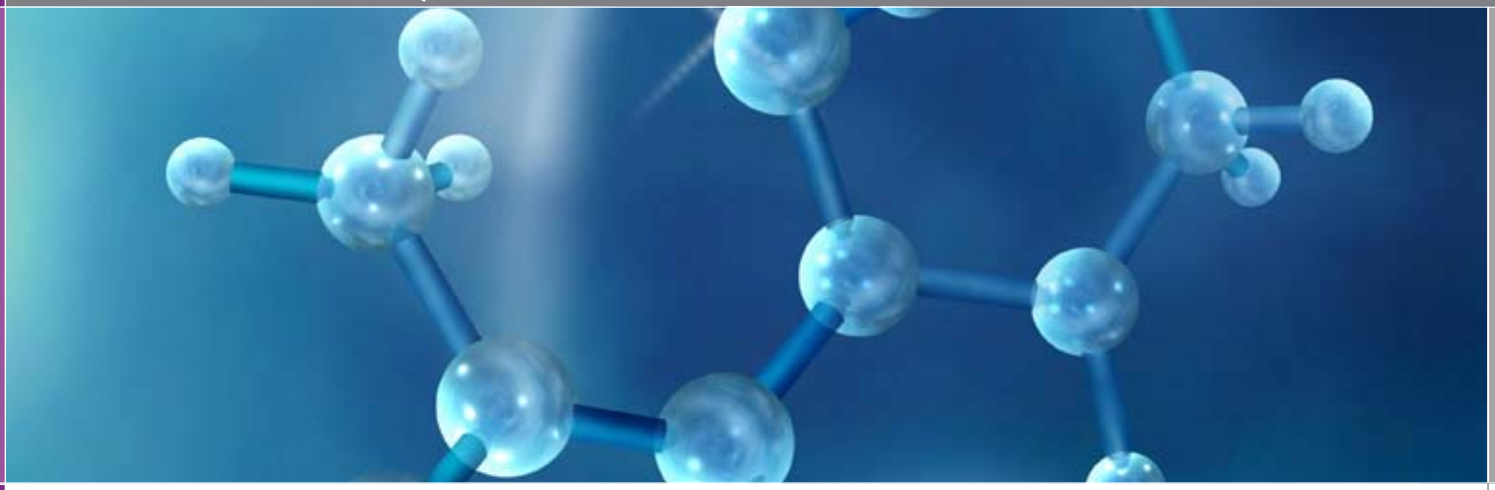
SOLUTION BRIEF

SGI® SOLUTIONS FOR QUANTUM MECHANICS



SGI® Solutions for Quantum Mechanics

Maximizing Performance and Flexibility for Demanding Computational Chemistry Problems

Solution Highlights

- Industry leading performance for high-throughput, high-performance and mixed use environments
- Flexible configurations to meet any budgetary requirement
- Superior TCO with optimized configurations, reduced system management and breakthrough energy efficiency

If you are using quantum mechanics, then you are solving the hardest computational chemistry problems with the highest level of accuracy. Whether you are using Gaussian, Jaguar, VASP, GAMESS or other quantum mechanics applications to study the surface properties of new materials or to understand bond angles in drug candidates, you need large amounts of computational power in cost effective solutions. SGI is the industry leader in developing and optimizing solutions for quantum mechanics, with configurations to match every workload and budget.

SGI Domain Expertise

Since the introduction of SGI® Power Challenge® systems in 1994, SGI solutions have been used to solve the most demanding quantum mechanics problems. During this period of time, SGI has worked with both commercial and open-source application developers to optimize per CPU performance and system scalability, enabling the solution of ever larger problems with higher theory levels.

Successful research at academic, government and industrial sites around the world including NSCCS, SAPAC, Donostia International Physics Center and Virginia Tech has been enhanced by SGI's knowledge of both the computational processes behind the leading quantum mechanics applications

as well as the discovery process at universities, national labs and industrial companies. SGI understands that not all quantum mechanics problems are created equal and that different solution methods, theory levels and problem sizes are required for different research and that each of these stress different aspects of system design. SGI leverages our deep domain expertise to ensure that the solution we propose for each customer is the best one for their current research plan and budget.

Scientific Workflow Solutions

SGI takes an individualized approach to creating solutions for scientific computing by looking at the research goals of an organization, the suite of applications being run to support that research and the budgetary constraints that are present. This approach, called a Scientific Workflow Solution, then combines a mix of different computing and data management platforms to optimally address these goals and constraints in a way that maximizes the ability to generate breakthrough results, supports a diverse organization and minimizes total cost of ownership (TCO).

At the individual or workgroup level this may mean selecting a single platform that runs all simulations well and gives headroom for growth while at the department or enterprise level it may mean integrating multiple platforms that are each configured to optimally run a specific portion of a quantum mechanics, computational chemistry or multi-disciplinary workload.

Individual / Workgroup Solutions

In quantum mechanics, many individual researchers have been using desktop PCs to run small simulations with low theory levels. These users are now ready to step up to running medium size simulations with medium theory levels. SGI® Altix® XE systems are cost effective solutions with up to 8 CPU cores, and are designed to optimize performance for this class of problem. With Intel® Xeon® 5200 and 5400 CPUs, these systems can provide up to 10 times more compute power and 32 times the memory of 2 year old PCs.

High-Throughput Departmental Solutions

Chemists, physicists and engineers often leverage semi-empirical or low-theory level ab-initio quantum mechanics to simulate a large number of small molecules. An SGI Altix XE cluster or SGI Altix ICE system with Intel Xeon processors is ideal for this environment since each model runs well on a single node with 4 to 8 cores and 8 to 32GBytes of memory.

High-Performance Departmental Solutions

Other departments have a need to understand the inner workings of large molecules with extremely high precision. These users typically have large models and use high-theory levels that leverage large numbers of CPUs, large amounts of memory and benefit from a unified I/O architecture. An SGI Altix system with 16 to 128 Intel® Itanium® 2 processor cores and 64GB to 256GB of memory is ideal for this environment since it delivers both the fastest per CPU core application performance and the best multi-core application scalability. Departments moving up from 2-year old Opteron based servers can expect to solve 10x larger problems and see 5x to 10x more application performance.

Minimizing Time To Solution with Hybrid Solutions

Many research groups have a mixture of small and large problems with both low and high theory levels. They also combine quantum mechanics with molecular mechanics simulations to increase the dynamic accuracy for large molecule simulations. When faced with a wide range of applications with varying compute, memory and I/O profiles, hybrid solutions that combine both high-throughput Altix XE clusters or Altix ICE systems with large memory, high-performance SGI Altix systems enable the solution of large, complex problems and provide the best time to solution for the overall workflow.

Minimizing Total Cost of Ownership

Total cost of ownership comes from purchase costs, direct operational expenses and personnel costs for system management, and SGI solutions for quantum mechanics are designed to enable organizations to live within the reality of their budget constraints. SGI minimizes up-front costs by building SGI Altix, SGI Altix ICE and SGI Altix XE systems from cost-effective, industry standard parts and then using our experience in building highly scalable systems to minimize potentially costly upgrades of computer room infrastructure. This results in systems that cost up to 50% less than similar systems from other vendors, take up less floor space, and place less of a load on the electrical and cooling infrastructure of the building. SGI's pioneering use of high-efficiency, single-stage power supplies and optional water cooled doors in highly scalable systems deliver leadership energy efficiency that can be as much as 40% below that of a similar number of cores in 1U servers. SGI also reduces operational expenses with shared memory systems that scale to up to 1,024 CPU cores and integrated cluster solutions that use SGI® Tempo software or ScaliManage® to greatly reduce system management burdens.

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