1.65 GHz IBM $e$server® OpenPower™ 710 Linux® HPC Benchmarks

Deep Computing Solutions Enablement Team

1.65 GHz OpenPower 710 Linux Performance: HPC ISV Benchmarks

Application	Application Description	Benchmark Problem Name(s)	Segment
CPMD Version 3.9.2	The CPMD code is a plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics.	Test Case 1: 32 water molecules Test Case2: 64 atom Si	Life Sciences Computational Chemistry
GAMESS Version Dec 12, 2003	GAMESS (General Atomic and Molecular Electronic Structure System) is a general ab initio quantum chemistry package	l-rotenone, luciferin, nicotine, siccc, tetrodotoxin	Life Sciences Computational Chemistry

1.65 GHz OpenPower 710 Performance:
Test Machine Specifications

- **Two 1.65 GHz IBM POWER5™ processors**
- **8GB RAM**
- **Work executed in a two-way striped file system**
- **Gigabit Ethernet switched network**
  - ➡ **Jumbo frame enabled**
  - ➡ **Tests run on up to four OpenPower 710 systems**
- **System software:**
  - ➡ **SLES 9**
  - ➡ **XLF V 9.1**
  - ➡ **VAC V 7.0**
  - ➡ **ESSL V 4.2**
  - ➡ **MASS V 4.1**
  - ➡ **MPICH V 1.2.5.2**
  - ➡ **LAM-MPI V 7.1.1**
  - ➡ **LAPACK V 3.0**

CPMD Version 3.9.2

- The CPMD code is a plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. Its first version was developed by Jurg Hutter at IBM Zurich Research Laboratory starting from the original Car-Parrinello codes and then developed in many groups around the world.
- The current version, 3.9, is copyrighted jointly by IBM Corp and by Max Planck Institute, Stuttgart and is distributed free of charge to non-profit organizations by the CPMD consortium.

Source of CPMD information: http://www.cpmd.org/

CPMD Version 3.9.2
Test Case 1: 32 water molecules
100 Ryd, 128x128x128 FFT grid, 50 steps
(Elapsed Time in seconds)

Platforms	1 MPI Task / # of Systems	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5 (SLES 9)	2003 / 1	1429 / 1	705 / 2	429 / 2

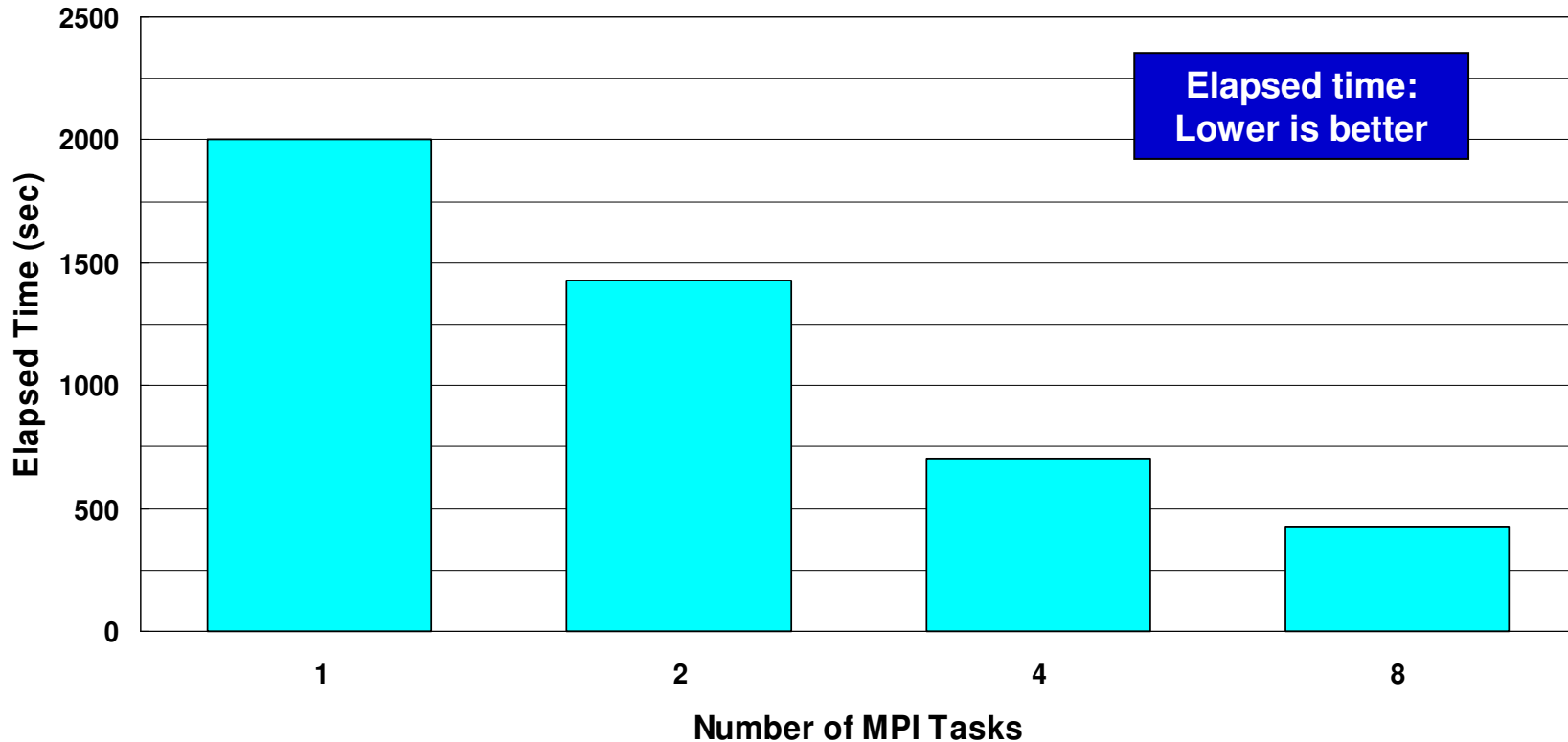**IBM data current as of January 17, 2005.**

CPMD Version 3.9.2
Test Case 1: 32 water molecules
100 Ryd, 128x128x128 FFT grid, 50 steps
(Elapsed Time in seconds)

■ **IBM OpenPower 710 1.65 GHz (SLES 9)**

**Elapsed time:
Lower is better**

Number of MPI Tasks

IBM data current as of January 17, 2005.

CPMD Version 3.9.2
Test Case 2: 64 atom Si
30 Ryd, mesh 64x64x64, 100 steps
(Elapsed Time in seconds)

Platforms	1 MPI Task / # of Systems	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5 (SLES 9)	353 / 1	206 / 1	159 / 2	107 / 4
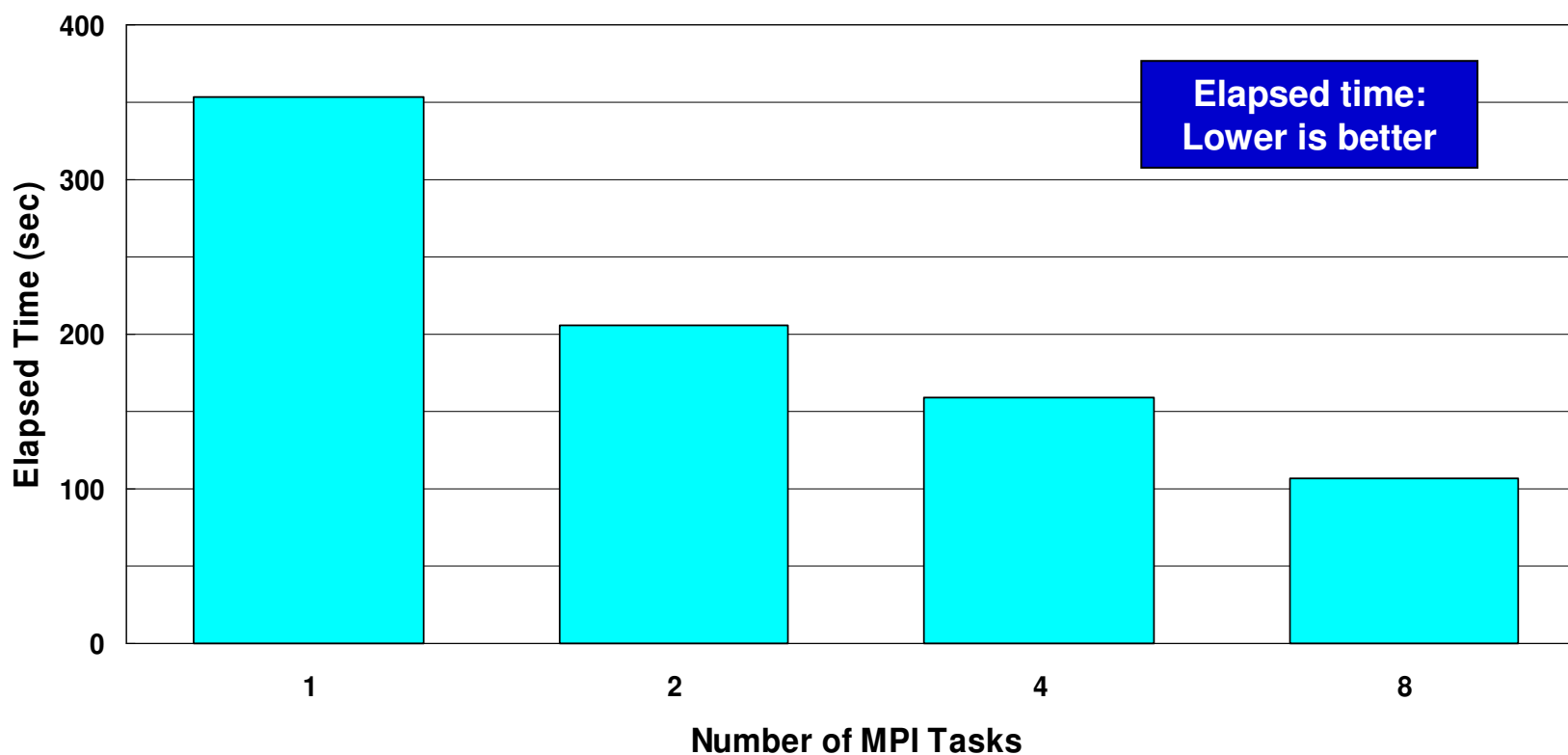
IBM data current as of January 17, 2005.

GAMESS V December 12, 2003

- GAMESS (General Atomic and Molecular Electronic Structure System) is a general ab initio quantum chemistry package maintained by the members of the Mark Gordon research group at Iowa State University

- GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include Configuration Interaction, second order perturbation theory, and Coupled-Cluster approaches, as well as the Density Functional Theory approximation. Analytic gradients are available, for automatic geometry optimization, transition state searches, or reaction path following. Computation of the energy hessian permits prediction of vibrational frequencies, with IR or Raman intensities. Solvent effects may be modeled by the discrete Effective Fragment Potentials, or continuum models such as the Polarizable Continuum Model. Numerous relativistic computations are available, including third order Douglas-Kroll scalar corrections, and numerous spin-orbit coupling options.

Source of GAMESS information:http://www.msg.ameslab.gov/GAMESS/GAMESS.html

GAMESS Version December 12, 2003
l-rotenone: Direct RHF, single point, 479 AO
(Elapsed Time in seconds)

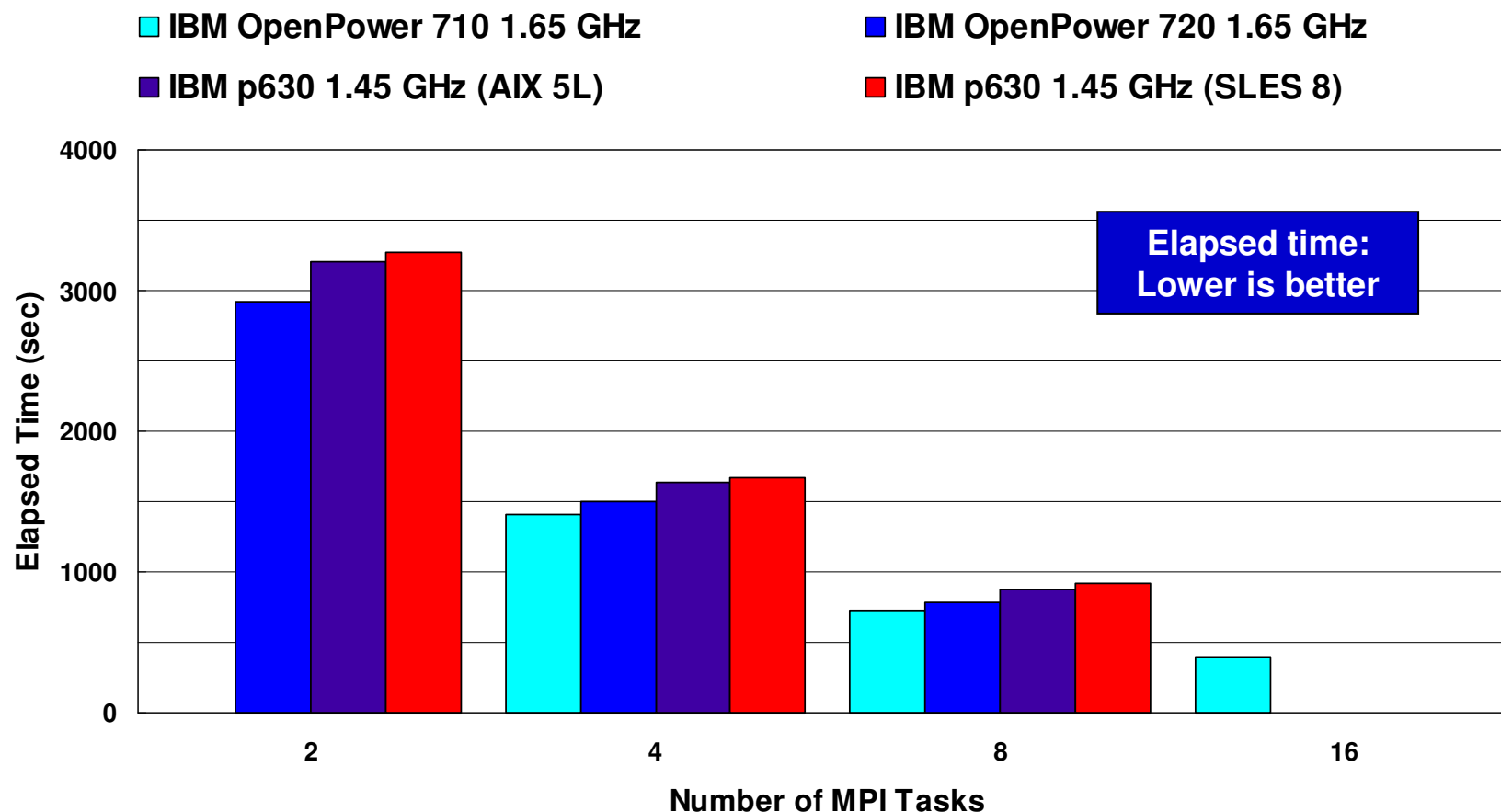| Platforms	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems	16 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5		1410 / 1	731 / 2	394 / 4
IBM OpenPower 720 1.65 GHz POWER5	2916 / 1	1497 / 1	782 / 1	
IBM p630 1.45 GHz POWER4+™ (AIX 5L™	3206 / 1	1640 / 1	878 / 1	
IBM p630 1.45 GHz POWER4+ (SLES 8)	3272 / 1	1676 / 1	917 / 1	

- •Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- •IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
l-rotenone: Direct RHF, single point, 479 AO
(Elapsed Time in seconds)

- IBM OpenPower 710 1.65 GHz
- IBM OpenPower 720 1.65 GHz
- IBM p630 1.45 GHz (AIX 5L)
- IBM p630 1.45 GHz (SLES 8)

Elapsed time: Lower is better

Elapsed Time (sec)

Number of MPI Tasks

- Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
luciferin: Direct RHF, gradient, 294 AO
(Elapsed Time in seconds)

Platforms	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems	16 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5		444 / 1	228 / 2	122 / 4
IBM OpenPower 720 1.65 GHz POWER5	916 / 1	467 / 1	241 / 1	
IBM p630 1.45 GHz POWER4+ (AIX 5L)	1030 / 1	525 / 1	272 / 1	
IBM p630 1.45 GHz POWER4+ (SLES 8)	1033 / 1	529 / 1	290 / 1	

- Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
luciferin: Direct RHF, gradient, 294 AO
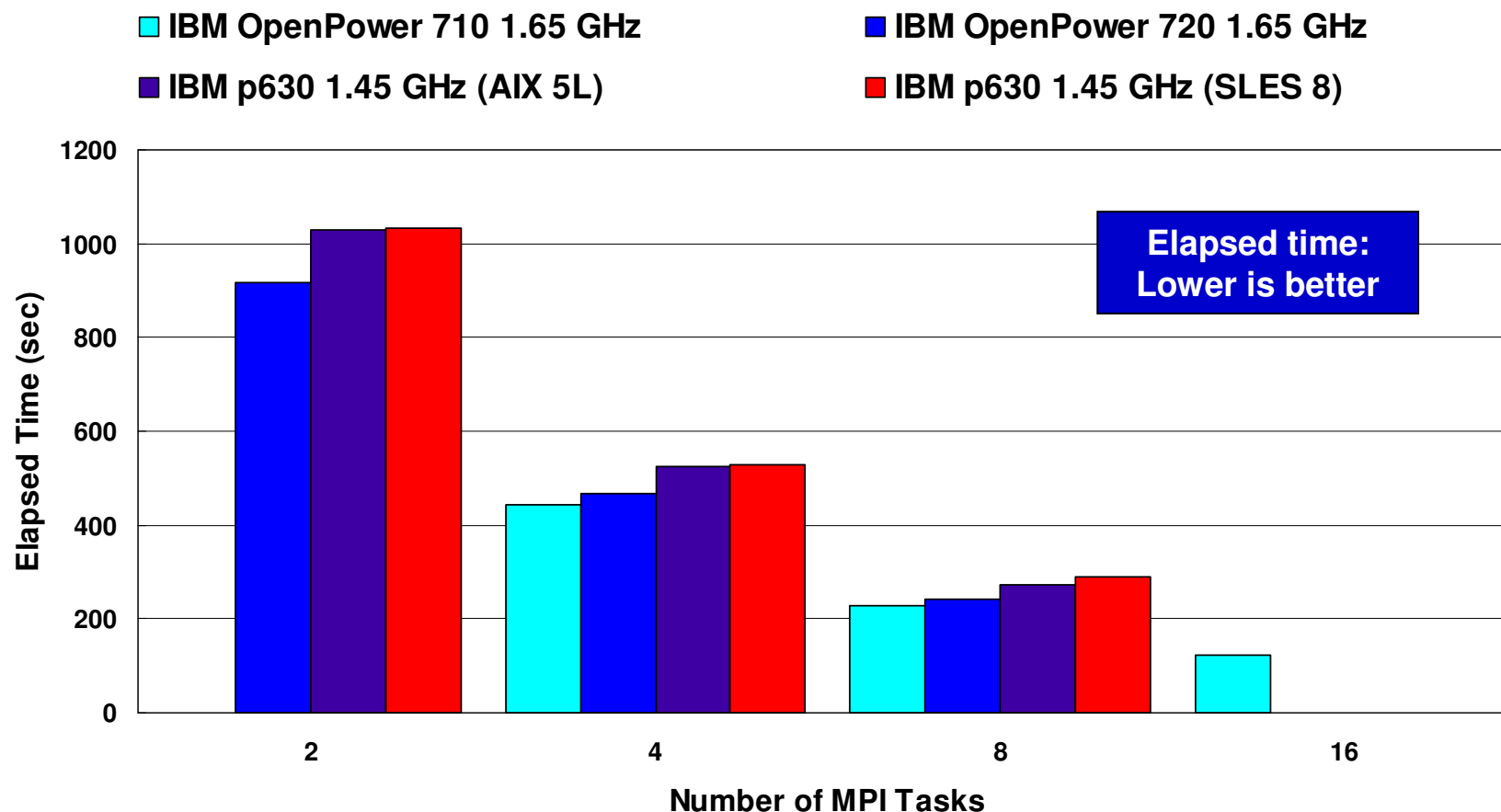## (Elapsed Time in seconds)

- **IBM OpenPower 710 1.65 GHz**
- **IBM OpenPower 720 1.65 GHz**
- **IBM p630 1.45 GHz (AIX 5L)**
- **IBM p630 1.45 GHz (SLES 8)**

Elapsed time: Lower is better

Number of MPI Tasks

Elapsed Time (sec)

- •Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- •IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
nicotine: Direct RHF, gradient, 208 AO
(Elapsed Time in seconds)

Platforms	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems	16 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5		198 / 1	103 / 2	56 / 4
IBM OpenPower 720 1.65 GHz POWER5	420 / 1	215 / 1	112 / 1	
IBM p630 1.45 GHz POWER4+ (SLES 8)	478 / 1	244 / 1	131 / 1	

- Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
nicotine: Direct RHF, gradient, 208 AO
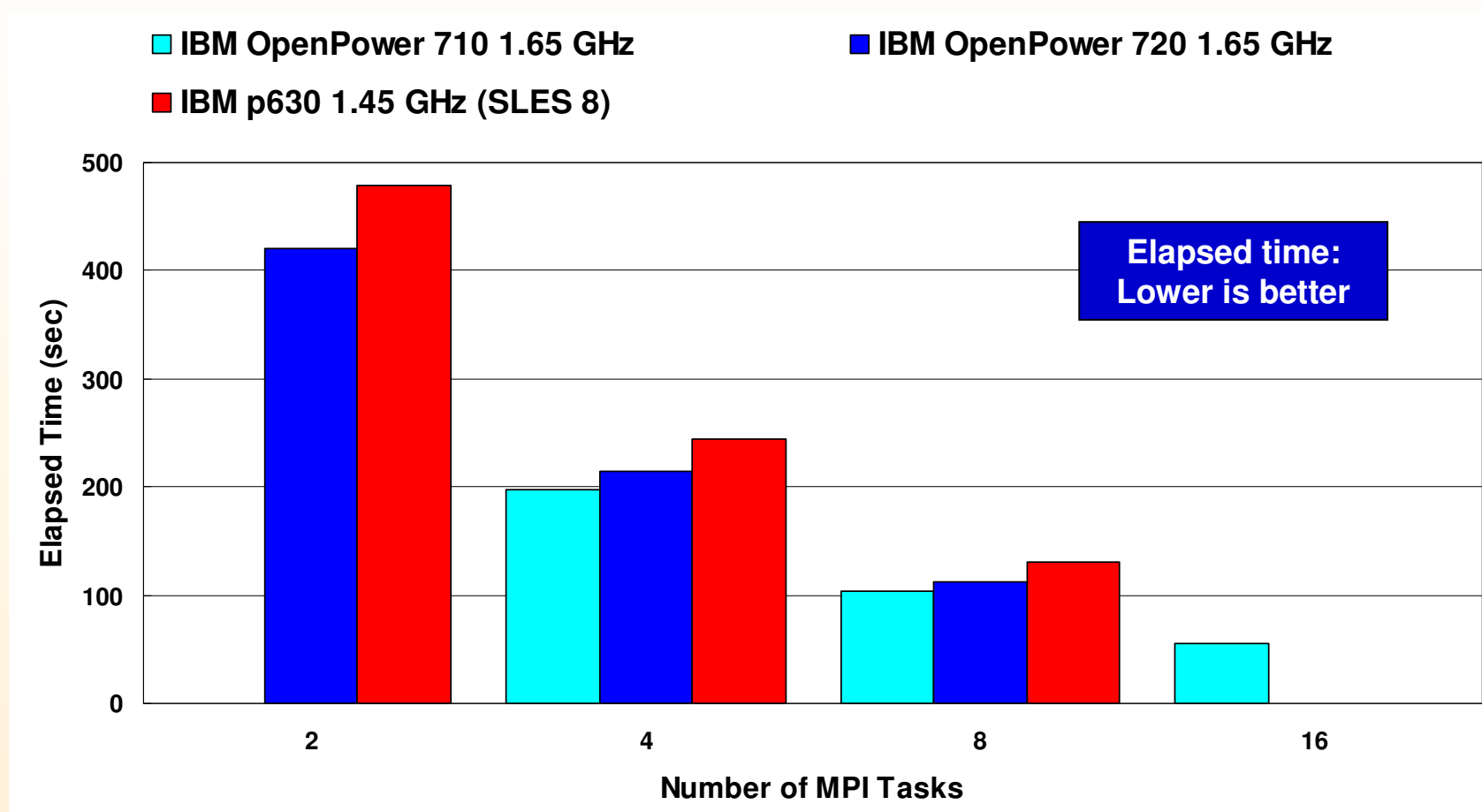### (Elapsed Time in seconds)

- Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
siccc: Direct GVB, Hessian, 180 AO
(Elapsed Time in seconds)

Platforms	2 MPI Tasks / # of Systems	4 MPI Tasks / # of Systems	8 MPI Tasks / # of Systems	16 MPI Tasks / # of Systems
IBM OpenPower 710 1.65 GHz POWER5		288 / 1	161 / 2	105 / 4
IBM OpenPower 720 1.65 GHz POWER5	598 / 1	331 / 1	189 / 1	

•Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
•IBM data current as of January 17, 2005.

GAMESS Version December 12, 2003
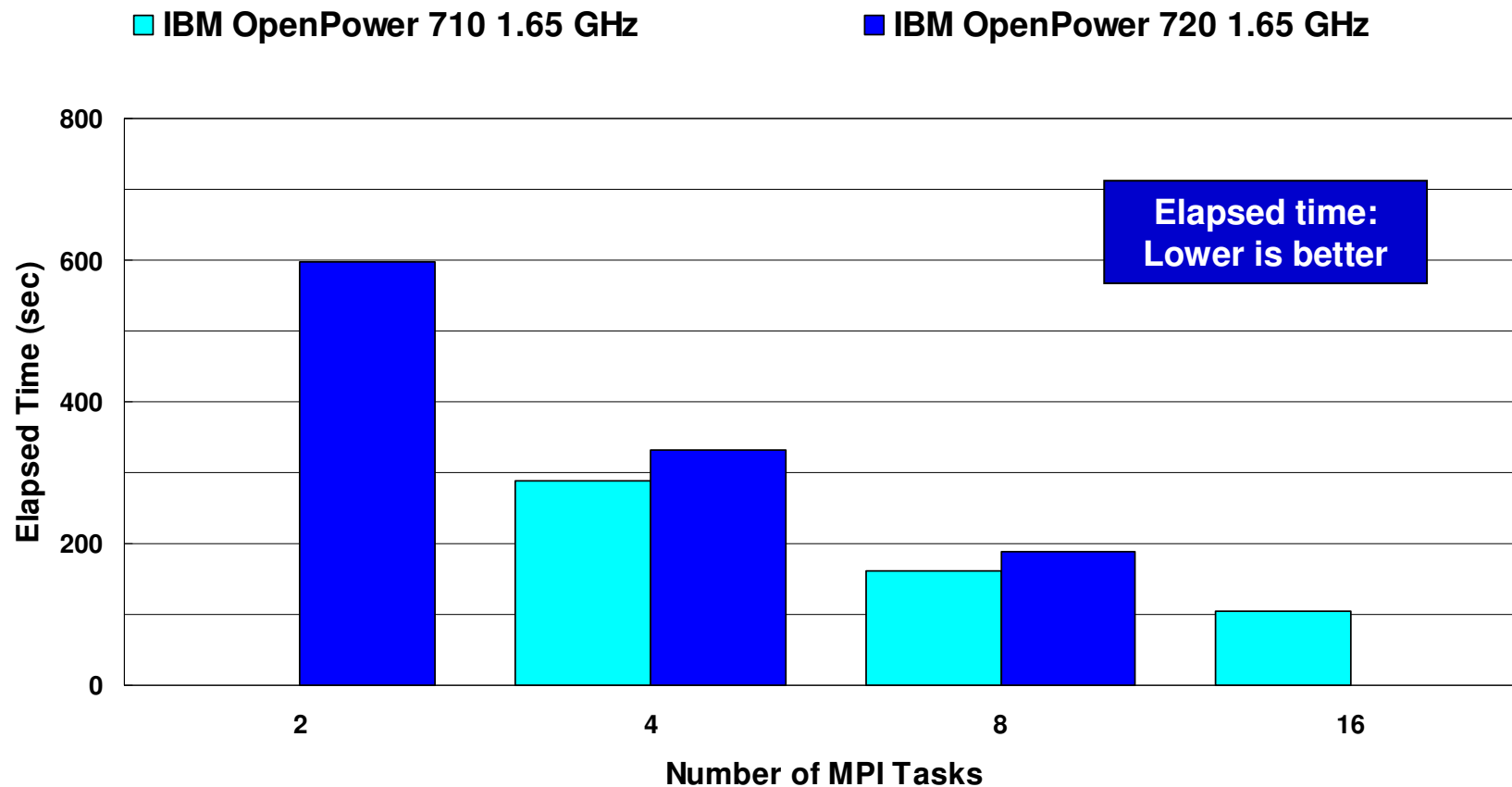# siccc: Direct GVB, Hessian, 180 AO
(Elapsed Time in seconds)

- IBM OpenPower 710 1.65 GHz
- IBM OpenPower 720 1.65 GHz

Elapsed time: Lower is better

Elapsed Time (sec)

Number of MPI Tasks

- Note: GAMESS creates 2N MPI tasks for what is effectively an N-way job.
- IBM data current as of January 17, 2005.

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Revised February 6, 2004

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Notes on Benchmarks and Values

The IBM benchmarks results shown herein were derived using particular, well configured, development-level and generally-available computer systems. Buyers should consult other sources of information to evaluate the performance of systems they are considering buying and should consider conducting application oriented testing. For additional information about the benchmarks, values and systems tested, contact your local IBM office or IBM authorized reseller or access the website of the benchmark consortium or benchmark vendor.

IBM benchmark results can be found in the IBM eServer p5, pSeries and IBM RS/6000 Performance Report at
http://www-1.ibm.com/servers/eserver/pseries/hardware/system_perf.html

Unless otherwise indicated for a system, the performance benchmarks were conducted using AIX V4.3 or AIX 5L. IBM C Set++ for AIX and IBM XL FORTRAN for AIX with optimization were the compilers used in the benchmark tests. The preprocessors used in some benchmark tests include KAP 3.2 for FORTRAN and KAP/C 1.4.2 from Kuck & Associates and VAST-2 v4.01X8 from Pacific-Sierra Research. The preprocessors were purchased separately from these vendors. Other software packages like IBM ESSL for AIX and MASS for AIX were also used in some benchmarks.

For a definition and explanation of each benchmark and the full list of detailed results, visit the web site of the benchmark consortium or benchmark vendor.

TPC   http://www.tpc.org
SPEC   http://www.spec.org
Linpack   http://www.netlib.org/benchmark/performance.pdf
Pro/E   http://www.proe.com
GPC   http://www.spec.org/gpc
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