (3.3, 3.5, 3.0, 4.0, 4.5, 5.0, 4.0, 3.0, 2.0, 1.0)

### Output

XYINT = -15.137 = 0.003 EEST

# SGLNQ and DGLNQ—Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature

These functions approximate the integral of a real valued function over a finite interval, using the Gauss-Legendre Quadrature method of specified order.

Table 156. Data Types		
a, b, Result	Subroutine	
Short-precision real	SGLNQ	
Long-precision real	DGLNQ	

### Syntax

Fortran	SGLNQ   DGLNQ (subf, a, b, n)
C and C++	sglnq   dglnq (subf, a, b, n);
PL/I	SGLNQ   DGLNQ (subf, a, b, n);

### On Entry

### subf

is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see "Programming Considerations for the SUBF Subroutine" on page 920.

Specified as: *subf* must be declared as an external subroutine in you application program. It can be whatever name you choose.

is the lower limit of integration, *a.* Specified as: a number of the data type indicated in Table 156.

is the upper limit of integration, *b*. Specified as: a number of the data type indicated in Table 156.

is the order of the quadrature method to be used. Specified as: a fullword integer; *n* = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

### On Return

### Function value

is the approximation of the integral. Returned as: a number of the data type indicated in Table 156.

### Notes

- Declare the DGLNQ function in your program as returning a long-precision real number. Declare the SGLNQ, if necessary, as returning a short-precision real number.
- 2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable *x*, described under "Function" on page 927, and

the argument *n* correspond to the *subf* arguments *t* and *n*, respectively. For details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 920.

**Function:** The integral is approximated for a real valued function over a finite interval, using the Gauss-Legendre Quadrature method of specified order. The region of integration is from a to b. The method of order n is theoretically exact for integrals of the following form, where f is a polynomial of degree less than 2n:

$$\int_{a}^{b} f(x) dx$$

The method of order n is a good approximation when your integrand is closely approximated by a function of the form f(x), where f is a polynomial of degree less than 2n. See references [26] and [86]. The result is returned as the function value.

### **Error Conditions**

Computational Errors: None

*Input-Argument Errors: n* is not an allowable value, as listed in the syntax for this argument.

**Example:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = x^2 + e^x$$

over the interval (0.0, 2.0), using the Gauss-Legendre method with 10 points:

$$\int_{0.0}^{2.0} (x^2 + e^x) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*)
DO 1 I=1,N
1 Y(I)=T(I)**2+EXP(T(I))
RETURN
END
```

Program Statements and Input

## SGLNQ and DGLNQ

# SGLNQ2 and DGLNQ2—Numerical Quadrature Performed on a Function Over a Rectangle Using Two-Dimensional Gauss-Legendre Quadrature

These functions approximate the integral of a real valued function of two variables over a rectangular region, using the Gauss-Legendre Quadrature method of specified order in each variable.

Table 157. Data Types		
a, b, c, d, Z, Result	Subroutine	
Short-precision real	SGLNQ2	
Long-precision real	DGLNQ2	

### Syntax

Fortran	SGLNQ2   DGLNQ2 (subf, a, b, n1, c, d, n2, z, ldz)
C and C++	sglnq2   dglnq2 ( <i>subf</i> , <i>a</i> , <i>b</i> , <i>n</i> 1, <i>c</i> , <i>d</i> , <i>n</i> 2, <i>z</i> , <i>ldz</i> );
PL/I	SGLNQ2   DGLNQ2 (subf, a, b, n1, c, d, n2, z, ldz);

### On Entry

subf

b

n1

C

d

is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with six arguments: *s*, *n*1, *t*, *n*2, *z*, and *ldz*. For details, see "Programming Considerations for the SUBF Subroutine" on page 920.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

is the lower limit of integration, *a*, for the first variable integrated. Specified as: a number of the data type indicated in Table 157.

is the upper limit of integration, *b*, for the first variable integrated. Specified as: a number of the data type indicated in Table 157.

is the order of the quadrature method to be used for the first variable integrated. Specified as: a fullword integer; n1 = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

is the lower limit of integration, *c*, for the second variable integrated. Specified as: a number of the data type indicated in Table 157.

is the upper limit of integration, *d*, for the second variable integrated. Specified as: a number of the data type indicated in Table 157.

*n2* is the order of the quadrature method to be used for the second variable integrated. Specified as: a fullword integer; n2 = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

is the matrix Z, containing the n1 rows and n2 columns of data used to evaluate the integrand function. (The output values from the subf subroutine

are placed in **Z**.) Specified as: an *ldz* by (at least) *n2* array, containing numbers of the data type indicated in Table 157.

ldz

is the size of the leading dimension of the array specified for z. Specified as: a fullword integer; Idz > 0 and  $Idz \ge n1$ .

#### On Return

### Function value

is the approximation of the integral. Returned as: a number of the data type indicated in Table 157 on page 929.

### **Notes**

- Declare the DGLNQ2 function in your program as returning a long-precision real number. Declare the SGLNQ2 function, if necessary, as returning a short-precision real number.
- 2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. For details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 920.

**Function:** The integral:

$$\int_{c}^{d} \int_{a}^{b} f(s,t) ds dt$$

is approximated for a real valued function of two variables *s* and *t*, over a rectangular region, using the Gauss-Legendre Quadrature method of specified order in each variable. The region of integration is:

$$(a, b)$$
 for  $s$   $(c, d)$  for  $t$ 

The method gives a good approximation when your integrand is closely approximated by a function of the form f(s, t), where f is a polynomial of degree less than 2(n1) for s and 2(n2) for t. See the function description for "SGLNQ and DGLNQ—Numerical Quadrature Performed on a Function Using Gauss-Legendre Quadrature" on page 926 and references [26] and [86]. The result is returned as the function value.

**Special Usage:** To achieve optimal performance in this subroutine and in the functional evaluation, specify the first variable integrated in this subroutine as the variable having more points. The first variable integrated is the variable in the inner integral. For example, in the following integration, *x* is the first variable integrated:

$$\int_{u_1}^{u_2} \int_{v_1}^{v_2} f(x, y) \, dx \, dy$$

This is the suggested order of integration if the x variable has more points than the y variable. On the other hand, if the y variable has more points, you make y the first variable integrated.

Because the order of integration does not matter to the resulting approximation, you may be able to reverse the order that x and y are integrated and get better performance. This can be expressed as:

$$\int_{u_1}^{u_2} \int_{r_1}^{r_2} f(x, y) \, dx \, dy = \int_{r_1}^{r_2} \int_{u_1}^{u_2} f(x, y) \, dy \, dx$$

Results are mathematically equivalent. However, because the algorithm is computed in a different way, results may not be bitwise identical.

Table 158 shows how to assign your variables to the \_GLNQ2 and *subf* arguments for the *x-y* integration shown on the left and for the *y-x* integration shown on the right. For examples of how to do each of these, see "Example 1" and "Example 2" on page 933.

Table 158. How to Assign Your Variables for x-y Integration Versus y-x Integration				
_GLNQ2 and SUBF Arguments	Variables for x-y Integration	Variables for y-x Integration		
For _GLNQ2: a b n1 c d n2	r1 r2 (order for x) u1 u2 (order for y)	u1 u2 (order for y) r1 r2 (order for x)		
For subf: s t n1 n2	x y (order for x) (order for y)	y x (order for y) (order for x)		

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $Idz \leq 0$
- 2. n1 > Idz
- 3. *n*1 or *n*2 is not an allowable value, as listed in the syntax for this argument.

**Example 1:** This example shows how to compute the integral of the function *f* given by:

$$f(x, y) = e^x \sin y$$

over the intervals (0.0, 2.0) for the first variable x and (-2.0, -1.0) for the second variable y, using the Gauss-Legendre method with 10 points in the x variable and 5 points in the y variable:

$$\int_{-2.0}^{-1.0} \int_{0.0}^{2.0} (e^x \sin y) dx dy$$

Because the variable x has more points, it is the first variable integrated. This allows the SGLNQ2 subroutine and the FUN1 evaluation to achieve optimal performance. Therefore, the x and y variables correspond to S and T in the FUN1 subroutine. Also, the x and y variables correspond to the A, B, N1 and C, D, N2 sets of arguments, respectively, for SGLNQ2.

Using Fortran for SUBF: The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (S,N1,T,N2,Z,LDZ)
   INTEGER*4 N1,N2,LDZ
   REAL*4 S(*),T(*),Z(LDZ,*)
   DO 1 J=1,N2
   DO 2 I=1,N1
      Z(I,J)=EXP(S(I))*SIN(T(J))
2
      CONTINUE
   RETURN
   END
```

**Note:** The computation for this user-supplied subroutine FUN1 can also be performed by using the following statements in place of the above DO loops, using T1 and T2 as temporary storage areas:

```
DO 1 I=1,N1
1
  T1(I)=EXP(S(I))
  DO 2 J=1,N2
2
    T2(J)=SIN(T(J))
  DO 3 J=1,N2
  DO 4 I=1,N1
4
     Z(I,J)=T1(I)*T2(J)
3
     CONTINUE
```

When coding your application, this is the preferred technique. It reduces the number of evaluations performed and, therefore, provides better performance.

Using C for SUBF: The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in C as follows:

```
void fun1(s, n1, t, n2, z, ldz)
float *s, *t, *z;
int *n1, *n2, *ldz;
     int i, j;
     for(j = 0; j < *n2; ++j, z += *ldz)
         for(i = 0; i < *n1; ++i)
         z[i] = exp(s[i]) * sin(t[j]);
}
```

Using C++ for SUBF: The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in C++ as follows:

```
void fun1(float *s, int *n1, float *t, int *n2, float *z, int *ldz)
{
    int i, j;
    for(j = 0; j < *n2; ++j, z += *ldz)
        {
        for(i = 0; i < *n1; ++i)
            z[i] = exp(s[i]) * sin(t[j]);
        }
}</pre>
```

Using PL/I for SUBF: The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in PL/I as follows:

```
FUN1: PROCEDURE(S,N1,T,N2,Z,LDZ) OPTIONS(FORTRAN,NOMAP);
DCL (N1,N2,LDZ,I,J) REAL FIXED BINARY(31,0);
DCL (S(10),T(10),Z(5,10)) REAL FLOAT DEC(16) ALIGNED CONNECTED;
DO J=1 TO N1;
   DO I=1 TO N2;
        Z(I,J)=EXP(S(J))*SIN(T(I));
   END;
END;
RETURN;
END FUN1;
```

### Program Statements and Input

**Example 2:** This example shows how to reverse the order of integration of the variables *x* and *y*. It computes the integral of the function *f* given by:

$$f(x, y) = \cos x \sin y$$

over the intervals (0.0, 1.0) for the variable x and (0.0, 20.0) for the variable y, using the Gauss-Legendre method with 5 points in the x variable and 48 points in the y variable. Because the order of integration does not matter to the approximation:

$$\int_{0.0}^{20.0} \int_{0.0}^{1.0} (\cos x \sin y) dx dy = \int_{0.0}^{1.0} \int_{0.0}^{20.0} (\cos x \sin y) dy dx$$

the variable y, having more points, is the first variable integrated (performing the integration shown on the right.) This allows the SGLNQ2 subroutine and the FUN1 evaluation to achieve optimal performance. Therefore, the x and y variables correspond to T and S in the FUN2 subroutine. Also, the x and y variables correspond to the C, D, N2 and A, B, N1 sets of arguments, respectively, for SGLNQ2.

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN2 (S,N1,T,N2,Z,LDZ)
  INTEGER*4 N1,N2,LDZ
  REAL*4 S(*),T(*),Z(LDZ,*)
  DO 1 J=1,N2
  DO 2 I=1,N1
      Z(I,J)=COS(T(J))*SIN(S(I))
1
      CONTINUE
  RETURN
  END
```

**Note:** The same coding principles for achieving good performance that are noted in "Example 1" on page 931 also apply to this user-supplied subroutine FUN2.

### Program Statements and Input

```
EXTERNAL FUN2.
                    A B N1 C
              SUBF
                                         D N2 Z LDZ
YXINT = SGLNQ2( FUN2 , 0.0 , 20.0 , 48 , 0.0 , 1.0 , 5 , Z , 48 )
FUN2
    =(see above)
Z
       =(not relevant)
Output
YXINT
       = 0.4981
```

# SGLGQ and DGLGQ—Numerical Quadrature Performed on a Function Using Gauss-Laguerre Quadrature

These functions approximate the integral of a real valued function over a semi-infinite interval, using the Gauss-Laguerre Quadrature method of specified order.

Table 159. Data Types	
a, b, Result	Subroutine
Short-precision real	SGLGQ
Long-precision real	DGLGQ

#### Syntax

Fortran	SGLGQ   DGLGQ (subf, a, b, n)	
C and C++	sglgq   dglgq (subf, a, b, n);	
PL/I	SGLGQ   DGLGQ (subf, a, b, n);	

#### On Entry

subf

is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see "Programming Considerations for the SUBF Subroutine" on page 920.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

а

has the following meaning, where:

If b > 0, it is the lower limit of integration.

If b < 0, it is the upper limit of integration.

Specified as: a number of the data type indicated in Table 159.

b

is the scaling constant b for the exponential. Specified as: a number of the data type indicated in Table 159; b > 0 or b < 0.

n

is the order of the quadrature method to be used. Specified as: a fullword integer; n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, or 64.

#### On Return

#### Function value

is the approximation of the integral. Returned as: a number of the data type indicated in Table 159.

#### Notes

- 1. Declare the DGLGQ function in your program as returning a long-precision real number. Declare the SGLGQ function, if necessary, as returning a short-precision real number.
- 2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this

ESSL subroutine. The variable x, described under "Function" on page 936, and the argument n correspond to the *subf* arguments t and n, respectively. For details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 920.

**Function:** The integral is approximated for a real valued function over a semi-infinite interval, using the Gauss-Laguerre Quadrature method of specified order. The region of integration is:

$$(a, \infty)$$
 if  $b > 0$   
 $(-\infty, a)$  if  $b < 0$ 

The method of order n is theoretically exact for integrals of the following form, where f is a polynomial of degree less than 2n:

$$\int_{a}^{\infty} f(x)e^{-bx}dx \qquad \text{if } b > 0$$

$$\int_{-\infty}^{a} f(x)e^{-bx}dx \qquad \text{if } b < 0$$

The method of order n is a good approximation when your integrand is closely approximated by a function of the form  $f(x)e^{-bx}$ , where f is a polynomial of degree less than 2n. See references [26] and [86]. The result is returned as the function value.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. b = 0
- 2. *n* is not an allowable value, as listed in the syntax for this argument.

**Example 1:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = \sin(3.0x)e^{-1.5x}$$

over the interval (-2.0, ∞), using the Gauss-Laguerre method with 20 points:

$$\int_{-2.0}^{\infty} \left( \sin(3.0x) e^{-1.5x} \right) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*)
DO 1 I=1,N
Y(I)=SIN(3.0*T(I))*EXP(-1.5*T(I))
RETURN
END
```

#### Program Statements and Input

**Example 2:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = \sin(3.0x)e^{1.5x}$$

over the interval  $(-\infty, -2.0)$ , using the Gauss-Laguerre method with 20 points:

$$\int_{-\infty}^{-2.0} \sin(3.0x) e^{1.5x} dx$$

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN2 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*),TEMP
DO 1 I=1,N
1 Y(I)=SIN(3.0*T(I))*EXP(1.5*T(I))
RETURN
END
```

#### Program Statements and Input

# SGRAQ and DGRAQ—Numerical Quadrature Performed on a Function Using Gauss-Rational Quadrature

These functions approximate the integral of a real valued function over a semi-infinite interval, using the Gaussian-Rational quadrature method of specified order.

Table 160. Data Types		
a, b, Result	Subroutine	
Short-precision real	SGRAQ	
Long-precision real	DGRAQ	

#### **Syntax**

Fortran	SGRAQ   DGRAQ (subf, a, b, n)	
C and C++	C and C++ sgraq   dgraq (subf, a, b, n);	
PL/I	SGRAQ   DGRAQ (subf, a, b, n);	

#### On Entry

#### subf

is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: *t*, *y*, and *n*. For details, see "Programming Considerations for the SUBF Subroutine" on page 920.

Specified as: *subf* must be declared as an external subroutine in your application program. It can be whatever name you choose.

а

has the following meaning, where:

If a+b > 0, it is the lower limit of integration.

If a+b < 0, it is the upper limit of integration.

Specified as: a number of the data type indicated in Table 160.

b

is the centering constant *b* for the integrand. Specified as: a number of the data type indicated in Table 160.

n

is the order of the quadrature method to be used. Specified as: a fullword integer; n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, 96, 128, or 256.

#### On Return

#### Function value

is the approximation of the integral. Returned as: a number of the data type indicated in Table 160.

#### **Notes**

- Declare the DGRAQ function in your program as returning a long-precision real number. Declare the SGRAQ function, if necessary, as returning a short-precision real number.
- 2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by *subf* must agree with the data types specified by this ESSL subroutine. The variable *x*, described under "Function," and the argument *n* correspond to the *subf* arguments *t* and *n*, respectively. For details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 920.

**Function:** The integral is approximated for a real valued function over a semi-infinite interval, using the Gauss-Rational quadrature method of specified order. The region of integration is:

$$(a, \infty)$$
 if  $a+b > 0$   
 $(-\infty, a)$  if  $a+b < 0$ 

The method of order n is theoretically exact for integrals of the following form, where f is a polynomial of degree less than 2n:

$$\int_{a}^{\infty} f\left(\frac{1}{x+b}\right) \frac{1}{\left(x+b\right)^{2}} dx \quad \text{if } a+b > 0$$

$$\int_{-\infty}^{a} f\left(\frac{1}{x+b}\right) \frac{1}{(x+b)^2} dx \quad \text{if } a+b < 0$$

The method of order n is a good approximation when your integrand is closely approximated by a function of the following form, where f is a polynomial of degree less than 2n:

$$f\left(\frac{1}{x+b}\right)\frac{1}{\left(x+b\right)^2}$$

See references [26] and [86]. The result is returned as the function value to a Fortran, C, C++, or PL/I program.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

1. 
$$a+b = 0$$

2. *n* is not an allowable value, as listed in the syntax for this argument.

**Example 1:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = (e^{1.0}/x) / x^2$$

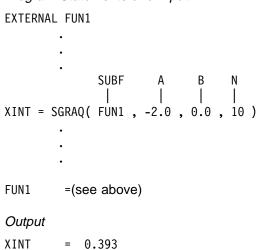
over the interval (-∞, -2.0), using the Gauss-Rational method with 10 points:

$$\int_{-\infty}^{-2.0} \left( \frac{e^{1.0/x}}{x^2} \right) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*),TEMP
DO 1 I=1,N
TEMP=1.0/T(I)
Y(I)=EXP(TEMP)*TEMP**2
RETURN
END
```

#### Program Statements and Input



**Example 2:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = (x-3.0)^{-2} + 10(x-3.0)^{-11}$$

over the interval (4.0, ∞), using the Gauss-Rational method with 6 points:

$$\int_{4.0}^{\infty} \left( \left( x - 3.0 \right)^{-2} + 10 \left( x - 3.0 \right)^{-11} \right) dx$$

The user-supplied subroutine FUN2, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN2 (T,Y,N)
   INTEGER*4 N
   REAL*4 T(*),Y(*),TEMP
   DO 1 I=1,N
        TEMP=1.0/(T(I)-3.0)
1
        Y(I)=TEMP**2+10.0*TEMP**11
   RETURN
   END
Program Statements and Input
EXTERNAL FUN2
              SUBF A B N | I | I
XINT = SGRAQ( FUN2 , 4.0 , -3.0 , 6 )
FUN2
        = (see above)
Output
XINT
        = 2.00
```

## SGHMQ and DGHMQ—Numerical Quadrature Performed on a **Function Using Gauss-Hermite Quadrature**

These functions approximate the integral of a real valued function over the entire real line, using the Gauss-Hermite Quadrature method of specified order.

Table 161. Data Types	
a, b, Result	Subroutine
Short-precision real	SGHMQ
Long-precision real	DGHMQ

#### **Syntax**

Fortran	SGHMQ   DGHMQ (subf, a, b, n)	
C and C++	sghmq   dghmq (subf, a, b, n);	
PL/I	SGHMQ   DGHMQ (subf, a, b, n);	

#### On Entry

#### subf

is the user-supplied subroutine that evaluates the integrand function. The subroutine should be defined with three arguments: t, y, and n. For details, see " Programming Considerations for the SUBF Subroutine" on page 920.

Specified as: subf must be declared as an external subroutine in your application program. It can be whatever name you choose.

is the centering constant a for the exponential. Specified as: a number of the data type indicated in Table 161.

is the scaling constant b for the exponential. Specified as: a number of the data type indicated in Table 161; b > 0.

is the order of the quadrature method to be used. Specified as: a fullword integer; n = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 64, or 96.

#### On Return

n

#### Function value

is the approximation of the integral. Returned as: a number of the data type indicated in Table 161.

#### Notes

- 1. Declare the DGHMQ function in your program as returning a long-precision real number. Declare the SGHMQ function, if necessary, as returning a short-precision real number.
- 2. The subroutine specified for *subf* must be declared as external in your program. Also, data types used by subf must agree with the data types specified by this ESSL subroutine. The variable x, described under "Function" on page 943, and the argument n correspond to the *subf* arguments t and n, respectively. For

details on how to set up the subroutine, see "Programming Considerations for the SUBF Subroutine" on page 920.

**Function:** The integral is approximated for a real valued function over the entire real line, using the Gauss-Hermite Quadrature method of specified order. The region of integration is from  $-\infty$  to  $\infty$ . The method of order n is theoretically exact for integrals of the following form, where f is a polynomial of degree less than 2n:

$$\int_{-\infty}^{\infty} f(x)e^{-b(x-a)^2} dx$$

The method of order n is a good approximation when your integrand is closely approximated by a function of the following form, where f is a polynomial of degree less than 2n:

$$f(x)e^{-b(x-a)^2}$$

See references [26] and [86]. The result is returned as the function value to a Fortran, C, C++, or PL/I program.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $b \le 0$
- 2. *n* is not an allowable value, as listed in the syntax for this argument.

**Example:** This example shows how to compute the integral of the function *f* given by:

$$f(x) = x^2 e^{-2(x+5.0)^2}$$

over the interval  $(-\infty, \infty)$ , using the Gauss-Hermite method with 4 points:

$$\int_{-\infty}^{\infty} \left( x^2 e^{-2(x+5.0)^2} \right) dx$$

The user-supplied subroutine FUN1, which evaluates the integrand function, is coded in Fortran as follows:

```
SUBROUTINE FUN1 (T,Y,N)
INTEGER*4 N
REAL*4 T(*),Y(*)
DO 1 I=1,N
V(I)=T(I)**2*EXP(-2.0*(T(I)+5.0)**2)
RETURN
END
```

```
Program Statements and Input
```

EXTERNAL FUN1 SUBF XINT = SGHMQ( FUN1 , -5.0 , 2.0 , 4 )

FUN1 =(see above)

Output

XINT = 31.646

## **Chapter 16. Random Number Generation**

The random number generation subroutines are described in this chapter.

#### Overview of the Random Number Generation Subroutines

Random number generation subroutines generate uniformly distributed random numbers or normally distributed random numbers (Table 162).

Table 162. List of Random Number Generation Subroutines			
Descriptive Name	Short- Precision Subroutine	Long- Precision Subroutine	Page
Generate a Vector of Uniformly Distributed Random Numbers	SURAND	DURAND	946
Generate a Vector of Normally Distributed Random Numbers	SNRAND	DNRAND	949
Generate a Vector of Long Period Uniformly Distributed Random Numbers	SURXOR	DURXOR	953

#### **Use Considerations**

If you need a very long period random number generator, you should use SURXOR and DURXOR, rather than SURAND and DURAND, respectively. The very long period of the generator used by SURXOR and DURXOR,  $2^{1279}$ –1, makes it useful in modern statistical simulations in which the shorter period of other generators can be exhausted during a single run. As a result, if you need a large number of random numbers, you can use these subroutines, because with this generator, you are not be requesting more than a small percentage of the entire period of the generator.

#### **Random Number Generation Subroutines**

This section contains the random number generation subroutine descriptions.

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# SURAND and DURAND—Generate a Vector of Uniformly Distributed Random Numbers

These subroutines generate vector  $\mathbf{x}$  of uniform (0,1) pseudo-random numbers, using the multiplicative congruential method with a user-specified seed.

Table 163. Data Types		
x	seed	Subroutine
Short-precision real	Long-precision real	SURAND
Long-precision real	Long-precision real	DURAND

**Note:** If you need a very long period random number generator, use SURXOR and DURXOR instead of these subroutines.

#### **Syntax**

Fortran	CALL SURAND   DURAND (seed, n, x)	
C and C++	surand   durand (seed, n, x);	
PL/I	CALL SURAND   DURAND (seed, n, x);	

#### On Entry

#### seed

is the initial value used to generate the random numbers. Specified as: a number of the data type indicated in Table 163. It should be a whole number; that is, the fraction part should be 0. (If you specify a mixed number, it is truncated.) Its value must be  $1.0 \le seed < (2147483647.0 = 2^{31}-1)$ .

**Note:** seed is always a long-precision real number, even in SURAND.

*n* is the number of random numbers to be generated. Specified as: a fullword integer;  $n \ge 0$ .

See "On Return."

#### On Return

#### seed

is the new seed that is to be used to generate additional random numbers in subsequent invocations of SURAND or DURAND. Returned as: a number of the data type indicated in Table 163. It is a whole number whose value is  $1.0 \le seed < (2147483647.0 = 2^{31}-1)$ .

is a vector of length *n*, containing the uniform pseudo-random numbers with values between 0 and 1. Returned as: a one-dimensional array of (at least) length *n*, containing numbers of the data type indicated in Table 163.

**Note:** In your C program, argument *seed* must be passed by reference.

**Function:** The uniform (0,1) pseudo-random numbers are generated as follows, using the multiplicative congruential method:

$$s_i = (a(s_{i-1})) \mod(m) = (a^i s_0) \mod(m)$$
  
 $x_i = s/m \text{ for } i = 1, 2, ..., n$ 

#### where:

 $s_i$  is a random sequence.

 $x_i$  is a random number.

 $s_0$  is the initial seed provided by the caller.

$$a = 7^5 = 16807.0$$

$$m = 2^{31} - 1 = 2147483647.0$$

*n* is the number of random numbers to be generated.

See references [70] and [74]. If n is 0, no computation is performed, and the initial seed is unchanged.

#### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2.  $seed < 1.0 \text{ or } seed \ge 2147483647.0$

**Example 1:** This example shows a call to SURAND to generate 10 random numbers.

Call Statement and Input

SEED = 80629.0

**Note:** It is important to note that SEED is a long-precision number, even though X contains short-precision numbers.

#### Output

**Example 2:** This example shows a call to DURAND to generate 10 random numbers.

#### **SURAND** and **DURAND**

0.1603607578018497, 0.1832563756887132, 0.9899062002030695, 0.3535068129904134)

# SNRAND and DNRAND—Generate a Vector of Normally Distributed Random Numbers

These subroutines generate vector  $\mathbf{x}$  of normally distributed pseudo-random numbers, with a mean of 0 and a standard deviation of 1, using Polar methods with a user-specified seed.

Table 164. Data Types		
<b>x</b> , aux	seed	Subroutine
Short-precision real	Long-precision real	SNRAND
Long-precision real	Long-precision real	DNRAND

#### Syntax

Fortran	CALL SNRAND   DNRAND (seed, n, x, aux, naux)	
C and C++	snrand   dnrand (seed, n, x, aux, naux);	
PL/I	CALL SNRAND   DNRAND (seed, n, x, aux, naux);	

#### On Entry

#### seed

is the initial value used to generate the random numbers. Specified as: a number of the data type indicated in Table 164. It must be a whole number; that is, the fraction part must be 0. Its value must be  $1.0 \le seed < (2147483647.0 = 2^{31}-1)$ .

**Note:** seed is always a long-precision real number, even in SNRAND.

n

is the number of random numbers to be generated. Specified as: a fullword integer; n must be an even number and  $n \ge 0$ .

Χ

See "On Return."

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size must be greater than or equal to n/2.

Specified as: an area of storage, containing numbers of the data type indicated in Table 164. They can have any value.

#### naux

is the size of the work area specified by *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, SNRAND and DNRAND dynamically allocate the work area used by the subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n/2$ .

#### On Return

seed

is the new seed that is to be used to generate additional random numbers in subsequent invocations of SNRAND or DNRAND. Returned as: a number of the data type indicated in Table 164. It is a whole number whose value is  $1.0 \le seed < (2147483647.0 = 2^{31}-1)$ .

Χ

is a vector of length n, containing the normally distributed pseudo-random numbers. Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 164 on page 949.

#### Notes

- 1. In your C program, argument seed must be passed by reference.
- 2. Vector **x** must have no common elements with the storage area specified for *aux*; otherwise, results are unpredictable.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** The normally distributed pseudo-random numbers, with a mean of 0 and a standard deviation of 1, are generated as follows, using Polar methods with a user-specified seed. The Polar method, which this technique is based on, was developed by G. E. P. Box, M. E. Muller, and G. Marsaglia and is described in reference [70].

- 1. Using *seed*, a vector of uniform (0,1) pseudo-random numbers,  $u_i$  for i = 1, n, is generated by calling SURAND or DURAND, respectively. These  $u_i$  values are then used in the subsequent steps.
- 2. All  $(y_j, z_j)$  for j = 1, n/2 are set as follows, where each (y, z) is a point in the square -1 to 1:

$$y_j = 2u_{2j-1} - 1$$
  
$$z_i = 2u_{2j} - 1$$

3. All  $p_j$  for j = 1, n/2 are set as follows, where each p measures the square of the radius of (y, z):

$$p_i = y_i^2 + z_i^2$$

If  $p_i \ge 1$ , then  $p_i$  is discarded, and steps 1 through 3 are repeated until  $p_i < 1$ .

4. All  $x_i$  for i = 1, n are set as follows to produce the normally distributed random numbers:

$$x_{2j-1} = y_j ((-2 \ln p_j) / p_j)^{0.5}$$
  
 $x_{2j} = z_j ((-2 \ln p_j) / p_j)^{0.5}$   
for  $j = 1$ ,  $n/2$ 

If *n* is 0, no computation is performed, and the initial seed is unchanged.

#### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

#### Input-Argument Errors

- 1. n < 0 or n is an odd number
- 2.  $seed < 1.0 \text{ or } seed \ge 2147483647.0$
- 3. Error 2015 is recoverable or *naux*≠0, and *naux* is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

Example 1: This example shows a call to SNRAND to generate 10 random numbers.

#### Call Statement and Input

Note: It is important to note that SEED is a long-precision number, even though X contains short-precision numbers.

#### Output

```
SEED
         = 48669425.0
Χ
       = (0.660649538,
             1.312503695,
             1.906438112,
             0.014065863,
            -0.800935328,
            -3.058144093,
            -0.397426069,
            -0.370634943,
            -0.064151444,
            -0.275887042)
```

Example 2: This example shows a call to DNRAND to generate 10 random numbers.

#### Call Statement and Input

Output

#### **SNRAND and DNRAND**

SEED = 48669425.0 Χ = (0.6606495655963802, 1.3125037758861060, 1.9064381379483730, 0.0140658628770495, -0.8009353314494653, -3.0581441239248530, -0.3974260845722100, -0.3706349643478605, -0.0641514443372939, -0.2758870630332470)

# SURXOR and DURXOR—Generate a Vector of Long Period Uniformly Distributed Random Numbers

These subroutines generate a vector  $\mathbf{x}$  of uniform [0,1) pseudo-random numbers, using the Tausworthe exclusive-or algorithm.

Table 165. Data Types		
x, vseed	iseed	Subroutine
Short-precision real	Integer	SURXOR
Long-precision real	Integer	DURXOR

#### Syntax

Fortran	CALL SURXOR   DURXOR (iseed, n, x, vseed)
C and C++	surxor   durxor (iseed, n, x, vseed);
PL/I	CALL SURXOR   DURXOR (iseed, n, x, vseed);

#### On Entry

#### iseed

has the following meaning, where:

If  $iseed \neq 0$ , iseed is the initial value used to generate the random numbers. You specify  $iseed \neq 0$  when you call this subroutine for the first time or when you changed vseed between calls to this subroutine.

If *iseed* = 0, *vseed* is used to generate the random numbers, where *vseed* was initialized by an earlier call to this subroutine. ESSL assumes you have not changed *vseed* between calls to this subroutine, when you specify *iseed* = 0.

Specified as: a fullword integer, as indicated in Table 165.

*n* is the number of random numbers to be generated. Specified as: a fullword integer;  $n \ge 0$ .

x See "On Return."

#### vseed

is the work area used by this subroutine and has the following meaning, where:

If iseed ≠ 0, vseed is not used for input. The work area can contain anything.

If *iseed* = 0, *vseed* contains the seed vector generated by a preceding call to this subroutine. *vseed* is used in this computation to generate the new random numbers. It should not be changed between calls to this subroutine.

Specified as: a one-dimensional array of (at least) length 10000, containing numbers of the data type indicated in Table 165.

#### On Return

#### iseed

is set to 0 for subsequent calls to SURXOR or DURXOR. Returned as: a fullword integer, as indicated in Table 165.

х

is a vector of length n, containing the uniform pseudo-random numbers with the following values:  $0 \le x < 1$ . Returned as: a one-dimensional array of (at least) length n, containing numbers of the data type indicated in Table 165.

#### vseed

is the work area used by these subroutines, containing the new seed that is to be used in subsequent calls to this subroutine. Returned as: a one-dimensional array of (at least) length 10000, containing numbers of the data type indicated in Table 165 on page 953.

#### Notes

- 1. You can generate the same vector *x* of random numbers by starting over and specifying your original nonzero *iseed* value.
- 2. Multiple calls to these subroutines with mixed sizes generate the same sequence of numbers as a single call the total length, assuming you specify the same initial *iseed* in both cases. For example, you can generate the same vector *x* of random numbers by calling this subroutine twice and specifying *n* = 10 or by calling this subroutine once and specifying *n* = 20. You need to specify the same *iseed* in the initial call in both cases, and *iseed* = 0 in the second call with *n* = 10.
- 3. Vector **x** must have no common elements with the storage area specified for *vseed*; otherwise, results are unpredictable.
- 4. In your C program, argument *iseed* must be passed by reference.

**Function:** The pseudo-random numbers uniformly distributed in the interval [0,1) are generated using the Tausworthe exclusive-or algorithm. This is based on a linear-feedback shift-register sequence. The very long period of the generator, 2<sup>1279</sup>–1, makes it useful in modern statistical simulations where the shorter period of other generators could be exhausted during a single run. If you need a large number of random numbers, you can use these subroutines, because with this generator you do not request more than a small percentage of the entire period of the generator.

This generator is based on two feedback positions to generate a new binary digit:

$$z_k = z_{(k-p)} \oplus z_{(k-q)}$$

where:

$$p > q$$
  
 $k = 1, 2, ...$   
 $z$  is a bit vector.  
and where:

 $\oplus$  is the bitwise exclusive - or operation.

For details, see references [50], [68], and [88]. The values of p and q are selected according to the criteria stated in reference [94].

The algorithm initializes a seed vector of length p, starting with *iseed*. The seed vector is stored in *vseed* for use in subsequent calls to this subroutine with iseed = 0.

If *n* is 0, no computation is performed, and the initial seed is unchanged.

**Special Usage:** For some specialized applications, if you need multiple sources of random numbers, you can specify different *vseed* areas, which are initialized with different seeds on multiple calls to this subroutine. You then get multiple sequences of the random number sequence provided by the generator that are sufficiently far apart for most purposes.

#### **Error Conditions**

Computational Errors: None.

Input-Argument Errors

- 1. n < 0
- 2. *iseed* = 0 and *vseed* does not contain valid data.

**Example 1:** This example shows a call to SURXOR to generate 10 random numbers.

Call Statement and Input

```
CALL SURXOR( ISEED , 10 , X , VSEED )
ISEED
         = 137
Output
ISEED
         = 0
       = (0.6440868,
            0.5105118,
            0.4878680,
             0.3209075,
             0.6624528,
             0.2499877,
             0.0056630,
             0.7329214,
             0.7486335,
             0.8050517)
```

**Example 2:** This example shows a call to SURXOR to generate 10 random numbers. This example specifies iseed = 0 and uses the vseed output generated from Example 1.

Call Statement and Input

```
ISEED N X VSEED

| | | | |
CALL SURXOR( ISEED , 10 , X , VSEED )

ISEED = 0
```

# Output ISEED = 0 X = (0.9930249, 0.0441873, 0.6891295, 0.3101060, 0.6324178, 0.3299408, 0.3553145, 0.0100013, 0.0214620, 0.8059390)

**Example 3:** This example shows a call to DURXOR to generate 20 random numbers. This sequence of numbers generated are like those generated in Examples 1 and 2.

#### Call Statement and Input

```
ISEED
                      N X VSEED
CALL DURXOR( ISEED , 20 , X , VSEED )
ISEED
         = 137
Output
ISEED
χ
             (0.64408693438956721,
              0.51051182536460882,
              0.48786801310787142,
              0.32090755617007050,
              0.66245283144861666,
              0.24998782843358081,
              0.00566308101257373,
              0.73292147005172925,
              0.74863359794102236,
              0.80505169697755319,
              0.99302499462139138,
              0.04418740640269125,
              0.68912952155409579,
              0.31010611495627916,
              0.63241786342211936,
              0.32994081459690583,
              0.35531452631408911,
              0.01000134413132581,
              0.02146199494672940,
              0.80593898487597615)
```

## Chapter 17. Utilities

The utility subroutines are described in this chapter.

## **Overview of the Utility Subroutines**

The utility subroutines perform general service functions that support ESSL, rather than mathematical computations (Table 166).

Table 166. List of Utility Subroutines		
Descriptive Name	Subroutine	Page
ESSL Error Information-Handler Subroutine	EINFO	960
ESSL ERRSAV Subroutine for ESSL	ERRSAV	963
ESSL ERRSET Subroutine for ESSL	ERRSET	964
ESSL ERRSTR Subroutine for ESSL	ERRSTR	966
Set the Vector Section Size (VSS) for the ESSL/370 Scalar Library	IVSSET‡	
Set the Extended Vector Operations Indicator for the ESSL/370 Scalar Library	IEVOPS‡	
Determine the Level of ESSL Installed	IESSL	967
Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines	STRIDE	969
Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode	DSRSM	979
For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DGKTRN	983
For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode	DSKTRN	989

<sup>‡</sup> This subroutine is provided for migration from earlier releases of ESSL and is not intended for use in new programs. Documentation for this subroutines is no longer provided.

#### **Use Considerations**

This section describes what you use the utility subroutines for.

## **Determining the Level of ESSL Installed**

IESSL gets the level of ESSL and returns it to your program. The level consists of the following: version number, release number, modification number, and number of the most recently installed ESSL PTF. You can use this function to verify that you are running on or using the capabilities of the desired level.

## Finding the Optimal Stride(s) for Your Fourier Transforms

STRIDE is used to determine optimal stride values for your Fourier transforms when using any of the Fourier transform subroutines, except \_RCFT and \_CRFT. You must invoke STRIDE for each optimal stride you want computed. Sometimes you need a separate stride for your input and output data. For the three-dimensional Fourier transforms, you need an optimal stride for both the

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second and third dimensions of the array. The examples provided for STRIDE explain how it is used for each of the subroutines listed above.

After obtaining the optimal strides from STRIDE, you should arrange your data using these stride values. After the data is set up, call the Fourier transform subroutine. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

### **Converting Sparse Matrix Storage**

DSRSM is used to migrate your existing program from sparse matrices stored by rows to sparse matrices stored in compressed-matrix storage mode. This converts the matrices into a storage format that is compatible with the input requirements for some ESSL sparse matrix subroutines, such as DSMMX.

DGKTRN and DSKTRN are used to convert your sparse matrix from one skyline storage mode to another, if necessary, before calling the subroutines DGKFS/DGKFSP or DSKFS/DSKFSP, respectively.

# **Utility Subroutines**

This section contains the utility subroutine descriptions.

#### **EINFO—ESSL Error Information-Handler Subroutine**

This subroutine returns information to your program about the data involved in a computational error that occurred in an ESSL subroutine. This is the same information that is provided in the ESSL messages; however, it allows you to check the information in your program at run time and continue processing. You pass the computational error code of interest to this subroutine in *icode*, and it passes back one or more pieces of information in the output arguments *inf1* and, optionally, *inf2*, as defined in Table 167. You should use this subroutine only for those computational errors listed in the table. It does not apply to computational errors that do not return information.

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see "Example of Handling Errors in a Multithreaded Application Program" on page 127.

Table 167.	. Computational I	Error Information Returned by EINFO
Error Code	Receiver	Type of Information
2100	inf1	Lower range of a vector
	inf2	Upper range of a vector
2101	inf1	Index of the eigenvalue that failed to converge
	inf2	Number of iterations after which it failed to converge
2102	inf1	Index of the last eigenvector that failed to converge
	inf2	Number of iterations after which it failed to converge
2103	inf1	Index of the pivot with zero value
2104	inf1	Index of the last pivot with nonpositive value
2105	inf1	Index of the pivot element near zero causing factorization to fail
2107	inf1	Index of the singular value that failed to converge
	inf2	Number of iterations after which it failed to converge
2109	inf1	Iteration count when it was determined that the matrix was not definite
2114	inf1	Index of the last eigenvalue that failed to converge
	inf2	Number of iterations after which it failed to converge
2115	inf1	Order of the leading minor that was discovered to have a nonpositive determinant
2117	inf1	Column number for which pivot value was near zero
2118	inf1	Row number for which pivot value was near zero
2120	inf1	Row number of empty row where factorization failed
2121	inf1	Column number of empty column where factorization failed
2126	inf1	Row number for which pivot value was unacceptable
2145	inf1	First diagonal element with zero value

#### Syntax

Fortran	CALL EINFO (icode[, inf1[, inf2]])
C and C++	einfo (icode, inf1, inf2);
PL/I	CALL EINFO (icode[, inf1[, inf2]]);

#### On Entry

#### icode

has the following meaning, where:

If icode = 0, this indicates that the ESSL error option table is to be initialized. (You specify this value once in the beginning of your program before calls to ERRSET.)

If *icode* has any of the allowable error code values listed in Table 167 on page 960, this is the computational error code of interest. (You specify one of these values whenever you want information returned about a computational error.)

Specified as: a fullword integer; *icode* = 0 or an error code value indicated in Table 167 on page 960.

#### inf1

See "On Return."

inf2

See "On Return."

#### On Return

#### inf1

has the following meaning, where:

If *icode* = 0, this argument is not used in the computation. In this case, *inf1* is an optional argument, except in C and C++ programs.

If  $icode \neq 0$ , then inf1 is the first information receiver, containing numerical information related to the computational error.

Returned as: a fullword integer.

#### inf2

has the following meaning, where:

If *icode* = 0, this argument is not used in the computation.

If  $icode \neq 0$ , then inf2 is the second information receiver, containing numerical information related to the computational error. It should be specified when the error code provides a second piece of information, and you want the information.

In both of these cases, *inf2* is an optional argument, except in C and C++ programs. For more details, see "Notes."

Returned as: a fullword integer.

#### Notes

1. If *icode* is not 0 and is not one of the error codes specified in Table 167 on page 960, this subroutine returns to the caller, and no information is provided in *inf1* and *inf2*.

- 2. If there are two pieces of information for the error and you specify one output argument, the second piece of information is not returned to the caller.
- 3. If there is one piece of information for the error and you specify two output arguments, the second output argument is not set by this subroutine.
- 4. In C and C++ programs you must code the inf1 and inf2 arguments, because they are not optional arguments.
- 5. In Fortran programs, inf1 and inf2 are optional arguments. This is an exception to the rule, because other ESSL subroutines do not allow optional arguments.
- 6. Examples of how to use EINFO are provided in Chapter 4 on page 111.

#### ERRSAV—ESSL ERRSAV Subroutine for ESSL

The ERRSAV subroutine copies an ESSL error option table entry into an 8-byte storage area that is accessible to your program.

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see "Example of Handling Errors in a Multithreaded Application Program" on page 127.

#### **Syntax**

Fortran	CALL ERRSAV (ierno, tabent)
C and C++	errsav (ierno, tabent);
PL/I	CALL ERRSAV (ierno, tabent);

#### On Entry

#### ierno

is the error number in the option table. The entry for *ierno* in the ESSL error option table is stored in the 8-byte storage area *tabent*. Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 26 on page 51.

#### tabent

is the storage area where the option table entry is stored. Specified as: an area of storage of length 8-bytes.

Note: Examples of how to use ERRSAV are provided in Chapter 4 on page 111.

#### ERRSET—ESSL ERRSET Subroutine for ESSL

The ERRSET subroutine allows you to control execution when error conditions occur. It modifies the information in the ESSL error option table for the error number indicated. For a range of error messages, you can specify the following:

- How many times a particular error is allowed to occur before the program is terminated
- How many times a particular error message is printed before printing is suppressed
- · Whether the ESSL error exit routine is to be invoked

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see "Example of Handling Errors in a Multithreaded Application Program" on page 127.

#### Syntax

Fortran	CALL ERRSET (ierno, inoal, inomes, itrace, iusadr, irange)
C and C++	errset (ierno, inoal, inomes, itrace, iusadr, irange);
PL/I	CALL ERRSET (ierno, inoal, inomes, itrace, iusadr, irange);

#### On Entry

#### ierno

is the error number in the option table. The entry for *ierno* in the ESSL error option table is updated as indicated by the other arguments. Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 26 on page 51.

#### inoal

indicates the number of errors allowed before each execution is terminated, where:

If  $inoal \le 0$ , the specification is ignored, and the number-of-errors option is not changed.

If inoal = 1, execution is terminated after one error.

If  $2 \le inoal \le 255$ , then *inoal* specifies the number of errors allowed before each execution is terminated.

If inoal > 255, an unlimited number of errors is allowed.

Specified as: a fullword integer, where:

If iusadr = ENOTRM, then  $2 \le inoal \le 255$ .

#### inomes

indicates the number of messages to be printed, where:

If inomes < 0, all messages are suppressed.

If *inomes* = 0, the number-of-messages option is not changed.

If  $0 < inomes \le 255$ , then *inomes* specifies the number of messages to be printed.

If inomes > 255, an unlimited number of error messages is allowed.

Specified as: a fullword integer.

#### itrace

this argument is ignored, but must be specified. Specified as: a fullword integer where, *itrace* = 0, 1, or 2 (for migration purposes).

#### iusadr

indicates whether or not the ESSL error exit routine is to be invoked, where:

If *iusadr* is zero, the option table is not altered.

If *iusadr* is one, the option table is set to show no exit routine. Therefore, standard corrective action is to be used when continuing execution.

If *iusadr* = ENOTRM, the option table entry is set to the ESSL error exit routine ENOTRM. Therefore, the ENOTRM subroutine is to be invoked after the occurrence of the indicated errors. (ENOTRM must appear in an EXTERNAL statement in your program.)

Specified as: a 32-bit integer in a 32-bit environment or the name of a subroutine; iusadr = 0, 1, or ENOTRM.

Specified as: a 64-bit integer in a 64-bit environment or the name of a subroutine; *iusadr* = 0 8, 1 8, or ENOTRM.

#### irange

indicates the range of errors to be updated in the ESSL error option table, where:

If *irange* < *ierno*, the parameter is ignored.

If  $irange \ge ierno$ , the options specified for the other parameters are to be applied to the entire range of error conditions encompassed by ierno and irange.

Specified as: a fullword integer.

#### Notes

- 1. Examples of how to use ERRSET are provided in Chapter 4 on page 111.
- 2. If you specify ENOTRM for *iusadr*, then *inoal* must be in the following range:  $2 \le inoal \le 255$ .

#### ERRSTR—ESSL ERRSTR Subroutine for ESSL

The ERRSTR subroutine stores an entry in the ESSL error option table.

For multithreaded application programs, if you want the error handling capabilities that this subroutine provides to be implemented on each thread created by your program, this subroutine must be called from each thread. If your application creates multiple threads, the action performed by a call to this subroutine applies to the thread that this subroutine was invoked from. For an example, see "Example of Handling Errors in a Multithreaded Application Program" on page 127.

#### Syntax

Fortran	CALL ERRSTR (ierno, tabent)
C and C++	errstr (ierno, tabent);
PL/I	CALL ERRSTR (ierno, tabent);

#### On Entry

#### ierno

is the error number in the option table. The information in the 8-byte storage area *tabent* is stored into the entry for *ierno* in the ESSL error option table. Specified as: a fullword integer; *ierno* must be one of the error numbers in the option table. For a list of these numbers, see Table 26 on page 51.

#### tabent

is the storage area containing the table entry data. Specified as: an area of storage of length 8-bytes.

Note: Examples of how to use ERRSTR are provided in Chapter 4 on page 111.

#### **IESSL—Determine the Level of ESSL Installed**

This function returns the level of ESSL installed on your system, where the level consists of a version number, release number, and modification number, plus the fix number of the most recent PTF installed.

#### Syntax

Fortran	CALL IESSL ()
C and C++	iessl ();
PL/I	CALL IESSL ();

#### On Return

Function value

is the level of ESSL installed on your system. It is provided as a fullword integer in the form *vvrrmmff*, where each two digits represents a part of the level:

- vv is the version number.
- rr is the release number.
- mm is the modification number.
- ff is the fix number of the most recent PTF installed.

Returned as: a fullword integer; vvrrmmff > 0.

#### Notes

- To use IESSL effectively, you must install your ESSL PTFs in their proper sequential order. As part of the result, IESSL returns the value ff of the most recent PTF installed, rather than the highest number PTF installed. Therefore, if you do not install your PTFs sequentially, the ff value returned by IESSL does not reflect the actual level of ESSL.
- 2. Declare the IESSL function in your program as returning a fullword integer value.

**Function:** The IESSL function enables you to determine the current level of ESSL installed on your system. It is useful to you in those instances where your program is using a subroutine or feature that exists only in certain levels of ESSL. It is also useful when your program is dependent upon certain PTFs being applied to ESSL.

**Example:** This example shows several ways to use the IESSL function. Most typically, you use IESSL for checking the version and release level of ESSL. Suppose you are dependent on a new capability in ESSL, such as a new subroutine or feature, provided for the first time in ESSL Version 3. You can add the following check in your program before using the new capability:

IF IESSL()  $\geq$  3010000

By specifying 0000 for *mmff*, the modification and fix level, you are independent of the order in which your modifications and PTFs are installed.

Less typically, you use IESSL for checking the PTF level of ESSL. Suppose you are dependent on PTF 2 being installed on your ESSL Version 3 system. You want

to know whether to call a different user-callable subroutine to set up your array data. You can add the following check in your program before making the call:

IF IESSL()  $\geq$  3010002

If your system support group installed the ESSL PTFs in their proper sequential order, this test works properly; otherwise, it is unpredictable.

# STRIDE—Determine the Stride Value for Optimal Performance in Specified Fourier Transform Subroutines

This subroutine determines an optimal stride value for you to use for your input or output data when you are computing large row Fourier transforms in any of the Fourier transform subroutines, except \_RCFT and \_CRFT. The strides determined by this subroutine allow your arrays to fit comfortably in various levels of storage hierarchy on your particular processor, thus allowing you to improve your run-time performance.

**Note:** This subroutine returns a single stride value. Where you need multiple strides, you must invoke this subroutine multiple times; for example, in the multidimensional Fourier transforms and, also, when input and output data types differ. For more details, see "Function" on page 970.

#### Syntax

Fortran	CALL STRIDE (n, incd, incr, dt, iopt)
C and C++	stride (n, incd, incr, dt, iopt);
PL/I	CALL STRIDE (n, incd, incr, dt, iopt);

#### On Entry

n

is the length n of the Fourier transform for which the optimal stride is being determined. The transform corresponding to n is usually a row transform; that is, the data elements are stored using a stride value.

Specified as: a fullword integer; n > 0.

incd

is the minimum allowable stride for the Fourier transform for which the optimal stride is being determined. For each situation in each subroutine, there is a specific way to compute this minimum value. This is explained in the examples starting on page 971.

Specified as: a fullword integer; incd > 0 or incd < 0.

incr

See "On Return" on page 970.

dt

is the data type of the numbers for the Fourier transform for which the optimal stride is being determined, where:

If dt = 'S', the numbers are short-precision real.

If dt = 'D', the numbers are long-precision real.

If  $dt = {}^{\mathsf{L}}\mathsf{C}^{\mathsf{L}}$ , the numbers are short-precision complex.

If dt = 'Z', the numbers are long-precision complex.

Specified as: a single character; dt = 'S', 'D', 'C', or 'Z'.

iopt

is provided only for migration purposes from ESSL Version 1 and is no longer used; however, you must still specify it as a dummy argument. Specified as: a fullword integer; iopt = 0, 1, or 2.

#### On Return

incr

is the stride that allows you to improve your run-time performance in your Fourier transform computation on your particular processor. In general, this value differs for each processor you are running on.

Returned as: a fullword integer; incr > 0 or incr < 0 and  $|incr| \ge |incd|$ , where incr has the same sign (+ or –) as incd.

#### Notes

- 1. In your C program, argument incr must be passed by reference.
- 2. All subroutines accept lowercase letters for the dt argument.
- 3. For each situation in each of the Fourier transform subroutines, there is a specific way to compute the value you should specify for the *incd* argument. Details on how to compute each of these values is given in the examples starting on page 971. See the example corresponding to the Fourier transform subroutine you are using.
- 4. Where different data types are specified for the input and output data in your Fourier transform subroutine, you should be careful to indicate the correct data type in the *dt* argument in this subroutine.
- 5. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

**Function:** This subroutine determines an optimal stride, *incr*, for you to use for your input or output data when computing large row Fourier transforms. The stride value returned by this subroutine is based on the size and structure of your transform data, using:

- The size of each data item (dt)
- The minimum allowable stride for this transform (incd)
- The length of the transform (n)

This information is used in determining the optimal stride for the processor you are currently running on. The stride determined by this subroutine allows your arrays to fit comfortably in various levels of storage hierarchy for that processor, thus giving you the ability to improve your run-time performance.

You get only one stride value returned by this subroutine on each invocation. Therefore, in many instances, you may need to invoke this subroutine multiple times to obtain several stride values to use in your Fourier transform computation:

- For multidimensional Fourier transforms using several strides, this subroutine
  must be called once for each optimal stride you want to obtain. Successive
  invocations should go from the lower (earlier) dimensions to the higher (later)
  dimensions, because the results from the lower dimensions are used to
  calculate the *incd* values for the higher dimensions.
- Where input and output data have different data types and you want to obtain optimal strides for each, this subroutine must be called once for each data type.

Where multiple invocations are necessary, they are explained in the examples starting on page 971. The examples also explain how to calculate the *incd* values

for each invocation. There are nine examples to cover the Fourier transform subroutines that can use the STRIDE subroutine.

After calling this subroutine and obtaining the optimal stride value, you then set up your input or output array accordingly. This may involve movement of data for input arrays or increasing the sizes of input or output arrays. To accomplish this, you may want to set up a separate subroutine with the stride values passed into it as arguments. You can then dimension your arrays in that subroutine, depending on the values calculated by STRIDE. For additional information on how to set up your data, see "Setting Up Your Data" on page 742.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $n \le 0$
- 2. incd = 0
- 3.  $iopt \neq 0, 1, or 2$
- 4.  $dt \neq S$ , D, C, or Z

Example 1—SCFT: This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the SCFT subroutine.

If inc2x = 1, the input sequences are stored in the transposed form as rows of a two-dimensional array X(INC1X,N). In this case, the STRIDE subroutine helps in determining a good value of inc1x for this array. The required minimum value of inc1x is m, the number of Fourier transforms being computed. To find a good value of *inc1x*, use STRIDE as follows:

Here, the arguments refer to the SCFT subroutine. In the following table, values of inc1x are given (as obtained from the STRIDE subroutine) for some combinations of *n* and *m* and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N	М	INC1X
128	64	64
240	32	32
240	64	65
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form (inc2y = 1). In that case, in the above example, inc1x is replaced by inc1y.

In computing column transforms (inc1x = inc1y = 1), the values of inc2x and inc2yare not very important. For these, any value over the required minimum of n can be used.

Example 2—DCOSF: This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the DCOSF subroutine.

If inc2x = 1, the input sequences are stored in the transposed form as rows of a two-dimensional array X(INC1X,N/2+1). In this case, the STRIDE subroutine helps in determining a good value of inc1x for this array. The required minimum value of inc1x is m, the number of Fourier transforms being computed. To find a good value of inc1x, use STRIDE as follows:

Here, the arguments refer to the DCOSF subroutine. In the following table, values of inc1x are given (as obtained from the STRIDE subroutine) for some combinations of n and m and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N	М	INC1X
128	64	64
240	32	32
240	64	64
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form (inc2y = 1). In that case, in the above example, inc1x is replaced by inc1y.

In computing column transforms (inc1x = inc1y = 1), the values of inc2x and inc2yare not very important. For these, any value over the required minimum of n/2+1 can be used.

Example 3—DSINF: This example shows the use of the STRIDE subroutine in computing one-dimensional row transforms using the DSINF subroutine.

If inc2x = 1, the input sequences are stored in the transposed form as rows of a two-dimensional array X(INC1X,N/2). In this case, the STRIDE subroutine helps in determining a good value of inc1x for this array. The required minimum value of inc1x is m, the number of Fourier transforms being computed. To find a good value of *inc1x*, use STRIDE as follows:

Here, the arguments refer to the DSINF subroutine. In the following table, values of inc1x are given (as obtained from the STRIDE subroutine) for some combinations of *n* and *m* and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N	М	INC1X
128	64	64
240	32	32
240	64	64
256	256	264
512	60	60
1024	64	65

The above example also applies when the output sequences are stored in the transposed form (inc2y = 1). In that case, in the above example, inc1x is replaced by inc1y.

In computing column transforms (inc1x = inc1y = 1), the values of inc2x and inc2yare not very important. For these, any value over the required minimum of n/2 can be used.

Example 4—SCFT2: This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SCFT2 subroutine.

If inc1y = 1, the two-dimensional output array is stored in the normal form. In this case, the output array can be declared as Y(INC2Y, N2), where the required minimum value of inc2y is n1. The STRIDE subroutine helps in picking a good value of *inc2y*. To find a good value of *inc2y*, use STRIDE as follows:

Here, the arguments refer to the SCFT2 subroutine. In the following table, values of inc2y are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with n1 = n2 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1	N2	INC2Y
64	64	64
128	128	136
240	240	240
512	512	520
840	840	848

If the input array is stored in the normal form (inc1x = 1), the value of inc2x is not important. However, if you want to use the same array for input and output, you should use inc2x = inc2y.

If inc2y = 1, the two-dimensional output array is stored in the transposed form. In this case, the output array can be declared as Y(INC1Y,N1), where the required minimum value of inc1y is n2. The STRIDE subroutine helps in picking a good value of inc1y. To find a good value of inc1y, use STRIDE as follows:

Here, the arguments refer to the SCFT2 subroutine. In the following table, values of inc1y are given (as obtained from the STRIDE subroutine) for some combinations

of n1 and n2 and for POWER2-P2SC with 64K level 1 cache using the POWER2 library for ESSL:

N1	N2	INC1Y
60	64	64
120	128	136
256	240	240
512	512	520
840	840	848

If the input array is stored in the transposed form (inc2x = 1), the value of inc1x is also important. The above example can be used to find a good value of inc1x, by replacing inc1y with inc1x. If both arrays are stored in the transposed form, a good value for inc1y is also a good value for inc1x. In that situation, the two arrays can also be made equivalent.

**Example 5—SRCFT2:** This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SRCFT2 subroutine.

For this subroutine, the output array is declared as Y(INC2Y,N2), where the required minimum value of inc2y is n1/2+1. The STRIDE subroutine helps in picking a good value of inc2y. To find a good value of inc2y, use STRIDE as follows:

Here, the arguments refer to the SRCFT2 subroutine. In the following table, values of inc2y are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with n1 = n2 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1	N2	INC2Y
240	240	121
420	420	211
512	512	257
840	840	421
1024	1024	513
2048	2048	1032

For this subroutine, the leading dimension of the input array (inc2x) is not important. If you want to use the same array for input and output, you should use  $inc2x \ge 2(inc2y)$ .

Example 6—SCRFT2: This example shows the use of the STRIDE subroutine in computing two-dimensional transforms using the SCRFT2 subroutine.

For this subroutine, the output array is declared as Y(INC2Y,N2), where the required minimum value of inc2y is n1+2. The STRIDE subroutine helps in picking a good value of inc2y. To find a good value of inc2y, use STRIDE as follows:

Here, the arguments refer to the SCRFT2 subroutine. In the following table, values of inc2y are given (as obtained from the STRIDE subroutine) for some two-dimensional arrays with n1 = n2 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1	N2	INC2Y
240	240	242
420	420	422
512	512	514
840	840	842
1024	1024	1026
2048	2048	2064

For this subroutine, the leading dimension of the input array (inc2x) is also important. In general, inc2x = inc2y/2 is a good choice. This is also the requirement if you want to use the same array for input and output.

Example 7—SCFT3: This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SCFT3 subroutine.

For this subroutine, the strides for the input array are not important. They are important for the output array. The STRIDE subroutine helps in picking good values of inc2y and inc3y. This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for inc2y. The minimum acceptable value for inc2y is n1.

Here, the arguments refer to the SCFT3 subroutine. Next, you should find a good value for inc3y. The minimum acceptable value for inc3y is (n2)(inc2y).

If inc3y turns out to be a multiple of inc2y, then Y can be declared a three-dimensional array as Y(INC2Y,INC3Y/INC2Y,N3). For large problems, this may not happen. In that case, you can declare the Y array as a two-dimensional array Y(0:INC3Y-1,0:N3-1) or a one-dimensional array Y(0:INC3Y\*N3-1). Using zero-based indexing, the element y(k1,k2,k3) is stored in the following location in these arrays:

- For the two-dimensional array, location (k1+k2\*inc2y,k3)
- For the one-dimensional array, location (k1+k2\*inc2y+k3\*inc3y)

In the following table, values of inc2y and inc3y are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with n1 = n2 = n3 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1,N2,N3	INC2Y	INC3Y
30	30	900
32	32	1032
64	64	4112
120	120	14400
128	136	17416
240	240	57608
256	264	67592
420	420	176400

As mentioned before, the strides of the input array are not important. The array can be declared as a three-dimensional array. If you want to use the same array for input and output, the requirements are  $inc2x \ge inc2y$  and  $inc3x \ge inc3y$ . A simple thing to do is to use inc2x = inc2y and make inc3x a multiple of inc2x not smaller than *inc3y*. Then X can be declared as a three-dimensional array X(INC2X,INC3X/INC2X,N3).

**Example 8—SRCFT3:** This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SRCFT3 subroutine.

For this subroutine, the strides for the input array are not important. They are important for the output array. The STRIDE subroutine helps in picking good values of inc2y and inc3y. This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for inc2y. The minimum acceptable value for inc2y is n1/2+1.

Here, the arguments refer to the SRCFT3 subroutine. Next, you should find a good value for inc3y. The minimum acceptable value for inc3y is (n2)(inc2y).

If inc3y turns out to be a multiple of inc2y, then Y can be declared a three-dimensional array as Y(INC2Y,INC3Y/INC2Y,N3). For large problems, this may not happen. In that case, you can declare the Y array as a two-dimensional array Y(0:INC3Y-1,0:N3-1) or a one-dimensional array Y(0:INC3Y\*N3-1). Using zero-based indexing, the element y(k1,k2,k3) is stored in the following location in these arrays:

- For the two-dimensional array, location (k1+k2\*inc2y,k3)
- For the one-dimensional array, location (k1+k2\*inc2y+k3\*inc3y)

In the following table, values of inc2y and inc3y are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with n1 = n2 = n3 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1,N2,N3	INC2Y	INC3Y
32	17	544
64	33	2112
120	61	7320
128	65	8328
240	121	29064
256	129	33032

As mentioned before, the strides of the input array are not important. The array can be declared as a three-dimensional array. If you want to use the same array for input and output, the requirements are  $inc2x \ge 2(inc2y)$  and  $inc3x \ge 2(inc3y)$ . A simple thing to do is to use inc2x = 2(inc2y) and make inc3x a multiple of inc2x not smaller than 2(inc3y). Then X can be declared as a three-dimensional array X(INC2X,INC3X/INC2X,N3).

Example 9—SCRFT3: This example shows the use of the STRIDE subroutine in computing three-dimensional transforms using the SCRFT3 subroutine.

The STRIDE subroutine helps in picking good values of *inc2y* and *inc3y*. This requires two calls to the STRIDE subroutine as shown below. First, you should find a good value for *inc2y*. The minimum acceptable value for *inc2y* is *n1*+2.

Here, the arguments refer to the SCRFT3 subroutine. Next, you should find a good value for inc3y. The minimum acceptable value for inc3y is (n2)(inc2y).

If inc3y turns out to be a multiple of inc2y, then Y can be declared a three-dimensional array as Y(INC2Y, INC3Y/INC2Y, N3). For large problems, this may not happen. In that case, you can declare the Y array as a two-dimensional array Y(0:INC3Y-1,0:N3-1) or a one-dimensional array Y(0:INC3Y\*N3-1). Using zero-based indexing, the element y(k1,k2,k3) is stored in the following location in these arrays:

- For the two-dimensional array, location (k1+k2\*inc2y,k3)
- For the one-dimensional array, location (k1+k2\*inc2y+k3\*inc3y)

In the following table, values of inc2y and inc3y are given (as obtained from the STRIDE subroutine) for some three-dimensional arrays with n1 = n2 = n3 and for POWER2-P2SC with 64KB level 1 cache using the POWER2 library for ESSL:

N1,N2,N3	INC2Y	INC3Y
32	34	1088
64	66	4224
120	122	14640
128	130	16656
240	242	58128
256	258	66064

### **STRIDE**

For this subroutine, the strides (inc2x and inc3x) of the input array are also important. In general, inc2x = inc2y/2 and inc3x = inc3y/2 are good choices. These are also the requirement if you want to use the same array for input and output.

# DSRSM—Convert a Sparse Matrix from Storage-by-Rows to Compressed-Matrix Storage Mode

This subroutine converts either m by n general sparse matrix  $\boldsymbol{A}$  or symmetric sparse matrix  $\boldsymbol{A}$  of order n from storage-by-rows to compressed-matrix storage mode, where matrix  $\boldsymbol{A}$  contains long-precision real numbers.

### Syntax

Fortran	CALL DSRSM (iopt, ar, ja, ia, m, nz, ac, ka, lda)
C and C++	dsrsm (iopt, ar, ja, ia, m, nz, ac, ka, lda);
PL/I	CALL DSRSM (iopt, ar, ja, ia, m, nz, ac, ka, lda);

### On Entry

iopt

indicates the storage variation used for sparse matrix **A** storage-by-rows:

If iopt = 0, matrix **A** is a general sparse matrix, where all the nonzero elements in matrix **A** are used to set up the storage arrays.

If iopt = 1, matrix **A** is a symmetric sparse matrix, where only the upper triangle and diagonal elements are used to set up the storage arrays.

Specified as: a fullword integer; iopt = 0 or 1.

ar

is the sparse matrix  $\mathbf{A}$ , stored by rows in an array, referred to as AR. The *iopt* argument indicates the storage variation used for storing matrix  $\mathbf{A}$ . Specified as: a one-dimensional array, containing long-precision real numbers. The number of elements, ne, in this array can be determined by subtracting 1 from the value in IA(m+1).

ja

is the array, referred to as JA, containing the column numbers of each nonzero element in sparse matrix A. Specified as: a one-dimensional array, containing fullword integers;  $1 \le (JA \text{ elements}) \le n$ . The number of elements, ne, in this array can be determined by subtracting 1 from the value in IA(m+1).

ia

is the row pointer array, referred to as IA, containing the starting positions of each row of matrix A in array AR and one position past the end of array AR. Specified as: a one-dimensional array of (at least) length m+1, containing fullword integers; IA(i+1)  $\geq$  IA(i) for i=1, m+1.

m

is the number of rows in sparse matrix **A**. Specified as: a fullword integer;  $m \ge 0$ .

nz

is the number of columns in output arrays AC and KA that are available for use. Specified as: a fullword integer; nz > 0.

ac

See "On Return" on page 980.

ka

See "On Return" on page 980.

lda

is the size of the leading dimension of the arrays specified for ac and ka. Specified as: a fullword integer;  $0 < Ida \le m$ .

#### On Return

nz

is the maximum number of nonzero elements, nz, in each row of matrix A, which is stored in compressed-matrix storage mode. Returned as: a fullword integer; (input argument)  $nz \le$  (output argument) nz.

ac

is the m by n general sparse matrix  $\boldsymbol{A}$  or symmetric matrix  $\boldsymbol{A}$  of order n stored in compressed-matrix storage mode in an array, referred to as AC. Returned as: an lda by at least (input argument) nz array, containing long-precision real numbers, where only the first (output argument) nz columns are used to store the matrix.

ka

is the array, referred to as KA, containing the column numbers of the matrix **A** elements that are stored in the corresponding positions in array AC. Returned as: an *Ida* by at least (input argument) *nz* array, containing fullword integers, where only the first (output argument) *nz* columns are used to store the column numbers.

#### **Notes**

- 1. In your C program, argument *nz* must be passed by reference.
- 2. The value specified for input argument nz should be greater than or equal to the number of nonzero elements you estimate to be in each row of sparse matrix A. The value returned in output argument nz corresponds to the nz value defined for compressed-matrix storage mode. This value is less than or equal to the value specified for input argument nz.
- 3. For a description of the storage modes for sparse matrices, see "Compressed-Matrix Storage Mode" on page 93 and "Storage-by-Rows" on page 99.

**Function:** A sparse matrix **A** is converted from storage-by-rows (using arrays AR, JA, and IA) to compressed-matrix storage mode (using arrays AC and KA). The argument *iopt* indicates whether the input matrix **A** is stored by rows using the storage variation for general sparse matrices or for symmetric sparse matrices. See reference [67].

This subroutine is meant for existing programs that need to convert their sparse matrices to a storage mode compatible with some of the ESSL sparse matrix subroutines, such as DSMMX.

### **Error Conditions**

Computational Errors: None

Input-Argument Errors

- 1.  $iopt \neq 0$  or 1
- 2. m < 0
- 3. Ida < 1
- 4. Ida < m
- 5.  $nz \leq 0$
- 6. IA(m+1) < 1
- 7. IA(i+1)-IA(i) < 0, for any i = 1, m
- 8. *nz* is too small to store matrix **A** in array AC, where:

- If iopt = 0, AC and KA are not modified.
- If *iopt* = 1, AC and KA are modified.

**Example 1:** This example shows a general sparse matrix **A**, which is stored by rows and converted to compressed-matrix storage mode, where sparse matrix A is:

Because there is a maximum of only two nonzero elements in each row of A, and argument nz is specified as 5, columns 3 through 5 of arrays AC and KA are not used.

Call Statement and Input

### Output

$$NZ = 2$$

$$AC = \begin{bmatrix} 11.0 & 14.0 & . & . & . \\ 22.0 & 24.0 & . & . & . \\ 33.0 & 34.0 & . & . & . \\ 44.0 & 0.0 & . & . & . \end{bmatrix}$$

**Example 2:** This example shows a symmetric sparse matrix **A**, which is stored by rows and converted to compressed-matrix storage mode, where sparse matrix A is:

Because there is a maximum of only four nonzero elements in each row of A, and argument nz is specified as 6, columns 5 and 6 of arrays AC and KA are not used.

Call Statement and Input

### Output

$$AC = \begin{bmatrix} 11.0 & 14.0 & 0.0 & 0.0 & . & . \\ 22.0 & 24.0 & 0.0 & 0.0 & . & . \\ 33.0 & 34.0 & 0.0 & 0.0 & . & . \\ 44.0 & 24.0 & 34.0 & 14.0 & . & . \end{bmatrix}$$

$$KA = \begin{bmatrix} 1 & 4 & 4 & 4 & . & . \\ 2 & 4 & 4 & 4 & . & . \\ 3 & 4 & 4 & 4 & . & . \\ 4 & 2 & 3 & 1 & . & . \end{bmatrix}$$

# DGKTRN—For a General Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode

This subroutine converts general sparse matrix  $\boldsymbol{A}$  of order n from one skyline storage mode to another—that is, between the following:

- · Diagonal-out skyline storage mode
- · Profile-in skyline storage mode

### Syntax

Fortran	CALL DGKTRN (n, au, nu, idu, al, nl, idl, itran, aux, naux)
C and C++	dgktrn (n, au, nu, idu, al, nl, idl, itran, aux, naux);
PL/I	CALL DGKTRN (n, au, nu, idu, al, nl, idl, itran, aux, naux);

### On Entry

n

is the order of general sparse matrix **A**. Specified as: a fullword integer;  $n \ge 0$ .

au

is the array, referred to as AU, containing the upper triangular part of general sparse matrix  $\boldsymbol{A}$ , stored as follows, where:

If ITRAN(1) = 0, **A** is stored in diagonal-out skyline storage mode.

If ITRAN(1) = 1,  $\mathbf{A}$  is stored in profile-in skyline storage mode.

Specified as: a one-dimensional array of (at least) length *nu*, containing long-precision real numbers.

nu

is the length of array AU. Specified as: a fullword integer;  $nu \ge 0$  and  $nu \ge (IDU(n+1)-1)$ .

idu

is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix  $\bf{A}$  in input array AU. Specified as: a one-dimensional array of (at least) length n+1, containing fullword integers.

al

is the array, referred to as AL, containing the lower triangular part of general sparse matrix A, stored as follows, where:

If ITRAN(1) = 0,  $\boldsymbol{A}$  is stored in diagonal-out skyline storage mode.

If ITRAN(1) = 1,  $\mathbf{A}$  is stored in profile-in skyline storage mode.

**Note:** Entries in AL for diagonal elements of **A** are assumed not to have meaningful values.

Specified as: a one-dimensional array of (at least) length *nl*, containing long-precision real numbers.

nl

is the length of array AL. Specified as: a fullword integer;  $nl \ge 0$  and  $nl \ge (IDL(n+1)-1)$ .

idl

is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix  $\bf{A}$  in input array AL. Specified as: a one-dimensional array of (at least) length n+1, containing fullword integers.

itran

is an array of parameters, ITRAN(i), where:

ITRAN(1) indicates the input storage mode used for matrix A. This
determines the arrangement of data in arrays AU, IDU, AL, and IDL on input,
where:

If ITRAN(1) = 0, diagonal-out skyline storage mode is used.

If ITRAN(1) = 1, profile-in skyline storage mode is used.

ITRAN(2) indicates the output storage mode used for matrix A. This
determines the arrangement of data in arrays AU, IDU, AL, and IDL on
output, where:

If ITRAN(2) = 0, diagonal-out skyline storage mode is used.

If ITRAN(2) = 1, profile-in skyline storage mode is used.

 ITRAN(3) indicates the direction of sweep that ESSL uses through the matrix A, allowing you to optimize performance (see "Notes" on page 985), where:

If ITRAN(3) = 1, matrix  $\mathbf{A}$  is transformed in the positive direction, starting in row or column 1 and ending in row or column n.

If ITRAN(3) = -1, matrix **A** is transformed in the negative direction, starting in row or column n and ending in row or column 1.

Specified as: a one-dimensional array of (at least) length 3, containing fullword integers, where:

```
ITRAN(1) = 0 or 1

ITRAN(2) = 0 or 1

ITRAN(3) = -1 or 1
```

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing *naux* long-precision real numbers. *naux* 

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DGKTRN dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge 2n$ .

### On Return

au

is the array, referred to as AU, containing the upper triangular part of general sparse matrix  $\boldsymbol{A}$ , stored as follows, where:

If ITRAN(2) = 0,  $\mathbf{A}$  is stored in diagonal-out skyline storage mode.

If ITRAN(2) = 1,  $\boldsymbol{A}$  is stored in profile-in skyline storage mode.

Returned as: a one-dimensional array of (at least) length *nu*, containing long-precision real numbers.

idu

is the array, referred to as IDU, containing the relative positions of the diagonal elements of matrix  $\bf{A}$  in output array AU. Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

al

is the array, referred to as AL, containing the lower triangular part of general sparse matrix A, stored as follows, where:

If ITRAN(2) = 0,  $\mathbf{A}$  is stored in diagonal-out skyline storage mode.

If ITRAN(2) = 1,  $\boldsymbol{A}$  is stored in profile-in skyline storage mode.

**Note:** You should assume that entries in AL for diagonal elements of **A** do not have meaningful values.

Returned as: a one-dimensional array of (at least) length *nl*, containing long-precision real numbers.

idl

is the array, referred to as IDL, containing the relative positions of the diagonal elements of matrix  $\boldsymbol{A}$  in output array AL. Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

### Notes

- 1. Your various arrays must have no common elements; otherwise, results are unpredictable.
- 2. The ITRAN(3) argument allows you to specify the direction of travel through matrix **A** that ESSL takes during the transformation. By properly specifying ITRAN(3), you can optimize the performance of the transformation, which is especially beneficial when transforming large matrices.

The direction specified by ITRAN(3) should be opposite the most recent direction of access through the matrix performed by the DGKFS or DGKFSP subroutine, as indicated in the following table:

Most Recent Computation Performed by DGKFS/DGKFSP	Direction Used by DGKFS/DGKFSP	Direction to Specify in ITRAN(3)
Factor and Solve	Negative	Positive (ITRAN(3) = 1)
Factor Only	Positive	Negative (ITRAN(3) = −1)
Solve Only	Negative	Positive (ITRAN(3) = 1)

- 3. For a description of how sparse matrices are stored in skyline storage mode, see "Profile-In Skyline Storage Mode" on page 103 and "Diagonal-Out Skyline Storage Mode" on page 101.
- You have the option of having the minimum required value for naux dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** A general sparse matrix **A**, stored in diagonal-out or profile-in skyline storage mode is converted to either of these same two storage modes. (Generally, you convert from one to the other, but the capability exists to specify the same

storage mode for input and output.) The argument ITRAN(3) indicates the direction in which you want the transformation performed on matrix  $\boldsymbol{A}$ , allowing you to optimize your performance in this subroutine. This is especially beneficial for large matrices.

This subroutine is meant to be used in conjunction with DGKFS and DGKFSP, which process matrices stored in these skyline storage modes.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

```
1. n < 0
2. nu < 0
3. IDU(n+1) > nu+1
4. IDU(i+1) \le IDU(i) for i = 1, n
5. IDU(i+1) > IDU(i)+i and ITRAN(1) = 0 for i = 1, n
6. IDU(i) > IDU(i-1)+i and ITRAN(1) = 1 for i = 2, n
7. nl < 0
8. IDL(n+1) > nl+1
9. IDL(i+1) \le IDL(i) for i = 1, n
10. IDL(i+1) > IDL(i)+i and ITRAN(1) = 0 for i = 1, n
11. IDL(i) > IDL(i-1)+i and ITRAN(1) = 1 for i = 2, n
12. ITRAN(1) \ne 0 or 1
13. ITRAN(2) \ne 0 or 1
14. ITRAN(3) \ne -1 or 1
15. Error 2015 is recoverable or naux \ne 0, and naux is too small—that is, less than
```

the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to convert a 9 by 9 general sparse matrix **A** from diagonal-out skyline storage mode to profile-in skyline storage mode. Matrix **A** is:

```
11.0 12.0 13.0 0.0 0.0 0.0
                               0.0
                                    0.0
                                         0.0
21.0 22.0 23.0 24.0 25.0 0.0 0.0
                                    0.0 29.0
31.0 32.0 33.0 34.0 35.0
                        0.0 37.0
                                    0.0 39.0
41.0 42.0 43.0 44.0 45.0 46.0 47.0
                                   0.0 49.0
0.0
     0.0 0.0 54.0 55.0 56.0 57.0 58.0 59.0
    62.0 63.0 64.0 65.0 66.0 67.0 68.0 69.0
0.0
     0.0 0.0 74.0 75.0 76.0 77.0
0.0
                                   78.0 79.0
          0.0 84.0 85.0 86.0 87.0
0.0
     0.0
                                   88.0
                                        89.0
91.0
    92.0 93.0 94.0 95.0 96.0 97.0 98.0
                                        99.0
```

Assuming that DGKFS last performed a solve on matrix A, the direction of the transformation is positive; that is, ITRAN(3) is 1. This provides the best performance here.

**Note:** On input and output, the diagonal elements in AL do not have meaningful values.

### Call Statement and Input

```
ΑU
                     NU
                          IDU
                                          IDL
                                                ITRAN
                                                        AUX
                                                              NAUX
                                ΑL
                                     NL
CALL DGKTRN(9, AU, 33, IDU, AL, 35, IDL, ITRAN, AUX,
          (11.0, 22.0, 12.0, 33.0, 23.0, 13.0, 44.0, 34.0, 24.0,
ΑU
             55.0, 45.0, 35.0, 25.0, 66.0, 56.0, 46.0, 77.0, 67.0,
            57.0, 47.0, 37.0, 88.0, 78.0, 68.0, 58.0, 99.0, 89.0,
            79.0, 69.0, 59.0, 49.0, 39.0, 29.0)
           (1, 2, 4, 7, 10, 14, 17, 22, 26, 34)
IDU
ΑL
           (.,.,21.0,.,32.0,31.0,.,43.0,42.0,41.0,.,
             54.0, . , 65.0, 64.0, 63.0, 62.0, . , 76.0, 75.0, 74.0,
             ., 87.0, 86.0, 85.0, 84.0, ., 98.0, 97.0, 96.0, 95.0,
            94.0, 93.0, 92.0, 91.0)
           (1, 2, 4, 7, 11, 13, 18, 22, 27, 36)
IDL
ITRAN
           (0, 1, 1)
Output
ΑU
           (11.0, 12.0, 22.0, 13.0, 23.0, 33.0, 24.0, 34.0, 44.0,
            25.0, 35.0, 45.0, 55.0, 46.0, 56.0, 66.0, 37.0, 47.0,
            57.0, 67.0, 77.0, 58.0, 68.0, 78.0, 88.0, 29.0, 39.0,
            49.0, 59.0, 69.0, 79.0, 89.0, 99.0)
IDU
          (1, 3, 6, 9, 13, 16, 21, 25, 33, 34)
ΑL
           (., 21.0, ., 31.0, 32.0, ., 41.0, 42.0, 43.0, ., 54.0,
             ., 62.0, 63.0, 64.0, 65.0, ., 74.0, 75.0, 76.0, .,
            84.0, 85.0, 86.0, 87.0, . , 91.0, 92.0, 93.0, 94.0, 95.0,
            96.0, 97.0, 98.0, . )
          (1, 3, 6, 10, 12, 17, 21, 26, 35, 36)
IDL
```

**Example 2:** This example shows how to convert the same 9 by 9 general sparse matrix **A** in Example 1 from profile-in skyline storage mode to diagonal-out skyline storage mode.

Assuming that DGKFS last performed a factorization on matrix A, the direction of the transformation is negative; that is, ITRAN(3) is -1. This provides the best performance here.

**Note:** On input and output, the diagonal elements in AL do not have meaningful values.

### Call Statement and Input

```
IDL
                            IDU
                                        NL
                                                    ITRAN
                                                            AUX
                                                                   NAUX
                                   ΑL
CALL DGKTRN( 9 , AU , 33 , IDU , AL , 35 , IDL , ITRAN , AUX , 18
ΑU
         =(same as output AU in Example 1)
IDU
         =(same as output IDU in Example 1)
ΑL
         =(same as output AL in Example 1)
         =(same as output IDL in Example 1)
IDL
ITRAN
         = (1, 0, -1)
```

### **DGKTRN**

### Output

AU =(same as input AU in Example 1)
IDU =(same as input IDU in Example 1)
AL =(same as input AL in Example 1)
IDL =(same as input IDL in Example 1)

# DSKTRN—For a Symmetric Sparse Matrix, Convert Between Diagonal-Out and Profile-In Skyline Storage Mode

This subroutine converts symmetric sparse matrix **A** of order *n* from one skyline storage mode to another—that is, between the following:

- · Diagonal-out skyline storage mode
- · Profile-in skyline storage mode

### Syntax

Fortran	CALL DSKTRN (n, a, na, idiag, itran, aux, naux)
C and C++	dsktrn (n, a, na, idiag, itran, aux, naux);
PL/I	CALL DSKTRN (n, a, na, idiag, itran, aux, naux);

### On Entry

n

is the order of symmetric sparse matrix A. Specified as: a fullword integer;  $n \ge 0$ .

а

is the array, referred to as A, containing the upper triangular part of symmetric sparse matrix A, stored as follows, where:

If ITRAN(1) = 0,  $\mathbf{A}$  is stored in diagonal-out skyline storage mode.

If ITRAN(1) = 1,  $\boldsymbol{A}$  is stored in profile-in skyline storage mode.

Specified as: a one-dimensional array of (at least) length *na*, containing long-precision real numbers.

na

is the length of array A. Specified as: a fullword integer;  $na \ge 0$  and  $na \ge (IDIAG(n+1)-1)$ .

### idiag

is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix **A** in input array A. Specified as: a one-dimensional array of (at least) length *n*+1, containing fullword integers.

#### itran

is an array of parameters, ITRAN(i), where:

• ITRAN(1) indicates the input storage mode used for matrix **A**. This determines the arrangement of data in arrays A and IDIAG on input, where:

If ITRAN(1) = 0, diagonal-out skyline storage mode is used.

If ITRAN(1) = 1, profile-in skyline storage mode is used.

• ITRAN(2) indicates the output storage mode used for matrix **A**. This determines the arrangement of data in arrays A and IDAIG on output, where:

If ITRAN(2) = 0, diagonal-out skyline storage mode is used.

If ITRAN(2) = 1, profile-in skyline storage mode is used.

• ITRAN(3) indicates the direction of sweep that ESSL uses through the matrix **A**, allowing you to optimize performance (see "Notes" on page 990), where:

If ITRAN(3) = 1, matrix  $\mathbf{A}$  is transformed in the positive direction, starting in row or column 1 and ending in row or column n.

If ITRAN(3) = -1, matrix **A** is transformed in the negative direction, starting in row or column n and ending in row or column 1.

Specified as: a one-dimensional array of (at least) length 3, containing fullword integers, where:

```
ITRAN(1) = 0 or 1

ITRAN(2) = 0 or 1

ITRAN(3) = -1 or 1
```

aux

has the following meaning:

If naux = 0 and error 2015 is unrecoverable, aux is ignored.

Otherwise, it is the storage work area used by this subroutine. Its size is specified by *naux*.

Specified as: an area of storage, containing *naux* long-precision real numbers. *naux* 

is the size of the work area specified by *aux*—that is, the number of elements in *aux*. Specified as: a fullword integer, where:

If naux = 0 and error 2015 is unrecoverable, DSKTRN dynamically allocates the work area used by this subroutine. The work area is deallocated before control is returned to the calling program.

Otherwise,  $naux \ge n$ .

### On Return

а

is the array, referred to as A, containing the upper triangular part of symmetric sparse matrix A, stored as follows, where:

If ITRAN(2) = 0,  $\mathbf{A}$  is stored in diagonal-out skyline storage mode.

If ITRAN(2) = 1,  $\mathbf{A}$  is stored in profile-in skyline storage mode.

Returned as: a one-dimensional array of (at least) length *na*, containing long-precision real numbers.

idiaq

is the array, referred to as IDIAG, containing the relative positions of the diagonal elements of matrix  $\bf{A}$  in output array A. Returned as: a one-dimensional array of (at least) length n+1, containing fullword integers.

### Notes

- 1. Your various arrays must have no common elements; otherwise, results are unpredictable.
- 2. The ITRAN(3) argument allows you to specify the direction of travel through matrix **A** that ESSL takes during the transformation. By properly specifying ITRAN(3), you can optimize the performance of the transformation, which is especially beneficial when transforming large matrices.

The direction specified by ITRAN(3) should be opposite the most recent direction of access through the matrix performed by the DSKFS or DSKFSP subroutine, as indicated in the following table:

Most Recent Computation Performed by DSKFS/DSKFSP	Direction Used by DSKFS/DSKFSP	Direction to Specify in ITRAN(3)
Factor and Solve	Negative	Positive (ITRAN(3) = 1)
Factor Only	Positive	Negative (ITRAN(3) = -1)
Solve Only	Negative	Positive (ITRAN(3) = 1)

- For a description of how sparse matrices are stored in skyline storage mode, see "Profile-In Skyline Storage Mode" on page 103 and "Diagonal-Out Skyline Storage Mode" on page 101.
- 4. You have the option of having the minimum required value for *naux* dynamically returned to your program. For details, see "Using Auxiliary Storage in ESSL" on page 31.

**Function:** A symmetric sparse matrix **A**, stored in diagonal-out or profile-in skyline storage mode is converted to either of these same two storage modes. (Generally, you convert from one to the other, but the capability exists to specify the same storage mode for input and output.) The argument ITRAN(3) indicates the direction in which you want the transformation performed on matrix **A**, allowing you to optimize your performance in this subroutine. This is especially beneficial for large matrices.

This subroutine is meant to be used in conjunction with DSKFS and DSKFSP, which process matrices stored in these skyline storage modes.

### **Error Conditions**

Resource Errors: Error 2015 is unrecoverable, naux = 0, and unable to allocate work area.

Computational Errors: None

Input-Argument Errors

- 1. n < 0
- 2. na < 0
- 3. IDIAG(n+1) > na+1
- 4.  $IDIAG(i+1) \leq IDIAG(i)$  for i = 1, n
- 5. IDIAG(i+1) > IDIAG(i)+i and ITRAN(1) = 0 for i = 1, n
- 6. IDIAG(i) > IDIAG(i-1)+i and ITRAN(1) = 1 for i = 2, n
- 7. ITRAN(1)  $\neq$  0 or 1
- 8. ITRAN(2)  $\neq$  0 or 1
- 9. ITRAN(3)  $\neq$  -1 or 1
- 10. *naux* Error 2015 is recoverable or *naux*≠0, and is too small—that is, less than the minimum required value. Return code 1 is returned if error 2015 is recoverable.

**Example 1:** This example shows how to convert a 9 by 9 symmetric sparse matrix **A** from diagonal-out skyline storage mode to profile-in skyline storage mode. Matrix **A** is:

```
11.0 12.0 13.0 14.0
                                                0.0
                        0.0
                              0.0
                                    0.0
                                          0.0
12.0 22.0
           23.0
                 24.0
                       25.0
                             26.0
                                    0.0
                                         28.0
                                                0.0
     23.0 33.0
13.0
                 34.0
                       35.0
                             36.0
                                    0.0
                                         38.0
                                                0.0
14.0
     24.0
           34.0
                 44.0
                       45.0
                             46.0
                                    0.0
                                         48.0
                                                0.0
 0.0
     25.0
           35.0
                  45.0
                       55.0
                             56.0
                                   57.0
                                         58.0
                                                0.0
     26.0
           36.0
                 46.0
                       56.0
                                   67.0
                                               69.0
 0.0
                             66.0
                                         68.0
 0.0
      0.0
            0.0
                  0.0 57.0
                             67.0
                                   77.0
                                         78.0
                                               79.0
 0.0
     28.0
           38.0
                  48.0
                       58.0
                             68.0
                                   78.0
                                         88.0
                                               89.0
 0.0
       0.0
            0.0
                  0.0
                        0.0
                             69.0
                                   79.0
                                         89.0
                                               99.0
```

Assuming that DSKFS last performed a factorization on matrix A, the direction of the transformation is negative; that is, ITRAN(3) is -1. This provides the best performance here.

Call Statement and Input

```
IDIAG
                                 ITRAN
                                         AUX
                                               NAUX
CALL DSKTRN(9, A, 33, IDIAG, ITRAN, AUX, 9)
        = (11.0, 22.0, 12.0, 33.0, 23.0, 13.0, 44.0, 34.0, 24.0,
Α
             14.0, 55.0, 45.0, 35.0, 25.0, 66.0, 56.0, 46.0, 36.0,
            26.0, 77.0, 67.0, 57.0, 88.0, 78.0, 68.0, 58.0, 48.0,
            38.0, 28.0, 99.0, 89.0, 79.0, 69.0)
IDIAG
        = (1, 2, 4, 7, 11, 15, 20, 23, 30, 34)
        = (0, 1, -1)
ITRAN
Output
          (11.0, 12.0, 22.0, 13.0, 23.0, 33.0, 14.0, 24.0, 34.0,
            44.0, 25.0, 35.0, 45.0, 55.0, 26.0, 36.0, 46.0, 56.0,
             66.0, 57.0, 67.0, 77.0, 28.0, 38.0, 48.0, 58.0, 68.0,
            78.0, 88.0, 69.0, 79.0, 89.0, 99.0)
IDIAG
        = (1, 3, 6, 10, 14, 19, 22, 29, 33, 34)
```

**Example 2:** This example shows how to convert the same 9 by 9 symmetric sparse matrix A in Example 1 from profile-in skyline storage mode to diagonal-out skyline storage mode.

Assuming that DSKFS last performed a solve on matrix A, the direction of the transformation is positive; that is, ITRAN(3) is 1. This provides the best performance here.

Call Statement and Input

```
IDIAG
                                  ITRAN
                                          AUX
                                                NAUX
CALL DSKTRN(9, A, 33, IDIAG, ITRAN, AUX,
Α
         =(same as output A in Example 1)
         =(same as output IDIAG in Example 1)
IDIAG
ITRAN
         = (1, 0, 1)
```

### Output

=(same as input A in Example 1) =(same as input IDIAG in Example 1) Α IDIAG

### **DSKTRN**

## Part 3. Appendixes

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## Appendix A. Basic Linear Algebra Subprograms (BLAS)

This appendix lists the ESSL subprograms corresponding to a subprogram in the standard set of BLAS.

## Level 1 BLAS

Table 168. Level 1 BLAS Included in ESSL		
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Position of the First or Last Occurrence of the Vector Element Having the Largest Magnitude	ISAMAX ICAMAX	IDAMAX IZAMAX
Sum of the Magnitudes of the Elements in a Vector	SASUM SCASUM	DASUM DZASUM
Multiply a Vector X by a Scalar, Add to a Vector Y, and Store in the Vector Y	SAXPY CAXPY	DAXPY ZAXPY
Copy a Vector	SCOPY CCOPY	DCOPY ZCOPY
Dot Product of Two Vectors	SDOT CDOTU CDOTC	DDOT ZDOTU ZDOTC
Euclidean Length of a Vector with Scaling of Input to Avoid Destructive Underflow and Overflow	SNRM2 SCNRM2	DNRM2 DZNRM2
Construct a Givens Plane Rotation	SROTG CROTG	DROTG ZROTG
Apply a Plane Rotation	SROT CROT CSROT	DROT ZROT ZDROT
Multiply a Vector X by a Scalar and Store in the Vector X	SSCAL CSCAL CSSCAL	DSCAL ZSCAL ZDSCAL
Interchange the Elements of Two Vectors	SSWAP CSWAP	DSWAP ZSWAP

## Level 2 BLAS

Table 169 (Page 1 of 2). Level 2 BLAS Included in ESSL		
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Matrix-Vector Product for a General Matrix, Its Transpose, or Its Conjugate Transpose	SGEMV CGEMV	DGEMV ZGEMV

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Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Rank-One Update of a General Matrix	SGER CGERU CGERC	DGER ZGERU ZGERC
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Matrix	SSPMV CHPMV SSYMV CHEMV	DSPMV ZHPMV DSYMV ZHEMV
Rank-One Update of a Real Symmetric or Complex Hermitian Matrix	SSPR CHPR SSYR CHER	DSPR ZHPR DSYR ZHER
Rank-Two Update of a Real Symmetric or Complex Hermitian Matrix	SSPR2 CHPR2 SSYR2 CHER2	DSPR2 ZHPR2 DSYR2 ZHER2
Matrix-Vector Product for a General Band Matrix, Its Transpose, or Its Conjugate Transpose	SGBMV CGBMV	DGBMV ZGBMV
Matrix-Vector Product for a Real Symmetric or Complex Hermitian Band Matrix	SSBMV CHBMV	DSBMV ZHBMV
Matrix-Vector Product for a Triangular Matrix, Its Transpose, or Its Conjugate Transpose	STPMV CTPMV STRMV CTRMV	DTPMV ZTPMV DTRMV ZTRMV
Solution of a Triangular System of Equations with a Single Right-Hand Side	STPSV CTPSV STRSV CTRSV	DTPSV ZTPSV DTRSV ZTRSV
Matrix-Vector Product for a Triangular Band Matrix, Its Transpose, or Its Conjugate Transpose	STBMV CTBMV	DTBMV ZTBMV
Triangular Band Equation Solve	STBSV CTBSV	DTBSV ZTBSV

## Level 3 BLAS

Table 170 (Page 1 of 2). Level 3 BLAS Included in ESSL		
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
Combined Matrix Multiplication and Addition for General Matrices, Their Transposes, or Conjugate Transposes	SGEMM CGEMM	DGEMM ZGEMM
Matrix-Matrix Product Where One Matrix is Real or Complex Symmetric or Complex Hermitian	SSYMM CSYMM CHEMM	DSYMM ZSYMM ZHEMM

Table 170 (Page 2 of 2). Level 3 BLAS Included in ESSL			
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram	
Triangular Matrix-Matrix Product	STRMM CTRMM	DTRMM ZTRMM	
Rank-K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYRK CSYRK CHERK	DSYRK ZSYRK ZHERK	
Rank-2K Update of a Real or Complex Symmetric or a Complex Hermitian Matrix	SSYR2K CSYR2K CHER2K	DSYR2K ZSYR2K ZHER2K	
Solution of Triangular Systems of Equations with Multiple Right-Hand Sides	STRSM CTRSM	DTRSM ZTRSM	

## Appendix B. LAPACK

This appendix lists the ESSL subroutines corresponding to subroutines in the standard set of LAPACK.

## **LAPACK**

Table 171. LAPACK Included in ESSL		
Descriptive Name	Short- Precision Subprogram	Long- Precision Subprogram
General Matrix Factorization	SGETRF CGETRF	DGETRF ZGETRF
General Matrix, Its Transpose, or Its Conjugate Transpose Multiple Right-Hand Side Solve	SGETRS CGETRS	DGETRS ZGETRS

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## **Glossary**

This glossary defines terms and abbreviations used in this publication. If you do not find the term you are looking for, refer to the index portion of this book. This glossary includes terms and definitions from:

- *IBM Dictionary of Computing*, New York: McGraw Hill (1-800-2MC-GRAW), 1994.
- American National Standard Dictionary for Information Systems, ANSI X3.172-1990, copyright 1990 by the American National Standards Institute (ANSI). Copies may be purchased from the American National Standards Institute, 11 West 42nd Street, New York, New York 10036.
   Definitions are identified by the symbol (A) after the definition.
- Information Technology Vocabulary, developed by Subcommittee 1, Joint Technical Committee 1, of the International Organization for Standardization and the International Electrotechnical Commission (ISO/IEC JTC1/SC1). Definitions from published sections of these vocabularies are identified by the symbol (I) after the definition. Definitions taken from draft international standards, committee drafts, and working papers being developed by ISO/IEC JTC1/SC1 are identified by the symbol (T) after the definition, indicating that final agreement has not yet been reached among the participating National Bodies of SC1.

**APAR**. Authorized Program Analysis Report. A report of a problem caused by a suspected defect in a current unaltered release of a program.

**argument**. A parameter passed between a calling program and a SUBROUTINE subprogram, a FUNCTION subprogram, or a statement function.

**array**. An ordered set of data items identified by a single name.

**array element**. A data item in an array, identified by the array name followed by a subscript indicating its position in the array.

**array name**. The name of an ordered set of data items that make up an array.

**assignment statement**. A statement that assigns a value to a variable or array element. It is made up of a variable or array element, followed by an equal sign (=), followed by an expression. The variable, array element, or expression can be character, logical, or arithmetic. When the assignment statement is processed, the

expression to the right of the equal sign replaces the value of the variable or array element to the left.

**Basic Linear Algebra Subprograms (BLAS).** A standard, public domain, set of mathematical subroutines that perform linear algebra operations.

**BLAS**. Basic Linear Algebra Subprograms.

**cache**. A special-purpose buffer storage, smaller and faster than main storage, used to hold a copy of instructions and data obtained from main storage and likely to be needed next by the processor. (T)

**character constant**. A string of one or more alphanumeric characters enclosed in apostrophes. The delimiting apostrophes are not part of the value of the constant.

**character expression**. An expression in the form of a single character constant, variable, array element, substring, function reference, or another expression enclosed in parentheses. A character expression is always of type character.

**character type**. The data type for representing strings of alphanumeric characters; in storage, one byte is used for each character.

**column-major order**. A sequencing method used for storing multidimensional arrays according to the subscripts of the array elements. In this method the leftmost subscript position varies most rapidly and completes a full cycle before the next subscript position to the right is incremented.

**complex conjugate even data**. Complex data that has its real part even and its imaginary part odd.

**complex constant**. An ordered pair of real or integer constants separated by a comma and enclosed in parentheses. The first real constant of the pair is the real part of the complex number; the second is the imaginary part.

complex type. The data type for representing an approximation of the value of a complex number. A data item of this type consists of an ordered pair of real data items separated by a comma and enclosed in parentheses. The first item represents the real part of the complex number; the second represents the imaginary part.

**constant**. An unvarying quantity. The four classes of constants specify numbers (arithmetic), truth values (logical), character data (character), and hexadecimal data.

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data type. The structural characteristics, features and properties of data that may be directly specified by a programming language; for example, integers, real numbers in Fortran; arrays in APL; linked lists in LISP; character string in SNOBOL.

decimation. The formation of a sequence containing every n-th element of another sequence.

dimension of an array. One of the subscript expression positions in a subscript for an array. In Fortran, an array may have from one to seven dimensions. Graphically, the first dimension is represented by the rows, the second by the columns, and the third by the planes. Contrast with rank. See also extent of a dimension.

direct access storage. A storage device in which the access time is in effect independent of the location of the data. (A)

divide-by-zero exception. The condition recognized by a processor that results from running a program that attempts to divide by zero.

double precision. Synonym for long-precision.

expression. A notation that represents a value: a primary appearing alone, or combinations of primaries and operators. An expression can be arithmetic, character, logical, or relational.

extent of a dimension. The number of different integer values that may be represented by subscript expressions for a particular dimension in a subscript for an array.

external function. A function defined outside the program unit that refers to it. It may be referred to in a procedure subprogram or in the main program, but it must not refer to itself, either directly or indirectly. Contrast with statement function.

**function**. In Fortran, a procedure that is invoked by referring to it in an expression and that supplies a value to the expression. The value supplied is the value of the function. See also external function, intrinsic function, and statement function. Contrast with subroutine.

function reference. A Fortran source program reference to an intrinsic function, to an external function, or to a statement function.

general matrix. A matrix with no assumed special properties such as symmetry. Synonym for matrix.

integer constant. A string of decimal digits containing no decimal point and expressing a whole number.

integer expression. An arithmetic expression whose values are of integer type.

**integer type**. An arithmetic data type capable of expressing the value of an integer. It can have a positive, negative, or 0 value. It must not include a decimal point.

intrinsic function. A function, supplied by Fortran, that performs mathematical or character operations.

leading dimension. For a two-dimensional array, an increment used to find the starting point for the matrix elements in each successive column of the array.

logical constant. A constant that can have one of two values: true or false. The form of these values in Fortran is: .TRUE. and .FALSE. respectively.

logical expression. A logical primary alone or a combination of logical primaries and logical operators. A logical expression can have one of two values: true or false.

**logical type**. The data type for data items that can have the value true or false and upon which logical operations such as .NOT. and .OR. can be performed. See also "data type."

long-precision. Real type of data of length 8. Contrast with single precision and short-precision.

main program. In Fortran, a program unit, required for running, that can call other program units but cannot be called by them.

mask. To use a pattern of characters to control the retention or elimination of portions of another pattern of characters. (I)

matrix. A rectangular array of elements, arranged in rows and columns, that may be manipulated according to the rules of matrix algebra. (A) (I)

multithreaded. There may be one or more threads in a process, and each thread is executed by the operating system concurrently. An application program is multithreaded if more than one thread is executed concurrently.

overflow exception. A condition caused by the result of an arithmetic operation having a magnitude that exceeds the largest possible number.

platform. A mainframe or a workstation.

primary. An irreducible unit of data; a single constant, variable, array element, function reference, or expression enclosed in parentheses.

program exception. The condition recognized by a processor that results from running a program that

improperly specifies or uses instructions, operands, or control information.

**PTF.** Program Temporary Fix. A temporary solution or by-pass of a problem diagnosed by IBM as resulting from a defect in a current unaltered release of the program. A report of a problem caused by a suspected defect in a current unaltered release of a program.

**pthread**. A thread that conforms to the POSIX Threads Programming Model.

**real constant**. A string of decimal digits that expresses a real number. A real constant must contain either a decimal point or a decimal exponent and may contain both. For example, the real constant 0.36819E+2 has the value +36.819.

**real type**. An arithmetic data type, capable of approximating the value of a real number. It can have a positive, negative, or 0 value.

**row-major order**. A sequencing method used for storing multidimensional arrays according to the subscripts of the array elements. In this method the rightmost subscript position varies most rapidly and completes a full cycle before the next subscript position to the left is incremented.

**scalar**. (1) A quantity characterized by a single number. (A) (I) (2) Contrast with vector.

**shape of an array**. The extents of all the dimensions of an array listed in order. For example, the shape of a three-dimensional array that has four rows, five columns, and three planes is (4,5,3) or 4 by 5 by 3.

**short-precision**. Real type data of length 4. Contrast with double precision and long-precision.

single precision. Synonym for short-precision.

**size of an array**. The number of elements in an array. This is the product of the extents of its dimensions.

SMP. Symmetric Multi-Processing.

**statement.** The basic unit of a program, that specifies an action to be performed, or the nature and characteristics of the data to be processed, or information about the program itself. Statements fall into two broad classes: executable and nonexecutable.

statement function. A procedure specified by a single statement that is similar in form to an arithmetic, logical, or character assignment statement. The statement must appear after the specification statements and before the first executable statement. In the remainder of the program it can be referenced as a function. A statement function may be referred to only in the

program unit in which it is defined. Contrast with external function.

**statement label**. A number of from one through five decimal digits that is used to identify a statement. Statement labels can be used to transfer control, to define the range of a DO, or to refer to a FORMAT statement.

statement number. See "statement label."

**stride**. The increment used to step through array storage to select the vector or matrix elements from the array.

**subprogram**. A program unit that is invoked by another program unit in the same program. In Fortran, a subprogram has a FUNCTION, SUBROUTINE, or BLOCK DATA statement as its first statement.

**subscript**. (1) A symbol that is associated with the name of a set to identify a particular subset or element. (A) (2) A subscript expression or set of subscript expressions, enclosed in parentheses and used with an array name to identify a particular array element.

**subscript expression**. An integer expression in a subscript whose value and position in the subscript determine the index number for the corresponding dimension in the referenced array.

**thread**. A thread is the element that is scheduled, and to which resources such as execution time, locks, and queues may be assigned. There may be one or more threads in a process, and each thread is executed by the operating system concurrently.

**thread-safe**. A subroutine which may be called from multiple threads of the same process simultaneously.

**type declaration**. The explicit specification of the type of a constant, variable, array, or function by use of an explicit type specification statement.

**underflow exception**. A condition caused by the result of an arithmetic operation having a magnitude less than the smallest possible nonzero number.

variable. (1) A quantity that can assume any of a given set of values. (A) (2) A data item, identified by a name, that is not a named constant, array, or array element, and that can assume different values at different times during program processing.

**vector**. A one-dimensional ordered collection of numbers.

**working storage**. A storage area provided by the application program for the use of an ESSL subroutine.

workstation. A workstation is a single-user, high-performance microcomputer (or even a minicomputer) which has been specialized in some way, usually for graphics output. Such a machine has a screen and a keyboard, but is also capable of extensive

processing of your input before it is passed to the host. Likewise, the host's responses may be extensively processed before being passed along to your screen. A workstation may be intelligent enough to do much or all the processing itself.

## **Bibliography**

This bibliography lists the publications that you may need to use with ESSL and describes how to obtain them.

#### References

Text books and articles covering the mathematical aspects of ESSL are listed in this section, as well as several software libraries available from other companies. They are listed alphabetically as follows:

- Publications are listed by the author's name. IBM publications that include an order number, other than an IBM Technical Report can be ordered through the Subscription Library Services System (SLSS). The non-IBM publications listed here should be obtained through publishers, bookstores, or professional computing organizations.
- Software libraries are listed by their product name.
   Each reference includes the names, addresses, and phone numbers of the companies from which they can be obtained.

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### **ESSL Publications**

This section lists the ESSL publications for each major task that you perform.

You can order the full set of ESSL for AIX publications through the Subscription Library Services System (SLSS) by specifying:

- The subject code 82
- The program number: 5765-C42

You can also order individual publications by specifying the individual order numbers. For example, to order a copy of the *ESSL Version 3 Release 1.1 Guide and Reference*, specify the order number SA22-7272.

Contact your IBM Marketing Representative or Systems Engineer to order manuals through SLSS.

### **Evaluation and Planning**

ESSL Products General Information, GC23-0529—provides detailed information helpful in evaluating and planning for ESSL: Parallel ESSL, ESSL for AIX, and ESSL/370.

### Installation

ESSL Version 3 Release 1.1 Installation Memo, GI10-0604-01—describes how to install ESSL on AIX. It is a packing list for the ESSL product when it is shipped. (One copy is delivered with each ESSL product.)

### **Application Programming**

ESSL Version 3 Release 1.1 Guide and Reference, SA22-7272—contains ESSL guidance information for designing, coding, and running programs using ESSL, and contains complete reference information for coding calls to the ESSL subroutines. This manual is available in HTML and PostScript format on the product medium.

ESSL Version 2 Release 2 Guide and Reference, SC23-0526—contains ESSL guidance information for designing, coding, and running programs using ESSL/370, and contains complete reference information for coding calls to the ESSL/370 subroutines.

Parallel ESSL Version 2 Guide and Reference, SA22-7273—contains Parallel ESSL guidance information for designing, coding, and running programs using Parallel ESSL, and contains complete reference information for coding calls to the Parallel ESSL subroutines. This manual is available in HTML and PostScript format on the Parallel ESSL product medium.

### **Related Publications**

The related publications listed below may be useful to you when using ESSL.

#### AIX for the RS/6000

IBM AIX Calls and Subroutines Reference for IBM RS/6000,(all volumes) SC23-2198

# AIX Version 4 Release 2 for the RS/6000

IBM AIX Version 4.1 and 4.2 Commands and Reference, (all volumes) SBOF-1851

IBM Version 4.1 and 4.2 General Programming Concepts: Writing and Debugging Programs, SC23-2533

IBM AIX Version 4.1 and 4.2 System Management Guide: Operating System and Devices, SC23-2525

# AIX Version 4 Release 3 for the RS/6000

For the latest updates, visit the RS/6000 web site at: http://www.rs6000.ibm.com/resource/aix\_resource/Pubs

AIX Version 4.3 Commands and Reference, (all volumes) SBOF-1877

AIX Version 4.3 General Programming Concepts:Writing and Debugging Programs, SC23-4128

| AIX Version 4.3 System Guide: Operating System and | Devices, SC23-4126

### XL Fortran

On the XL Fortran Version 5 Release 1.1 CD ROM and the XL High Performance Fortran Version 1 Release 3.1 tape, you may reference the following document available in both PostScript and HTML formats, which describes the changes for those releases: *Changes to XL Fortran for AIX and XL High Performance Fortran for AIX* 

IBM XL Fortran for AIX User's Guide Version 5.1, SC09-2606

IBM XL Fortran for AIX Language Reference Version 5.1, SC09-2607

### PL/I

IBM PL/I Set for AIX Programming Guide, SC26-8456

IBM PL/I Set for AIX Language Reference, SC26-8455

### Workstation Processors

RS/6000 POWERstation and POWERserver Hardware Technical Reference Information—General Architectures, SA23-2643

## **IBM 3838 Array Processor**

IBM 3838 Array Processor Functional Characteristics GA24-3639

OS/VS1 and OS/VS2 MVS Vector Processing Subsystem Programmer's Guide, GC24-5125

MVS Extended Architecture Vector Processing Subsystem Application Programmer's Guide, SC28-1202

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