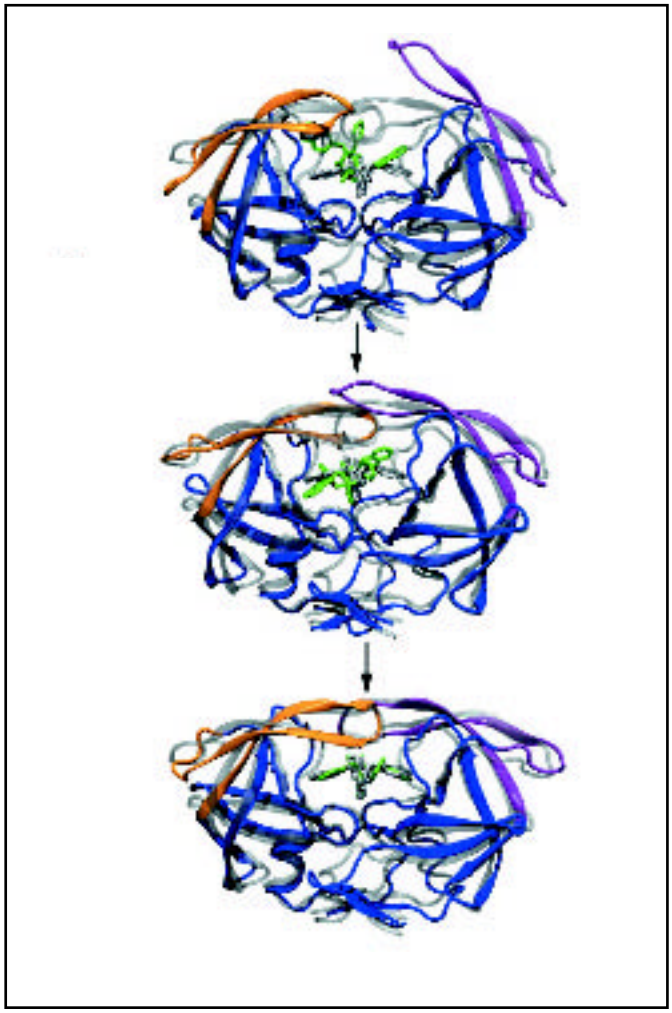
Efficient mining of genomic data for better drug discovery

Michael G. Brown of Silicon Graphics, Inc (SGI) explains how new computer technologies have emerged in recent years to provide more efficient genome processing systems, leading to increased efficiencies in drug discovery.

Several new technologies have emerged over the past few years to support gene sequencing and related biosciences work. In particular, cluster computer systems based on the X86 architecture, like the new SGI® Altix® XE clusters from Silicon Graphics, Inc (SGI) are now used as dedicated genome processing systems. These systems have the advantage of offering high CPU speed and low cost per CPU but with more complex system and storage management environments. A more recent development has been the emergence of FPGA-based algorithms for genetic sequencing.

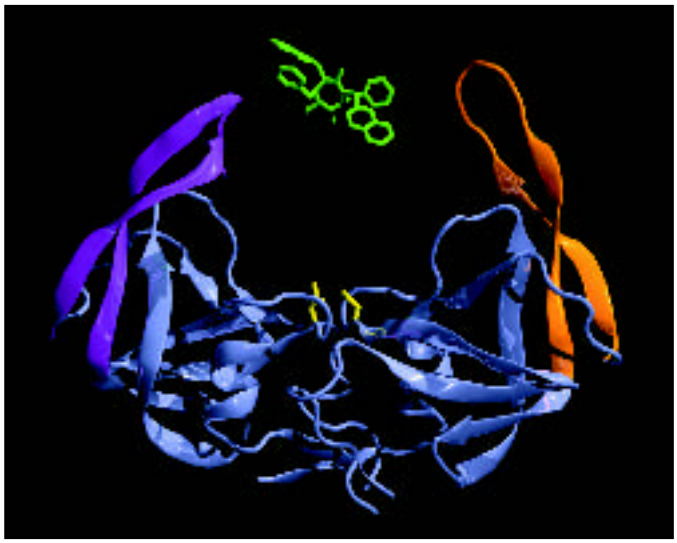


Working on an SGI Altix system, researchers at Stony Brook University can simulate an HIV protease molecule to view the moments at which 'starter molecules' for HIV are most vulnerable to new drugs. Seen here are the three states of thr HIV protease molecule: open, semi-open, and closed. (Image courtesy of Stony Brook University).

MEET MICHAEL G. BROWN OF SGI

Michael G. Brown is Sciences Segments marketing team manager at SGI with over 20 years of experience with scientific computing and visualisation. He joined SGI to launch the RISC revolution in the supercomputing industry, and later became marketing team manager for Visualization and Visual Supercomputing. Before joining SGI, he held product marketing and sales positions for Digital Equipment Corporation in both the USA and Europe and a research and development position at Lawrence Livermore National Laboratory. He holds a BS in Electrical Engineering and BA in Philosophy from Swarthmore College, an MS in Electrical Engineering from the University of Illinois Champaign-Urbana, and an MBA from The Wharton School at the University of Pennsylvania.

SGI, headquartered in Mountain View, California, USA, is a leader in high-performance computing, providing solutions for a very broad range of industries and service sectors, including health care, oil exploration, climate studies, security and defence, and, of course, life sciences. The company has recently worked with an application partner to achieve a greater than



Experiments have been unable to show how drugs gain access to the active site near the centre of the protease, but the simulations run on an SGI Altix system revealed transient events in which the binding site opens and an inhibitor can enter. (Image courtesy of Stony Brook University).

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100 times speed-up on BLAST using a single SGI® RASC™ RC100 blade on an Altix 4700. Since many of these can be combined together in a single system, a gene sequencing site could be looking at a single computing system that could deliver 1,000 times or greater application speed-up, effectively creating a gene sequencing factory.

"SGI was established in 1982 by a team of engineers from Stanford led by Jim Clark in 1982. SGI's initial focus on 3D graphics required it to develop highly parallel computational systems with robust I/O infrastructure, which was perfect for computational chemistry and later on for genetic sequencing," says Michael G. Brown, SGI's Sciences Segments marketing team manager. "SGI currently delivers computing and storage management solutions in government, education, sciences, energy, media and manufacturing markets that allow users to simplify complex data-intensive computing and storage environments. SGI's differentiation is our ability to integrate a mix of flexible, large-memory computer servers, X86 clusters, high-performance 'appliances', NAS storage and Data Lifecycle Management solutions into a solution that is both tailored to the user's current workflow and is flexible enough to address future changes in that workflow. We have seen significant interest in each of these solutions and have had several orders over the past year."

Introducing new solutions

SGI recently introduced an all-new range of cluster solutions based on Dual-Core Intel® Xeon® processor 5100, and has introduced the SGI® Altix® 450 mid-range blade server based on dual-core Intel® Itanium® 2 processors. The company has also doubled the performance of its SGI® Altix® 4700 servers. SGI says these developments reflect its new strategy to significantly extend its presence within its existing high-performance computing markets, and to introduce SGI solutions to new customers.

SGI has also introduced SGI® Altix® XE, a new family of Linux® OS-based servers and factory-integrated clusters powered by the new Dual-Core Intel Xeon processor 5100. SGI Altix XE servers are driven by a pair of dual-core Intel Xeon processor 5150 CPUs, with a total of four processor cores and supporting up to 32GB of memory in each server.

The company is also equipping its SGI® Altix® 4700 blade server line with new dual-core Intel® Itanium® 2 processors. SGI says the new Linux systems will deliver at least double the performance of Altix servers at no additional system cost to users, while drawing less power and offering more density and flexibility for demanding, data-intensive applications.

Supporting growth in drug discovery

So how do these developments impact on the drug discovery sector? Brown explains:

"We see significant growth in the overall drug discovery business - not just in gene sequencing - that is driven by the growth of powerful yet affordable computing and data management solutions that allow even small to medium-sized research groups directly participate in the development of new pharmaceuticals. We are always looking for opportunities to partner with new application providers and integrators in this and other fields.

"Drug discovery is about much more than just gene sequencing. Success requires a powerful computational infrastructure, data management environment, and data archiving capabilities to meet regulatory requirements. Leading research establishments need to develop an integrated, workflow-oriented approach that automates much of the data and computing management and allows their scientists to focus on science instead of on computing. SGI is focused on delivering these capabilities, and delivering solutions that simplify complex data-intensive computing and data management environments," he says. sp²

FURTHER INFORMATION

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