Application Brief

State University of New York at Buffalo Teams up with SGI for Next-Level Supercomputing Site

New Facility Brings Exciting Science and Competitive Edge to University

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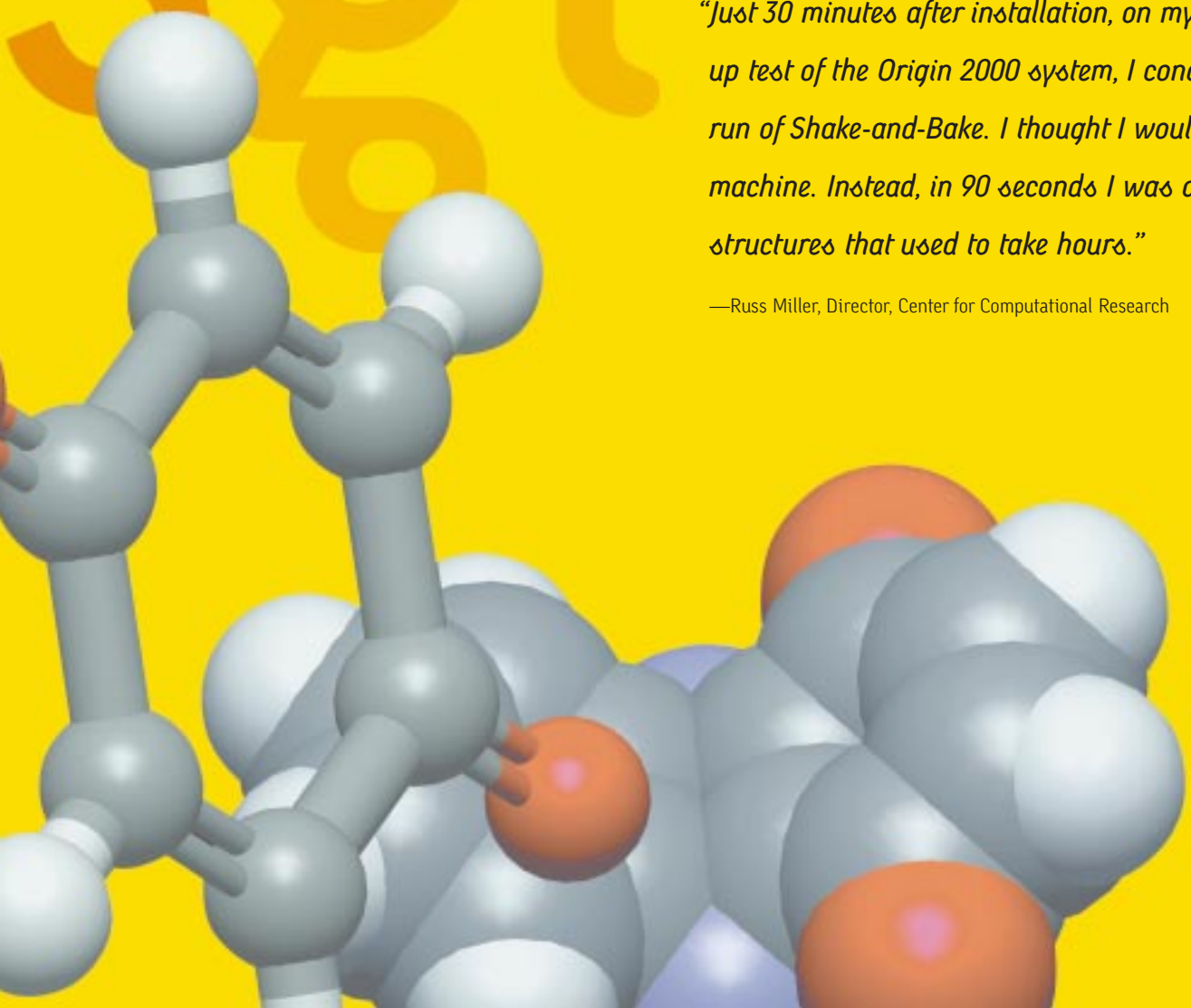

"The center puts UB on the map. It takes us from being a major research university completely lacking in high-performance computing to the ranks of the nation's top 10 academic supercomputing sites."

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Need:
A heavy-duty interactive computing and visualization environment for conducting advanced computational science and attracting world-class research opportunities.

Solution:
A 64-processor Origin 2000 system, as part of the new $7 million Center for Computational Research founded with grants and assistance from government and the private sector, including SGI.

Benefits:
In addition to powering today's most complex computational-based research, the center has become a magnet for recruiting top-notch faculty and students. Plus, it is creating opportunities for partnerships within western New York, thereby attracting additional public and private funding.

In January 1998, Dr. Russ Miller of the State University of New York at Buffalo (UB) was charged with leading a large, multidisciplinary task force to evaluate the campus' research infrastructure. After four months of thorough investigation, the verdict was in: while UB had a solid track record and well-established reputation for conducting high-quality science, the university lacked the computing infrastructure to elevate its research to the next level. And because of that, not only was the university's ability to tackle compute-intensive research severely limited, but its capacity to attract top-quality faculty and students as well as external funding was restricted, too. To make that leap, Miller's group advised, would require the high-end parallel computing firepower and interactive visualization that are driving leading-edge computational research sites worldwide. With a tenacious motivation to put UB in those elite ranks, Miller and his group began the arduous process of formulating proposals and grant applications that would make their vision a reality. A year later, with the support of the provost and in a unique partnership of public- and private-sector organizations, including the National Science Foundation, SUNY, SGI, and other technology companies, UB's $7 million Center for Computational Research (CCR) was born. Now, along with a reputation for quality research, the university has a world-class facility to help its research faculty solve some of the world's toughest problems.

From left to right:
Dr. Russ Miller, Director, Center for Computational Research
Corky Brunskill, Director of UB's Science and Engineering Node Services
Dr. Thomas Furlani, Associate Director, Center for Computational Research

Exciting Science

From the moment the initial installations were complete, a tremendous amount of what Miller and Associate Director Dr. Thomas Furlani call "exciting science" was enabled. Anchored by a 64-processor SGI™ Origin™ 2000 supercomputer and several high-end visual workstations, the center boasts the aggregate power to carry out 60 billion operations per second (60 Gflops)—the kind of computing muscle requisite to computational science and high-performance computing applications. "Work in computational science is leading to advances in a surprising variety of fields—structural biology, drug design, materials science, high-energy physics, industrial design, and global climate change, to name just a few," observes Miller. "It is radically changing the way scientists perform their research." At its most effective, computational science is benefited by a computer interface that encourages interaction between people and data. "As a visual company, SGI is a natural player in this arena," says Furlani. "It makes doing this kind of science much more interactive."

A Campus-Wide Resource

The university's new center is not affiliated with any single department, but is open to requests from all university researchers. "Our goal is to reach out to all who can benefit from high-end computing and visualization," notes Miller. Accordingly, CCR resources are available across campus, and, indeed, across western New York. After the center is fully established, Miller envisions a broad range of university departments—as well as off-campus commercial partners—taking advantage of its substantial time-saving and insight-provoking potential. In addition to research science, a number of applications in medicine, biophysics, mechanical engineering, geology and earthquake studies, and even music and the arts are planned. For the moment, six research groups are using the facility, with another eight waiting in the wings. "Lack of interest has not been a problem," jokes Miller.

Among the center's inaugural projects is a study to determine the molecular structure of proteins and antibiotics in order to provide a basis for designing more effective drugs. Propelled by "Shake-and-Bake," an innovative crystallography algorithm jointly

developed by Miller and New York's Hauptman-Woodward Medical Research Institute, this project is able to look at and solve larger molecular structures than was previously possible. And because of the bottleneck-busting architecture of SGI™ Origin™ that optimizes parallel processing performance, it is doing it in much less time than ever before. "Just 30 minutes after installation, on my first power-up test of the Origin 2000 system, I conducted a trial run of Shake-and-Bake," says Miller. "I thought I would crash the machine. Instead, in 90 seconds I was able to analyze structures that used to take hours."

Bridge to the Community

Key to the ongoing success of the center will be its ability to forge partnerships with business and industry. In its first few months, the CCR is already a big draw for cooperative ventures in the competitive arena of sponsored research. Major industrial and research organizations voicing interest in utilizing the facility include Eastman Kodak, Occidental Chemical, Calspan, Innovative Business Communications, and the Roswell Park Cancer Institute. "The sophisticated visualization we are developing with SGI is an absolute requirement for effectively evaluating the huge quantities of data produced in today's research," says Miller. Although companies recognize that advanced visualization makes it much easier to quickly identify innovative solutions, they are not always able to justify the investment. "In partnership with the CCR, it is now feasible for local companies and research institutions to take advantage of the facilities on a collaborative basis," he adds. A bit down the road, Miller sees the center as the focal point for technology transfer and scientific discovery within western New York—not to mention an important source of funding for the university.

Speedy Setup, Speedy Results

The enormous data analysis capacity of the UB center will speed discovery in areas as diverse as designing new catalysts for environmental and energy innovations and synthesizing chemicals for pharmaceuticals. The engine central to this massive compute capability is an SGI Origin 2000 supercomputer with 64 250 MHz MIPS® R10000® processors, 16GB of memory, and 120GB of Fibre Channel disk storage. Because of its cache-coherent nonuniform memory architecture (ccNUMA), which combines the best features of shared memory systems with those of scalable, distributed systems, Origin 2000 eliminates the memory bus bottlenecks of other multiprocessor systems. But unlike distributed systems from other companies, each processor in the Origin 2000 system has direct

64-Processor SGI Origin 2000

A Full Plate of Research

The Origin 2000 supercomputer at the heart of UB's new Center for Computational Research enables researchers to tackle important, computationally intensive problems in areas ranging from molecular structure determination to computational fluid dynamics. From the day its doors were first opened, the CCR has had its plate full with several important projects.

Cellular Biology

Using programs developed at UB, researchers are studying ion channels—the small pores in cell membranes that open and close when stimulated. By discovering the mechanism by which these "transistors" function to control the flow of electric current in cells, researchers will better understand movement, our senses, and perhaps the physiological basis of thought. Medical applications may include the development of drugs to prevent heart attacks and treatments that slow the deterioration of nerve cells from multiple sclerosis.

Computational Chemistry

Tapping the efficient parallel processing power of Origin, researchers are applying novel computational techniques to understand the complex chemistry of the upper atmosphere. Consequently, a better understanding of this chemistry will lead to more reliable predictions of global climate changes.

Industrial Design Optimization

The university's industrial design group is focusing on the development of a series of computational tools aimed at helping industry improve the process of model design and optimization. Using virtual models, this research will enable engineers to test automobile designs against several safety parameters simultaneously. These studies will reduce testing time and the cost of prototyping, and their findings may prove instrumental to improving automobile safety and promoting fuel efficiency through aerodynamics.

Molecular Structure

SnB, from UB and Hauptman-Woodward Medical Research Institute, is a computer program based on Shake-and-Bake, a direct-methods procedure for determining crystal structures. The program is being used to solve difficult structures that could not be solved by traditional reciprocal-space routines based on the tangent formula.

access to the entire machine memory via a high-speed CrayLink™ interconnect. This architecture makes Origin 2000 a powerful and scalable solution for the speedy analysis of the vast sums of data produced by computational scientists. To the delight of the technical unit supporting the new facility, the SGI system is also fast in other ways. "The Origin 2000 system fit right in, without any special disk allocations or hassles migrating password files," comments Corky Brunskill, director of UB's Science and Engineering Node Services. "It's extremely user-friendly, and because of its built-in administration tools, we were up and running in less than an hour." Brunskill adds that he was very surprised at being able to configure the system, install the user accounts, and bring it online using only one administrator, and a newly designated one at that. And now that it's running, the same solo systems administrator cares for the entire system. "I only wish other platforms were this easy," says Brunskill.

Dr. Russ Miller works at one of the several high-end visual workstations, anchored by a 64-processor SGI Origin 2000 supercomputer.

What's Ahead?

"It's like eating peanuts—you can't stop," says Brunskill about what's in store for the Center for Computational Research. "Once the university and the community catch on to its tremendous potential, things will really take off." That potential is fostered by UB's wide-open perspective. From Director Miller on down, everyone involved is approaching the enterprise without any constraining preconceptions. "We see an unlimited future with the potential for satisfying the ever-increasing demand for high-performance computing and high-end visualization," says Miller. To that end, he plans to build on the center's relationship with SGI to keep current with technical advances, adding industry-leading Silicon Graphics® Onyx® visualization and future product upgrades. Further, his vision portends a gathering spot where visualization and interaction will drive synergy and build community. "Traditionally, research science is an isolated affair," he notes. "We see the center as a space for bringing teachers, students, researchers, and partners together to share information and work faster and smarter. The center will not just be a processing factory. There will be many breakthroughs here with lots of exciting science to come." Word about that vision is already out: after just a few months, UB's new computational research facility has become a magnet, drawing inquiries from industrial partners and visits from potential students and a high-quality faculty from far and wide.

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