Success Story

Wichita State University's HPC Center

Combining Capacity and Capability with an SGI® Altix® Hybrid Cluster for Linux®

"We could easily have bought the clusters separately. But we found value in using SGI Technology Solutions to build us a hybrid system."

—John Matrow
HPC Center Director

The names of Boeing, Beech (now Raytheon), Cessna, and Learjet are synonymous in many minds with Wichita, Kansas – a hotbed of aeronautical design and innovation. The National Institute for Aviation Research (NIAR), supported by public and industry funding, has long played a major role on the Wichita State University campus. By the late 1990s, the wide-ranging needs of NIAR and WSU researchers moved faculty members to raise the level of research on campus by setting up an HPC center with federal and state funding assistance. A 16-processor Origin® 2000® compute server was installed as the centerpiece of the new High Performance Computing Center (HiPeCC) in April 1999 and later upgraded to 24 processors.

The number of users, the demand for compute cycles, and the size of simulation models continued to grow relentlessly. In 2003, HiPeCC decided to make the leap to open-source computing. It wanted its next-generation Linux® os-based solution to offer its users a choice of resources: the capability of the most powerful shared-memory HPC technology available and the capacity of massively parallel clusters. HiPeCC met with potential vendors and ultimately focused on SGI. "We asked SGI the question: Will you give us both these things in one package? And they stepped up to the plate," says HiPeCC Director John Matrow. "We could easily have bought the clusters separately. But we found value in using SGI Technology Solutions to build us a hybrid system."

SGI® Technology Solutions: Installing A Cross-Platform Powerhouse

The SGI Altix Hybrid Cluster solution, installed by SGI Technology Solutions in July 2003, is two platforms in one – an SGI® Altix® 3700 compute server with 32 64-bit Intel® Itanium® 2 processors, and two 32-bit Atipa Technologies clusters, each with 17 dual-processor Intel® Xeon™ nodes. SGI worked closely with Wild Open Source, Inc. to implement the cluster solution. A terabyte of storage on an SGI® TP9100 RAID is accessible to all nodes via NFS filesystem. HiPeCC's 130-plus users, who include faculty members, research associates, graduate students, and postdoctoral fellows, submit jobs to the hybrid system through the Origin 2000 server using a simple, flexible interface.

Success Story

The Altix Hybrid Cluster solution fills a dual need faced by many research organizations today: 32-bit cluster technology can provide lower-cost capacity for distributed processing applications, but users running large, resource-intensive jobs (often with more sophisticated applications) can be far more productive in the record-breaking 64-bit shared-memory environment of the SGI® Altix® 3000 series. Together they vastly increase HiPeCC's compute horsepower.

"When the 24-processor Origin 2000 system was our primary resource, it was considered fast," says Matrow. "The new system is seven times faster. The Origin system was rated at about 11GFLOPs. I haven't benchmarked the Altix Hybrid cluster, but it's unofficially rated at 300GFLOPs."

Suiting the Platform to the Job

WSU faculty members are using the SGI system for a great variety of studies, including the potential of ultra-high speed quantum computing, the molecular structure of ionized liquids, and the influence of magnetic force on flow fields. The system runs five primary applications - Gaussian®, LS-DYNA™, Abaqus®, Cobalt, and Fluent® – for researchers working in computational aa chemistry, computational fluid dynamics, finite element analysis, , and other specialties. All but Cobalt (limited to the 32-bit platform) are currently running on both the 64-bit Altix® platform and the 32-bit clusters, but at varying performance levels. "Some of these applications work well on the Xeon clusters, and others want the shared-memory platform of the Altix system," says Matrow. "That's primarily why we went with a hybrid system."

Users are able to see which resources are in use before they submit jobs and make decisions accordingly. Because most applications can run on either side of the system, they can choose the most efficient way to run a job. For example: a user has a job that would occupy four Itanium 2 processors on the Altix platform, but all are in use and there is a queue. On the other hand, nodes are available on one of the 32-bit clusters. The job can be converted to eight-processor format and submitted on the cluster side.

The WSU Chemistry Department is a major user of the SGI system, with a primary research focus on light-sensitive molecules. Over the last four years, the Department has published six papers a year on related subjects. Assistant Professor Dr. Yuri Illitchev works with nitrobenzyl compounds, which serve to protect biologically active molecules but can be removed by the application of light, and with melanins, which supply the pigmentation in human skin and are also light-sensitive. Illitchev runs Gaussian models in his study of these molecules, primarily using the 32-bit clusters but switching to the Altix platform if he has a particularly complex job or needs results quickly.

"This system is much faster than our old system," says Illitchev. "I can now generate more data in a month than I did all last year. Now my major problem is that I don't have enough time to analyze data and create new jobs."

Professor Mel Zandler runs molecular models in Gaussian to determine the properties of light-collecting molecules. His results are used by the Analytical and Supramolecular Chemistry group under Professor Francis D'Souza to link Carbon C60 molecules (Bucky balls) to porphyrins to emulate and modify the photosynthesis process found in green plants. Professor Zandler uses 20 desktop computers to make Gaussian runs that can last up to six months.

"When I'm in a hurry, I submit the job to the SGI Altix system and they'll give me four or

eight processors," says Zandler. "They're about twice as fast as the fastest desktop processors I'm using, so instead of getting one iteration a day, I might get one an hour, and the whole job usually takes hours instead of weeks. Gaussian just works very well on that computer. The Chemistry Department has been dominating the available time over there recently." Other groups within the department are also working with light-sensitive molecules and using a large share of available time on the Altix and the 32-bit clusters.

What does the future hold for HiPeCC? Matrow is keeping an eye on demand and utilization to see when the Altix 3700 system, which has virtually unlimited scalability, will need an upgrade. In the meantime, he is actively promoting grid computing and the use of Internet2 to share research computing resources with other universities. He cites as an example the current $6 million upgrade to the university's famous Olive N. Beech Wind Tunnel, which will provide data and video streaming of tests to remote sites.

Clearly, major scientific questions in chemistry, aeronautics and othe disciplines will keep the HPC Center's SGI Altix Hybrid Cluster productive in the years to come.

sgi

Corporate Office
1500 Crittenden Lane
Mountain View, CA 94043
(650) 960-1980
www.sgi.com

North America 1 (800) 800.7441
Latin America (52)5267.1300
Europe (44)118.925.75.00
Japan (81)3.5488.1811
Asia Pacific (67)6771.0290

3681 [11.2004]

J14644