The Ultimate in Productivity Computing: SGI Scalability and 64-Bit Performance Drives the Future in Life and Chemical Science Research

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Whether simulating large protein structures or delivering predictive measures of catalysts, 64-bit computing and system scalability have become critical requirements for delivering timely and accurate results. This class of calculations demonstrates the advantages that large memory in single-system image computers can deliver.

Scalability

Many computational chemistry jobs demand scalable systems to deliver results in reasonable time frames. Being able to return a calculation over 100 times faster by efficient utilization of both scalable computers and parallelized software allows a scientist to run more jobs in the same time period and allows broader testing of experimental options.

For example, CASTEP, the density functional theory application from Accelrys, has been demonstrated to achieve a 112 times speedup on the same experiment when using tuned software and a 128-processor SGI® Origin® server, part of a family of single system image supercomputers that can deliver up to 1TB of memory.

For explorations of the properties of complex chemical reactions or predictions for new formulation criteria for tomorrow's nanomaterials, it is critical to take full advantage of whole-system parallelism in a 64-bit environment to enable quick turnaround of high- precision jobs.

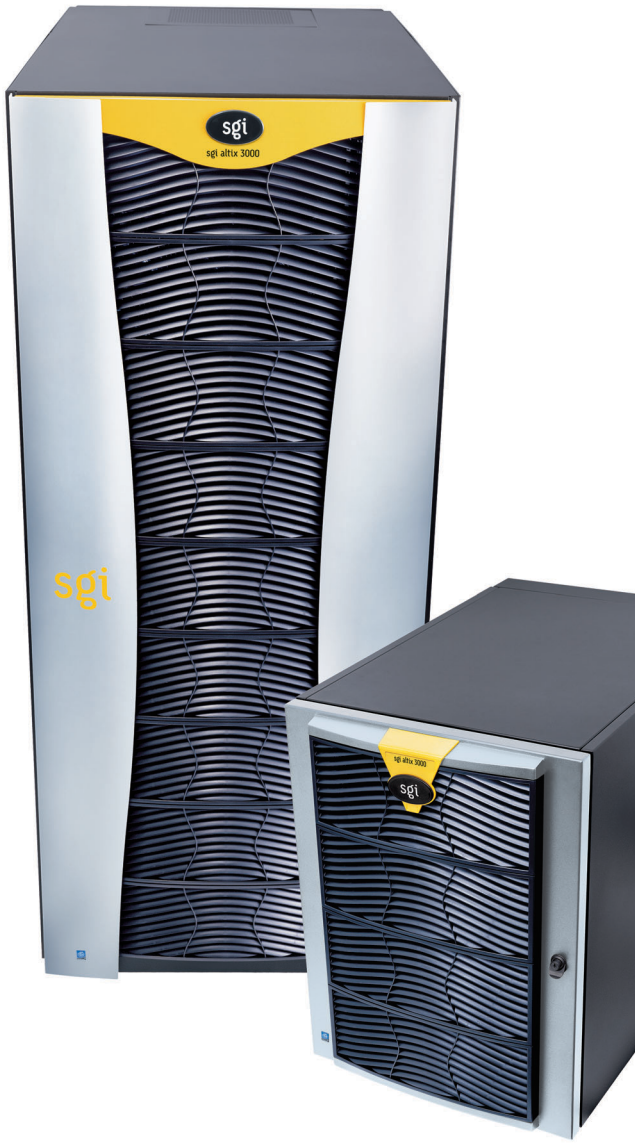
64-Bit Performance

A trend in technical computing in the past two years has been the rapid adoption of the Linux® operating system, especially in the life sciences. In tasks that range from computational chemistry and molecular simulations to bioinformatics, the advantages of the open-source Linux operating system have been demonstrated.

Sequence database searching is among the most computationally demanding activities in bioinformatics, most notably the Smith-Waterman algorithm, which continues to provide the most rigorous way to search biological databases for local sequence similarities.

Superior parallel performance of major bioinformatics applications on a 64-processor SGI® Altix™ server running the 64-bit Linux operating system demonstrates the capability of Linux in a 64-bit, scalable computing environment, in which databases nearing half a terabyte may be held resident in the same single system image. Key applications are now available for the Altix 64-bit Linux systems, including Gaussian®, GAMESS, Amber®, BLAST®, and FastA'.

This breakthrough for Linux systems will speed big computational jobs at improved price points and will end the requirement to break and rebuild sequence databases for efficient database searching protocols—saving overall time and costs in unifying database searching procedures.



For further details on the SGI Origin family of servers, the world's most scalable microprocessor-based supercomputers, visit *www.sgi.com/origin/3000*, and for information on the recently launched SGI Altix family of Linux OS-based servers, visit *www.sgi.com/servers/altix*.

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