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HP's supercomputer will greatly aid research at IGIB

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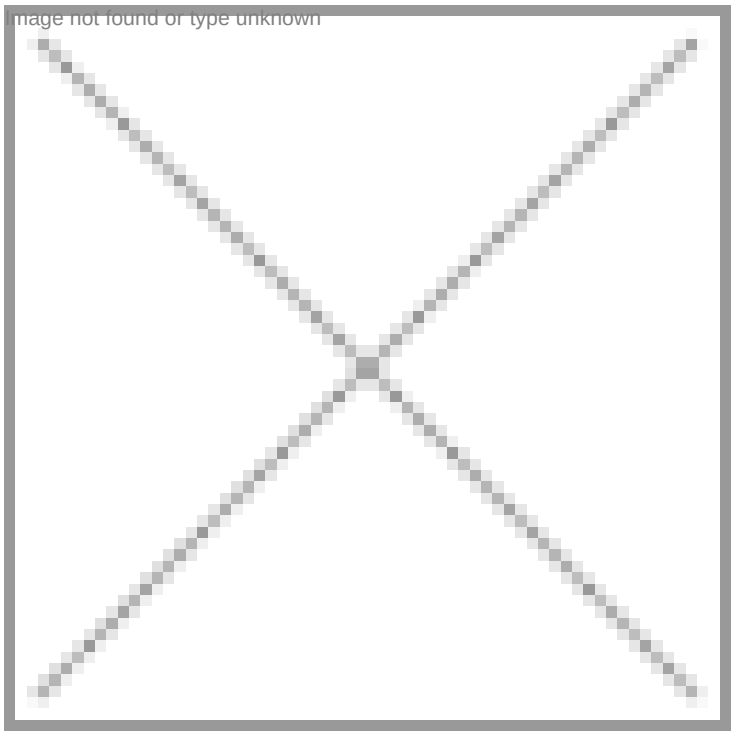

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The facility at IGIB has put India in the Top 500 global computational list

Life sciences companies and those institutions involved at the cutting-edge of life science research face fierce competition and rising R&D costs as they work amidst various challenges to bring a breakthrough drug to market. Technology, especially in Informatics and Computational Sciences has an important role to play in helping further research in life sciences. The IT infrastructure must align with constantly changing business and research requirements. Many companies are implementing low-cost, high-technology IT infrastructures that can integrate with current environments, adapt quickly, and accelerate business and research processes with minimal or no disruption to operations.

Life science research advances beyond the area of genomics is the next great challenge. This deals with life systems delving in genes to proteins, biotechnology to pharmaceuticals and to personalized medicine. The computational demands increase exponentially, necessitated by identifying and understanding all proteins and how their complexes in living beings interact with drug molecules. To meet these challenges, the Institute of Genomics and Integrative Biology (IGIB) was looking to acquire the computational power for research in complex molecular dynamics simulations, protein structure, interaction experiments and in-silico toxicity studies.

Mapping complex requirements

To realize these huge, complex computational challenges with very large data sizes will lead to the generation of complete physiological simulations that integrative system biology experiments will demand, necessitating the setting up of ultra scalable systems that reach to 4Teraflops and beyond. The IGIB has taken its first step with its 4+ TFlops supercomputer joining the world's leading supercomputing centers adopting life science supercomputing solutions. The IGIB 4 TFlops facility is built from open standard systems and platforms that deliver top efficiency. This allows the IGIB to quickly develop complex bioinformatics algorithms on the platform that facilitates easy sharing, painless adoption and joint collaboration with the best tier institutions around the world.

"HP's Cluster Platform provides a scalable architecture that allows us to complete large simulation experiments such as molecular interactions and dynamics of protein folding much more quickly. This technology combined with HP's experience and expertise in life sciences helps IGIB speedy access to information, knowledge and new levels of efficiency."

Dr Samir Brahmachari, director, IGIB

The new Hewlett-Packard supercomputer will be used to meet the increasingly complex needs of life sciences research that has advanced beyond genomics. "HP's Cluster Platform provides a scalable architecture that allows us to complete large simulation experiments such as molecular interactions and dynamics of protein folding much more quickly," says Dr Samir Brahmachari, director, IGIB. "This technology combined with HP's experience and expertise in life sciences helps IGIB speedy access to information, knowledge and new levels of efficiency, which we hope will ultimately culminate in the discovery of new drug targets and predictive medicine for complex disorders. Using the HP supercomputer, in a short time we have been able to scan entire viral genome database to discover human miRNAs that can target crucial genes in HIV-1 and H5N1 bird flu influenza virus.

The IGIB High Performance Computing Facility (HPC) is a 288-node Cluster Platform 3000 based on Intel Xeon HP ProLiant servers running the Linux operating system. The high-speed InfiniBand 10Gbps cluster interconnect is used and HP's XC System Software provides cluster management capability. In addition, this center will also have a 24-node, high-performance HP ProLiant cluster running Linux, a powerful HP Itanium based server that will be used for experimental projects by the students/developer community. The systems are supported by 12 Terabytes of HP StorageWorks Enterprise Virtual Array 5000 (EVA5000) storage and a MSL6060 tape library. The facility will also host a powerful scalable Integrity Superdome, an SMP server and 12 Terabyte storage capacity. To help customers manage and visualise the large volumes of data created by computational analysis, HP's Unified Cluster Portfolio, which includes entry-level HP Integrity and ProLiant servers and an enhanced HP StorageWorks Scalable File Share, provide a common implementation across Linux and servers based on industry-standard processors (Intel Xeon , Itanium 2 and AMD Opteron).

Furthering the cause of medical issues

"Partnering with HP will help to further advancements in research and speed progress in the discovery of new drug target and predictive medicines for complex disorders", adds Dr Brahmachari. "This will enable us to attract the best young minds of the country through attractive fellowships and world-class supercomputing environment. This partnership will ensure that the hassle of such a large and complex computing environment will be managed by professionals from HP."

HP's most powerful supercomputer in Asia will be based out of IGIB's new facility and will be a national facility available to all researchers, scientists, companies and other organizations who need high end computational systems to address and contribute to help find solutions to critical medical issues. HP, under the partnership, will facilitate the investigation of collaborative research projects with its partners, institutions, other COEs and scientific communities (e.g. EPFL, SIB and Partners) in bioscience research.

Ensuring maximum value creation

This supercomputing facility at IGIB has put India in the Top 500 global computational list and as a leading center globally in the life sciences domain, while fostering excellence for research in life sciences. This infrastructure has helped IGIB join the Top 500 club, the HP Supercomputer being one of only a handful in India to make the list. Due to the seamless integration of IT into business operations, early identification of promising compounds will be possible, leading to a faster time-to-market and giving a higher return on investment. Large simulation experiments such as molecular interactions/dynamics, protein folding, virtual drug screening, discovering RNA therapeutics, etc. will be completed with faster turnaround times. This will not only accelerate discovery of new drugs and targets with minimum side effects but also enable solving fundamental problems of gene regulatory network and host pathogen specificity.

Computational life science algorithms need both capability and capacity computational models. These involve multiple tasks that may demand simultaneous throughput. The IGIB can use intelligent resource management, provided as inbuilt in to the HP supercomputing cluster. The IGIB parallel algorithms require a highly scalable SMP server like HP's Integity Superdome SMP server. These highly scalable, parallelized applications pose the ultimate test to inherent scalability and parallel efficiency of a well- tuned HPC cluster.

With HPC, IGIB can now accelerate the pace of innovation while driving greater cost savings, productivity and responding quickly to new opportunities and change, with complete, supported, highly scalable cluster solutions. Further, HP's leadership position in health systems innovation will help life sciences researchers and product developers at IGIB to speedily access new discoveries and aid in developing new therapeutics.