Deep Computing Capacity on Demand: Life Sciences Industry

Highlights

- *Addresses peak workload demands for high performance computing*
- *Offers flexible pricing, allowing customers to pay only for the capacity reserved and avoid up-front capital investment*
- *Helps create a flexible, scalable and responsive IT infrastructure*

IBM Deep Computing

IBM Deep Computing can address the needs of customers who require powerful solutions to address their most complex and challenging business needs. These customers include scientists, engineers, knowledge workers, and other professionals whose core business or research relies on high performance computing (HPC) for deep levels of computation, data access, visualization, and communications. Deep Computing is more than traditional HPC hardware, software and services. It also embraces emerging strategic technologies, research initiatives, open standards, industry and customer partnerships, and industry expertise. IBM Deep Computing takes a comprehensive approach to helping our customers gain insight and transform their business and organizations. Industries and business segments include Life Sciences, Digital Media, Financial Services, Petroleum, Electronics, Automotive, Aerospace, Government and Higher Education.

Using HPC in the Life Sciences industry

The Life Sciences industry, ranging from discovery of targets and leads, to development of new drugs, diagnostics and therapeutics, to the delivery of leading-edge patient care is well-suited to take advantage of an on demand computing and storage model. High Performance Computing (HPC) supports key research, business, clinical, manufacturing and regulatory processes in Biotechnology,

Pharmaceutical, Academic, Government, Provider and Payer roles. Scientists and physicians increasingly employ HPC capabilities and assets directly or indirectly:

- *Researchers across a range of disciplines seek to identify and validate targets and leads*
- *Clinicians work to match genome and phenome to proteome*
- *Clinical trials managers and regulators aim to reduce development cost and time and produce a flawless submission*
- *Payers and providers strive to match data to actionable, accurate, timely diagnoses to drive better patient outcomes at lower lifetime cost*
- *Physicians work to target treatment solutions to their individual patients instead of populations*

As research, development and diagnostic environments have become increasingly digital, accompanied by a rapid pace of experimentation, innovation and advance, it may not be economical for an individual entity to build HPC capacity to meet its peak demand.

IBM's offerings for on demand delivery of high performance computing demand can help Life Sciences constituents meet peak demands for HPC capacity, while providing a better way to manage capital and operating costs. Life Sciences constituents can achieve attractive price/performance for compute- and data-intensive applications and processing large data volumes—distributed, federated, warehoused, or consolidated. Organizations may reduce the administrative costs associated with managing distributed systems and data, allowing them to focus on their core research, development, clinical and business activities, rather than on IT cost recovery or infrastructure complexity.

Meeting Life Sciences research, development, clinical and business challenges

Life Sciences companies, institutions and agencies face increasing requirements for HPC capacity in order to process, manage and mine ever-expanding quantities of data to aid discovery, development and diagnostic decisions. These requirements are exacerbated by the need to improve productivity; namely to fill the pipeline, "fail sooner and faster," derive insight and repeatable results from heterogeneous data via directed and non-directed searches and analysis. Life Sciences companies have to meet a broad range of objectives:

- *Review, manage and analyze a larger portfolio of research and clinical data assets in a shorter time in response to scientific, regulatory, patient and business needs*
- *Build better and more accurate protein models*
- *Cross-tabulate breakthrough mass-spec data to corresponding genomic, phenotypic and genealogical data to identify potential targets and leads faster*
- *Reduce the time to derive key decisions such as whether/how/why to proceed to the next phase of a trial*
- *Capture, cleanse, analyze and report clinical trial data, nominal and adverse, in a close to real time environment to support an adaptive trial structure*
- *Manipulate and mine huge volumes of expression data in hours instead of weeks to stem a potential outbreak*

Such activities, requiring high peak loads to satisfy unpredictable demands, can be critical to the continued success of research, commercial, academic, clinical and regulatory players in the Life Sciences industry as they endeavor to use scarce and valuable resources in the most effective manner, while containing costs, mitigating risks and driving optimum patient outcomes.

Successes in discovery, development and delivery can be uncertain, and the Life Sciences industry is beginning to show symptoms of economic stress as research, health care and accompanying IT expenses are rising faster than results fill the pipeline; patents expire faster than the pipeline fills and health care costs continue to rise. Both the current 'blockbuster' model and an encroaching targeted treatment solution model require the industry to embark on significant transformation in order for desired growth, profitability and results to drive sustaining funding and investment. Research is shifting from in-vivo and in-vitro to in-silico, with much to be discovered and proven, yielding a lab and IT environment increasingly but unpredictably dependent on massive computing capacity and huge, often dispersed data volumes. Mandates from the governing bodies (e.g. HIPAA) are placing additional process, skills, risk and economic pressures on an increasingly cost-constrained, security-conscious patient-care industry, especially as it continues its shift from analog to digital media. For providers, shifts in patient portfolios and payer reimbursement have exerted downward pressure on capital budgets, squeezed operating margins and constricted operating cash. Payers, public and private, speak of increasing cost and price controls across Life Sciences (Biotechnology and Pharmaceutical) and Health Care (private providers) in response to public and interest group pressures—actions which would materially disrupt the current fiscal models.

The Life Sciences industry is facing voluntary and mandatory process and model transformations that are driving an increasing, unpredictable and variable demand for HPC capacity. Planning against such fluctuating demand becomes inherently difficult. Companies must provide services quickly, efficiently and cost-effectively. The successful companies are those that meet the fluctuating needs of the Life Science constituencies while helping to control costs, advance science/medicine and improve profit margins. Using IBM cluster services to obtain HPC capacity on demand can contribute to this success.

IBM can help the Life Sciences industry meet these research, clinical and business challenges by helping to maximize capacity flexibility while minimizing capital investment. IBM offerings for delivering HPC on demand are based on state-of-the-art cluster technologies and services, and leverage IBM's industry and technology expertise.

Examining HPC requirements for the Life Sciences industry

Providing HPC resources on demand requires an infrastructure of high-speed processors and storage that can provide measurable compute and data storage capacity in a flexible, scalable and highly secure manner. Users require seamless access

to these resources, regardless of where the physical systems may reside. An HPC infrastructure for Life Sciences has the following objectives:

Scalability: Applications and databases often exceed the capacity of even the largest single systems, with companies and institutions quickly outgrowing these systems.

Security: Life Sciences researchers and developers need a data, information and knowledge sharing environment that is highly secure, yet enables collaboration in an environment accustomed to physical and logical partitions.

Flexibility: While they focus on controlling costs, Life Sciences companies need increased flexibility in a rapidly changing environment.

Significant processing capacity: As processing requirements continue to grow, more and more companies are finding that they can benefit from using clustered servers and Grid computing. Clusters link separate nodes to create a single, powerful, scalable system, while Grid computing increases overall compute resource sharing and utilization.

Flexible financial and delivery models: Life sciences companies can benefit from balancing their fixed and variable IT infrastructure and operations costs and choosing between onsite owned/operated versus offsite hosted IT solutions.

Clustering and Grid computing, combined with a wide range of server and storage technologies, are designed to provide:

- *High availability with failover protection*
- *Scalability with minimal downtime*
- *Large-capacity data volumes*
- *Capability to handle peaks in workload, permitting flexible responses to changing scientific and business requirements*

Providing high performance computing on demand

Fundamentally, providing HPC capacity on demand is a simple concept. Instead of purchasing computers to meet peak demands, companies can procure sufficient hardware for average demand and then contract remote processing power to help meet peak loads, or offload all processing to a remote facility. In practice this process can be more complex. However, IBM can help shield customers from much of this complexity—one of the primary advantages of a hosted on demand environment.

High performance computing can have many different requirements, and purchasing the sufficient hardware can become expensive. Some problems are computationally parallel, and a large number of servers working in parallel can solve the problem quickly and efficiently. Other problems require ultrafast interprocess communication or a single large memory model. A hosted environment can supply access to these resources, and instead of paying for equipment that

may be underutilized, customers simply pay for the cycles and compute or storage resources that they reserve for a specified period of time.

IBM provides a scalable, highly secure and extensible environment designed to handle peak workloads. This solution combines the best of IBM technologies and open standards with on demand computing, providing an infrastructure that enables customers to help meet their goals of increased scalability, flexibility, and processing capacity.

Building a world class infrastructure to support Life Sciences

IBM has a comprehensive approach to deliver on demand computing for Life Sciences markets. IBM's advanced clustering capabilities and services can help reduce the time, effort and expense required to capture, compile and analyze the broad spectrum of Life Sciences data.

The HPC infrastructure is based on the IBM @server™ Cluster 1350, an innovative Linux-based cluster that provides a robust, highly scalable compute facility centrally managed and controlled by IBM. The Cluster 1350 combines the power of IBM @server xSeries® Intel Xeon™ processor 32-bit and IBM @server AMD Opteron™ processor 32-bit/64-bit compute servers with IBM Cluster Systems Management (CSM) software, IBM TotalStorage® products, and leading third-party networking components to enable powerful, flexible solutions for high performance computing. IBM also offers clusters of IBM @server pSeries® POWER™ 64-bit compute nodes running AIX 5L™ or Linux. IBM plans to offer other models, platforms and technologies over time.

Customers can access virtual dedicated Cluster 1350 cluster capacity based on the xSeries 335 a 2-way Intel Xeon processor-based server or IBM @server 325 AMD Opteron processor-based server. The xSeries 345 or IBM @server 325 is used as a management node for centralized control of the system. Each virtual cluster has its own dedicated management node. Customers can also access virtual cluster capacity based on the pSeries 655 4-way server with a pSeries management node.

Optional Fibre Channel or SCSI external disk storage capacity can be provided. Customers also have access to an IBM 3590, LTO or DLT serially shared tape server for loading data and performing backups.

Customers have full control of the compute and storage resources within their assigned environment, and each virtual cluster has a dedicated cluster and management network. A robust networking infrastructure is designed to allow customer data and applications to be highly available and secure, and a virtual private network (VPN) service provides remote access to the facility. Customers pay for their assigned compute and storage capacity for the length of time that they use it.

Advanced systems management and Grid-enabling software

IBM Cluster Systems Management (CSM) for Linux software provides robust capabilities for resource monitoring, automated operations, remote hardware control, distributed command execution, configuration file management and parallel network

installation. Access to the system is accomplished through a remote shell interface. Customers may use CSM directly to perform remote management tasks, install and use their own management tools, or request comprehensive management and monitoring services from IBM.

The IBM General Parallel File System (GPFS) for Linux and AIX®, offered as an option, is a high performance scalable file system—ideal for Life Sciences companies that manage extremely large data files. GPFS can provide an enhanced layer of scalability, availability and performance. Optional dynamic job scheduling and workload management tools are also planned to be available to optimize cluster resources and help increase job throughput.

Customers supply the additional software required to run their workloads; this software may include in-house, open source, or IBM and third party applications and tools. Customers can use Grid software and services, acquired separately from IBM or a third party, to develop new applications or run existing applications in a Grid environment. The open source Globus Toolkit™ is designed to provide the underlying elements for Grid security, communication, information infrastructure, resource management and portability. The IBM Grid Toolbox for Linux and AIX is an integrated set of tools and software based on the Globus Toolkit that facilitates the building of Grids and development of Grid applications. In addition to running production workloads, customers may run benchmarks or perform other types of analysis.

Services for delivering HPC on demand

IBM offers a variety of services to support IBM-supplied hardware, software, and networking components and infrastructure. Base services include the facility, provisioning and deployment of resources, security, virtual private network, monitoring, maintenance, and help desk support. Customers can benefit from a range of fee-based custom services, such as enhanced VPN bandwidth, software deployment and customization, advanced monitoring and management, storage management and backup, Grid-related services, and more.

Delivering dynamic HPC resources

IBM offers dynamic HPC resources on demand that are designed to match customer requirements for scalability and capacity. The on demand computing model is economical, enabling customers to enjoy flexible pricing and terms and helping them to realize lower operational and infrastructure fixed costs. This computing model also can help reduce infrastructure complexity, IT training and staffing and ongoing maintenance and upgrades. Customers can focus on their core research and business and be insulated from rapid information technology shifts.

IBM is extending its leadership in high performance computing to the on demand environment. By combining leading IBM @server technologies, advanced cluster and systems management capabilities, growth and innovation in Grid and autonomic computing, and demonstrated industry expertise, IBM is delivering solutions designed to enable Life Sciences customers to conduct their research and business more efficiently and effectively in a highly competitive market.

Figure A. Possible technical components: Deep Computing Capacity on Demand for the Life Sciences Industry

Component	Features/Benefits
HARDWARE	
IBM @server Cluster 1350	• Combines IBM @server servers, IBM TotalStorage storage and leading third-party networking components to create powerful, flexible solutions for HPC and commercial application environments • Uses xSeries 335 (1U) and xSeries 345 Intel Xeon 32-bit dual processor nodes • Uses BladeCenter Intel Xeon 32-bit dual processor nodes • Uses IBM @server 325 (1U) AMD Opteron 32-bit/64-bit dual processor nodes • Runs the Linux operating system standard • Runs the Windows operating system by exception • Uses CSM for central management
AMD Opteron Technology	• Runs 32-bit and 64-bit applications simultaneously • Easy migration to 64-bit computing capability with software investment protection • Extreme price/performance design—high performance at affordable pricing • Runs Linux and Windows
IBM pSeries Technology	• Features POWER 64-bit processors in an ultra-dense packaged server for high performance computing • Includes the AIX 5L operating system and a rich suite of cluster software
IBM TotalStorage	• FAStT Fibre Channel and SCSI disk options • 3590, LTO, and DLT tape server and cartridges options
SOFTWARE	
Operating Systems	• Linux and Windows provided by customer • AIX provided by IBM
IBM Cluster Systems Management (CSM)	• Provides robust, powerful management from a central point of control • Simplifies administrative tasks and may reduce life-cycle costs • Offers a highly reliable infrastructure and event monitoring • Provides software installation and updates, remote hardware control, distributed command execution, configuration file management, and diagnostics
IBM General Parallel File System (GPFS) (optional)	• Provides shared access to files across multiple disk drives on multiple nodes • Provides a common file system abstraction for data shared among multiple nodes • Allows applications to easily access files using standard POSIX (Portable Operating System Interface for UNIX®) file system interfaces • Enables parallel applications to simultaneously access either the same or different files • Provides high availability through automatic recovery from node and disk failures
Job scheduling (optional) (planned availability)	• Provides dynamic job scheduling and workload management • Designed to optimize cluster resources and increase job throughput • Works with CSM to facilitate management of cluster resources
SERVICES	
IBM Global Services	• Support Deep Computing Capacity on Demand with a full range of services for solution customization • Provide Grid enablement services, including Grid Innovation Workshops, Grid Pilot Implementation Services, and Grid Rollout Implementation Services

For more information

To learn more about Deep Computing Capacity on Demand for the Life Sciences Industry, contact your IBM representative.

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