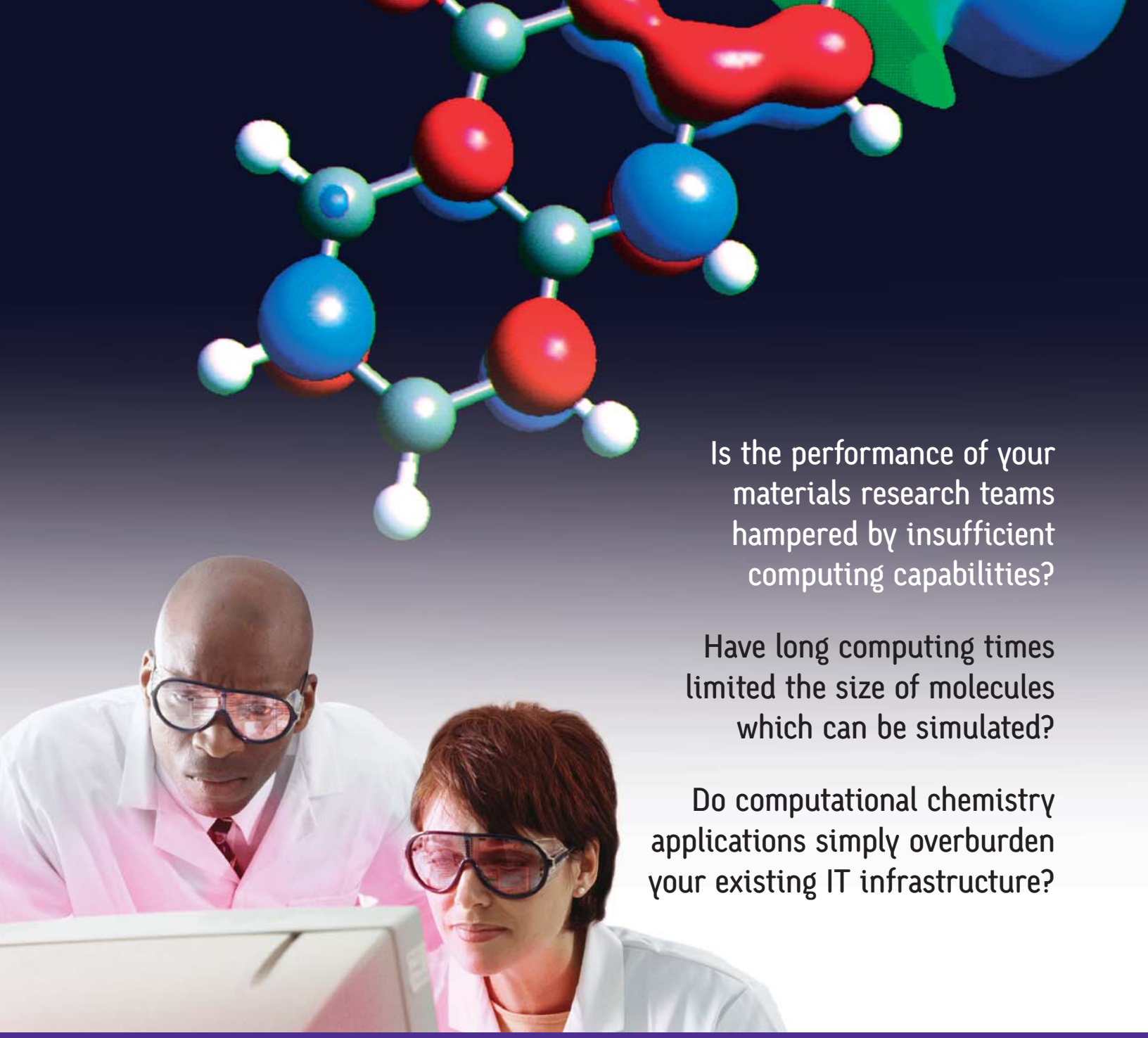

Is the performance of your materials research teams hampered by insufficient computing capabilities?

Have long computing times limited the size of molecules which can be simulated?

Do computational chemistry applications simply overburden your existing IT infrastructure?

Driving innovation
in materials research

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The field of computational materials science has become a key driver in facilitating effective modeling and analysis for the materials research community. However, despite significant advances in both software development and numerical algorithms, material scientists are reliant on access to a flexible computational infrastructure that can scale to accommodate increased molecular complexity. The inability of typical cluster technologies to provide this support has resulted in unacceptably long calculation times and the need to 'decompose' jobs into more consumable sections before running simulations.

Remove the Barriers to Productivity

The SGI® Altix® family of HPC servers, clusters, and supercomputers offers a unique computational infrastructure to optimize your material science applications. With an advanced parallel system architecture and large globally addressable memory, the SGI Altix provides the high throughput (rate at which multiple jobs are processed) and fast turnaround (how quickly an individual job is completed) that maximizes the productivity of today's material science applications. Based on the industry-leading SGI NUMAflex™ shared-memory system architecture, the SGI Altix enables material scientists to significantly improve both the scale and precision of computational simulations for complex molecular systems:

"The ability to routinely do large calculations in a reasonable timeframe would create a lot of opportunities for us to look at systems that we couldn't previously approach. Right now we have to break up problems into little pieces and use a time-consuming, mosaic approach."

Gerry Zajac – Innovene Research Associate

Global Shared Memory Access: With the NUMAflex shared-memory architecture, multiple processors have access to all available data in the system's combined memory space to perform demanding analytic and data-intensive applications. This minimizes the movement of data through I/O or networking bottlenecks that typically stretch delivery times for large model results to days and weeks. By harnessing the entire computer's thinking power, memory, and visualization resources into a single, communal space, material scientists can address larger, complete models direct from memory.

Parallel Processing Power: The Intel® Itanium® 2 Processor delivers superior floating-point performance to execute multiple instructions simultaneously, enabling more users to access departmental compute resources. The explicitly parallel architecture of the Itanium 2 Processor, including its massive execution resources, gives it the ability to accelerate calculations and analysis for large molecular simulations. Internal resources include a massive on-die cache, 128 floating-point registers, and memory management features that enable more effective management of large data sets.

"The speedup achieved with Itanium 2 and the Altix platform makes our simulation codes applicable to bigger systems than ever before. This brings us closer to bridging the gap between the engineering world and the molecular world with far-reaching implications."

Keith Glassford, Director, Materials Science Marketing, Accelrys

Bringing Complex Problems into the Realm of Routine Computation

The SGI Altix family of servers provides research departments with a computing solution that delivers a clear roadmap for cost-effective productivity and growth. Customers can configure systems with 16, 32, and 64 processors that are ideal for departmental application servers, and scale as required up to 512 processors and 6 terabytes of memory under one copy of the operating system. Users can also 'expand on demand' by independently scaling CPU, memory, and I/O resources to create the most scalable, fast, and complete materials science solution on Linux today.

SGI has also worked closely with materials research software developers so that key applications are tuned and optimized for performance and scalability on SGI's Altix. These include, but are not limited to, the DMol^3 and CASTEP applications from Accelrys®, Gaussian, VASP, Schrödinger® Jaguar, GAMESS, NWChem, and ADF. The result is the fastest time-to-solution for chemistry applications and the best job throughput for mixed capacity workloads – claims that have been consistently demonstrated both in industry standard benchmarks and real-world application results. The SGI Altix provides researchers with the capabilities to explore all analysis options, and to bring the largest problems into the realm of routine computation.

To find out more about exciting SGI solutions available for running computational chemistry applications:
Call **1-800-800-SGI1** (7441), e-mail to **eleads@sgi.com** or contact your authorized regional SGI partner.

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