



Computing expansion

UB center to spend \$9 million on upgrades to serve growing clientele of researchers in medical, variety of other wide-ranging fields

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The University at Buffalo's downtown supercomputer center is an impressive electronic powerhouse.

The center, which has won \$11.45 million in grants in the past year, helps university professors and other researchers run myriad projects. But with supercomputer centers around the world chasing funding and talent, there is no room for complacency.

“It’s tough to stay on the leading edge, and you have to keep working at it,” said Thomas Furlani, director of the Center for Computational Research, its official name.

The center will install \$9 million in new equipment this year, improvements that will ramp up capabilities while aiming to reduce energy consumption.

The upgrades will bolster computing capacity — to 6,000 from 2,000 processors—and expand electronic memory by a factor of more than 20.

The center handles about 1,000 projects per day, running them automatically from a queue when the required number of processors opens up. It typically runs at about 90 percent capacity.

Furlani offers this measure of its capability: If you let your personal computer run for one day, that counts as a one central processing unit day, or CPU-day. Last year, the center delivered 720,000 CPU-days.

The center employs a staff of 13, but Furlani described jobs as only one measure of its impact. Its computing horsepower helps researchers win grants and carry out their work, not to mention acting as a UB recruiting tool for faculty and graduate students.

The center sits on the first floor of the New York State Center of Excellence in Bioinformatics and Life Sciences, on the Buffalo Niagara Medical Campus. Its location is more than symbolic. Economic development officials see the campus — also home to Roswell Park Cancer Institute, Hauptman-Woodward Medical Research Institute and Kaleida Health, among others — as a source of growth, amid job losses in such traditional high-wage sectors as manufacturing.

The center was established in 1999 on the UB North Campus and moved downtown four years ago, making its resources more accessible to a wider range of users. The center helps scientists on the medical campus improve their chances of securing federal funding, Furlani said.

According to UB, more than \$30 million in funding was awarded last year to UB faculty using the center’s resources.

Furlani said a shift in the world of science has bolstered the center’s value. Computers have become increasingly important for all kinds of research, beyond just the natural sciences, and the center allows the massive data generated by scientific machines to be analyzed, he said.

Fifteen or 20 years ago, Furlani said, only a handful of researchers would have needed access to this type of resource. Nowadays, researchers in all types of fields use it.

“It provides the university faculty with tools, with a resource that they couldn’t afford to support on their own, to enable them to be able to carry out advanced studies,” he said. “And that means increased grant dollars, which means increased employees, it means training new students, it means hiring postdoctoral researchers, it means support staff. So it’s all tied together.”

The center serves a variety of areas, including chemistry, engineering and health care.

It, for instance, can support the design of pharmaceuticals, helping researchers narrow down potential candidates for drug molecules. That prevents researchers from having to go into a laboratory and synthesize them first, only to discover that the molecules are the wrong shape or size to inhibit a particular protein, Furlani said.

The center also can be used to improve automobile or airplane aerodynamics, to improve fuel efficiency, without having to build costly and time-consuming prototypes for wind tunnel testing, he said.

Buffalo BioBlower Technologies is one of the businesses that has tapped into the center. The company, which created a device to sterilize high-volume airstreams, is using the center to research air flows in environments such as hospital rooms, said John Lordi, chief executive officer and co-inventor.

Using the computer center has proven a faster and cheaper alternative to conducting experiments, Lordi said. "Experiments tend to be far more expensive than computations."

Kinex Pharmaceuticals, located in the bioinformatics building, might use the center's services for the chemistry portion of a project now getting under way with Hauptman-Woodward. "It's a significant resource," said Allen Barnett, Kinex's CEO. "It's good to have them there."

Kinex moved into the bioinformatics building four years ago and has formed ties with UB, Roswell Park, Hauptman-Woodward and AHRM Inc., which monitors its clinical studies. Those associations have opened Kinex up to new ideas and helped move its research along more efficiently, Barnett said.

Among the fastest

UB's computer system has previously been ranked by Top500.org, which lists the world's fastest machines, but it has not appeared on it since fall 2007. Five editions of the list have come out since then.

UB's supercomputer center is expected to rejoin the top 500 after its upgrades. But Furlani said speed is only one measure of what a such a center can do.

A chemist working on a breakthrough project, for instance, might need access to a large database but a relatively small number of processors, not necessarily one of the fastest systems, he said. Furlani sees greater value in providing a combination of staff expertise, high-performance storage and advanced computer technology, qualities he says the UB center has.

Furlani said continuing to upgrade the center is important since other supercomputer centers are also striving to improve. The center is part of the Coalition for Academic Scientific Computation, which Furlani said has grown to more than 60 members from 25 about five years ago.

"Everyone else is applying for these grants, and they're all good, too," he said.

Keeping the UB center competitive for grants, he said, depends on a mix of staff—which he says is relatively large for a university center — faculty and technology.

“Once you show that you’re capable of doing good, important research, you apply for grants for larger equipment,” Furlani said.

The \$11.45 million in grants the center was awarded includes \$7.75 million over five years from the National Science Foundation. The center also won a \$2.5 million grant from the National Institutes of Health and a \$1.2 million grant from the New York State Energy Research and Development Authority.

“Our mission over the next few years will be to see if we can’t continue to enhance and grow our reputation and at the same time, facilitating research,” Furlani said.

The National Science Foundation grant relates to the Tera- Grid, which supports more than 4,000 users at more than 200 universities, enabling scientists to carry out advanced research in a host of fields.

The grant will allow the center to develop software tools to make sure the grid continues to run as efficiently as possible.

‘Solid proposal’

Barry I. Schneider, program director at the National Science Foundation, credited the center with having a “solid proposal and a good team.”

“Basically, the Buffalo proposal provided an excellent vehicle for an independent auditing service for TeraGrid,” Schneider said.

In the past year, the center has added six staff members to its core 13 staffers, largely because of the new grants it has secured.

The growth of the medical campus, with the supercomputer center as a component, is encouraging to Furlani. He grew up on nearby Goodrich Street, where the Clinical Translation and Research Center is now under construction.

“I think this has a chance to be very successful, and I think it has been so far,” he said. “And the future I think is very bright. As a Buffalo native, it’s exciting because you believe in the city and you want it to succeed.”

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