Boosting Shared Memory Supercomputing

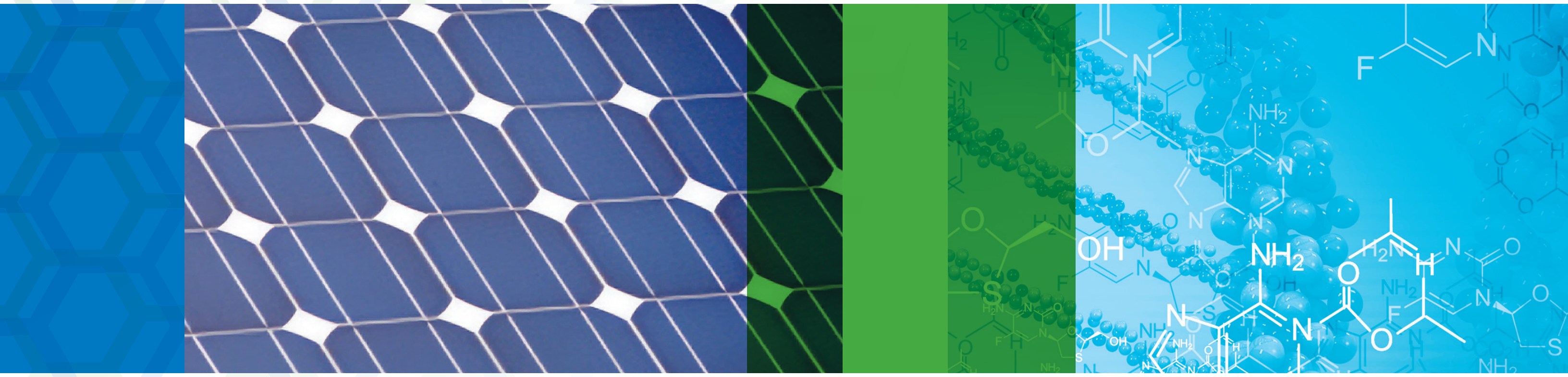
NCSA Doubles Performance and Nearly Triples Memory Capacity with SGI UV 1000

Key Facts

Organization:
National Center for Supercomputing Applications

Location:
Urbana, IL

Industry:
Higher Education & Research



As one of the premier high-performance computing (HPC) research institutions in the U.S., the National Center for Supercomputing Applications (NCSA) provides HPC resources for a wide range of scientific applications, including many where performance needs require highly parallel shared memory architecture. NCSA recently replaced its previous shared memory system, an SGI Altix® 4700 supercomputer, with an SGI Altix UV 1000 system based on the Intel® Xeon® E7 processor family, with 256 cores and 8TB of memory. NCSA representatives say that the new system, called Ember, is more powerful in many ways than the previous system.

Ember supports applications that require large-scale shared memory architecture, especially in the fields of chemistry and solid and fluid mechanics. In computational chemistry, for example, large shared memory nodes that can reliably handle long-running *ab initio* calculations enable material property predictions to occur more efficiently than in comparable distributed memory systems.

Ember Solves the Challenge of Rising Demand on an Aging System

At nearly six years old, NCSA's Intel® Itanium® processor-based Altix 4700 supercomputer could not keep up with the increasing demands of its users. NCSA needed an easily deployable, supportable and fast system that could be accessed by a multitude of users doing a wide variety of work. "Our allocation requests for shared memory systems consistently exceeded the available resources, by as much as seven times in one review of requests," states John Towns, NCSA's Director of Persistent Infrastructure, whose team supports the system.

Shared memory server systems are able to maximize data-intensive performance. The open x86 architecture of UV leverages the power of standard Intel® Xeon® processors and off-the-shelf Linux® or Windows® software, enabling customers to solve complex challenges more rapidly and effectively than ever before.

NCSA configured the system to provide maximum memory bandwidth per core for parallel shared memory computing with large datasets, and chose the Linux operating system, along with the SGI ProPack for Linux enhancement, for Ember. SGI ProPack for Linux focuses on features that accelerate applications, enable development of parallel and real-time applications, and manage system resources for large scalable servers, clusters and storage from SGI.

The SGI UV provides more economy, more speed and greater capacity, with 13.5 GB per second of I/O bandwidth, helping scientists accelerate progress on a variety of complex and important problems. Towns states, "Our expectation was that we'd see a baseline of maybe a 20 to 50 or 70 percent increase in application performance over the previous system. What we found is that many applications are seeing a factor of 200 percent increase in performance, and sometimes more!"

The UV also provides cost and energy savings, consuming half as much power as the previous platform while delivering double the performance. This ratio equates to four times more performance per watt. The system also has just four racks of compute nodes, making it four times denser than its predecessor, freeing up valuable space in the data center.

A High Performance Resource for Memory-Intensive Applications

Parallel shared memory servers are crucial resources for HPC applications in areas such as computational chemistry, fluid dynamics and solid mechanics – and the demand for those resources is growing. Few organizations understand that demand better than NCSA, a national leader in providing an advanced infrastructure for open scientific discovery. Towns says that Ember is an essential tool for shared memory applications, particularly those where memory bandwidth can be a major constraint on performance.

"When we purchased this system, we made several choices that were important to support parallel shared applications in a shared memory environment more effectively," Towns explains. "The specific processor, configuration, DIMM size, core count and other factors are all aimed at maximizing memory bandwidth. Ember also provides researchers with approximately 5.33GB of memory per core," he says.

The SGI UV 1000 lets researchers take full advantage of the SGI NUMAlink® 5 interconnect, optimizing shared memory performance between 384 processor cores on the Ember system. This gives researchers access to a 2TB pool of shared memory. To handle this massive storage requirement, the system connects to two SGI InfiniteStorage™ 15000 controllers with 700TB of capacity

Organic Chemistry Experiments Conducted

Don Aue, Ph.D., at University of California Santa Barbara (UCSB), conducts research in organic chemistry on the system. "We calculate the energies and properties of organic and organometallic molecules for comparison with experimental results," states Aue. "These results are used on a variety of projects."

Aue explains some of the experiments he conducted on Ember. "We did calculations of carbocation stabilities for comparison with our gas-phase experimental stabilities; calculations on mechanisms of catalytic organogold reactions for organic synthesis and drug synthesis, where we have found additional examples of unusual bifurcation mechanisms; and calculations on mechanisms of organocopper reactions of great importance in synthetic chemistry, "green" chemistry and drug synthesis (in collaboration with Prof. Bruce Lipshutz, UCSB). These and other projects we've conducted work really well on a shared memory system."

Aue continues, "We have used other supercomputer systems over many years, as well as locally available workstations for smaller calculations. We continue to use local workstations, but the SGI supercomputer allowed us to use new quantum mechanical methods like G4 and CCSD(T)-F12 codes, within the Gaussian and Molpro software packages for molecules of small and moderate size. This has provided us with the capability of calculating highly accurate energies for these molecules, comparable to experimental accuracy."

Students Research Solar Cells on Ember[1]

Solar energy has the potential to be the perfect renewable energy source. Unfortunately, modern solar cells are too inefficient and too expensive to achieve the technology's potential. Researchers are hard at work to change that, however, by searching for alternative materials that could change the solar energy landscape, and they're doing it with high-performance computing. "Organic materials provide several benefits over their inorganic analogs," explains Aimée Tomlinson, a chemistry researcher at North Georgia College & State University. Tomlinson and her colleague, Malika Jeffries-El at Iowa State University, are working with several undergraduate chemistry students to study organic materials that could function as solar cells.

According to Tomlinson, producing organic materials for solar cells is less detrimental for the environment. These materials also have plastic-like properties, such that they can be molded into a variety of shapes. That plasticity also means they are less breakable. "On the flip side, they are less efficient than the inorganic variety, which is why a great many scientists all over the world are working on identifying materials which will give rise a more efficient organic solar cell," Tomlinson explains.

Tomlinson and her students used Ember and other computing resources to study possible chemical structures for use in organic, hydrocarbon-based solar cells. "Quantum mechanical computations that could take as long as a week to solve on a typical computer can be solved in as little as an hour on a supercomputer," says Tomlinson. Because of the researchers' access to advanced computing, they were able to identify a few compounds that show particular promise for use in solar cells.

About NCSA

The National Center for Supercomputing Applications was established in 1986 as one of the original sites for the National Science Foundation's Supercomputer Centers Program. Located at the University of Illinois at Urbana-Champaign, NCSA is supported by the state of Illinois, the University of Illinois, the National Science Foundation and grants from other federal agencies. NCSA is a leader in deploying robust high-performance computing resources and in working with research communities to develop new computing and software technologies. For more information about NCSA, please visit www.ncsa.illinois.edu.

[1]http://www.hpcwire.com/hpcwire/2011-09-08/ember_sheds_light_on_solar_cell_research.html

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