Center of Synergy

Computational Research Center a boon for biomedical studies

This past fall, the entire infrastructure for UB's Center for Computational Research (CCR), including a 2,000-processor supercomputer, was moved from the university's North Campus into UB's New York State Center of Excellence in Bioinformatics and Life Sciences on the Buffalo Niagara Medical Campus in downtown Buffalo. The center has also quadrupled its computing power, upgraded its high-performance storage system and installed a new state-of-the-art visualization room.

While CCR staff and users enjoy the increase in power, as well as the center's new home, Thomas R. Furlani, PhD, CCR's director, says the real dividend from the move, has come from new synergies it is generating with researchers in the Center of Excellence and its partners, Roswell Park Cancer Institute (RPCI) and the Hauptman-Woodward Medical Research Institute.

By Ellen Goldbaum

"THE CCR STAFF has dramatically increased its interactions with medical researchers since the move, and this has been highly beneficial to Buffalo's life-sciences projects," notes Bruce A. Holm, PhD, senior vice provost and executive director of the Center of Excellence. "Dr. Furlani has done an outstanding job of educating our researchers about the possibilities open to them via CCR resources, and we are now seeing an increase in NIH grant applications that include CCR staff and services as part of their budgets."

At the same time, CCR is ensuring that the needs of its existing users remain a priority and is staffing two full-time satellite offices on the North Campus in Amherst.

Since the move downtown, and partly as a result of energetic outreach efforts by CCR staff, existing partnerships with local medical institutions have intensified and become more productive, especially with the increase in computing power. As a result, CCR recently added a dozen or so new users, primarily in the life sciences.

Ironically, in a field that is driven by virtual connections, sheer physical proximity to one's collaborators has turned out to be a valuable asset for researchers in specific disciplines. Daniel Gaile, PhD, UB assistant professor of biostatistics whose office in the Center of Excellence is steps away from CCR, has noticed the change.

"I think we're really on an upswing now; there's some energy that has come just from CCR being located down here," he says. "There's been a definite increase in the number of life-sciences collaborations involving the CCR."

Gaile and Furlani agree that a key factor driving collaboration is CCR's proximity to faculty members in the Department of Biostatistics who have offices in the Center of Excellence and proximity to the adjacent Roswell Park Center for Genetics and Pharmacology, where RPCI's microarray facilities soon will be housed.

"This provides for one-stop shopping for researchers interested in conducting experiments and studies that require collaborations with all three groups," says Gaile. "They will not have to worry about coordinating their efforts across three disconnected groups; we are now very connected."

These connections are critical because the large amounts of data generated by microarray researchers in the fields of genomics and proteomics—jointly referred to as "omics"—must be analyzed and managed by biostatisticians, operations that are greatly enhanced by access to CCR's hardware and expertise.

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Daniel Gaile, PhD, right, assistant professor of biostatistics, has an office that is steps away from the Computational Research Center.

PHOTO BY DOUG LEVERE

manner requires both high-performance computing and high-throughput storage," says Furlani.

"Fortunately, the increase in computing power and storage at CCR over the past year has allowed us to provide better service to the Center of Excellence and UB researchers."

But fast machines and large storage arrays are only part of the story, Furlani points out.

CCR staff members also provide a broad range of support for users, including software engineering, graphical-user interface development, advanced-database engineering, scientific programming and modeling, algorithm optimization, bioinformatics expertise, scientific and medical visualization, and advanced computing administration.

"We provide faculty with the hardware, software and human resources necessary to help enable their research, including custom software development," Furlani says.

Marc Halfon, PhD, UB assistant professor of biochemistry and biological sciences and a researcher in the Center of Excellence, provides a case in point.

Using the fruit fly as a model system, Halfon studies the gene regulatory elements in DNA sequences, the mechanisms that govern when genes are turned on and off. Information on what regulates genes is critical to understanding diseases, including birth defects and evolutionary processes.

But little information had been gathered on regulatory elements, and what was known pertained only to single elements.

"We wanted to know, 'Are there general principles involved in regulatory elements en masse that could be discerned from what we do know, rather than having to study them one at a time?'" says Halfon.

That question was the impetus behind REDfly, a database of *Drosophila* gene regulatory elements that Halfon established with initial funding from the National Institutes of Health and about which he recently published a paper on in *Bioinformatics*.

Before establishing the database, fewer than 60 regulatory elements had been annotated, or described in detail as to their function. Halfon and his colleagues now have collected well over 600 and the database is not finished.

"Our resource is important not just for collecting the information, but it allows us to start doing computational studies on regulatory elements as a class and that was impossible before," he says.

Halfon notes that while his research did not require supercomputers, it did require expertise in databases, so he contacted CCR to see if staff could recommend a graduate student who could assist him.

"Instead, they said 'We can do that for you; let's set up a meeting,'" he recalls. "They ended up doing the entire computational end of it."

Halfon explains that Steve Gallo helped design a database schema, developed a Web-based interface and handled the back-end programming. CCR maintains REDfly on its computers (see http://redfly.ccr.buffalo.edu).

The level of service that CCR provides, Halfon says, would not have been possible if he had had to hire a part-time computer technician.

"THIS WAS NOT a hardware issue at all, but rather a service issue," he says. "I think there is some uniqueness to CCR, as supercomputing centers go, because they don't just provide access; they provide expertise."

Ping Liang, assistant professor of oncology in the Department of Cancer Genetics at RPCI, had a similarly positive experience with CCR when he received an urgent request from a collaborator at another institution.

Liang is working on a project that aims to identify the critical genetic factors responsible for the biological differences—including susceptibility to diseases—between humans and primates. The goal is to help prevent and treat human diseases, including AIDS and cancer.

Liang needed to conduct comparative genomics studies of more than 3 billion nucleotide sequences base by base—a job that could only be done by high-performance computers.

Even with the short time frame, CCR readily accepted the job. CCR staff member Cynthia Cornelius worked nights and weekends, providing Liang with access to U2, a high-performance computer cluster with 800 nodes.

"Not including set up and testing, it took U2 only one night to complete the job," says Liang. "It would have taken my small computer cluster months."

The individual attention that comes from CCR computational scientists and staff, such as Matt Jones, Zihua Hu, Steve Gallo and Martins Innus, all of whom work one-on-one with faculty members, has been well received.

This spring, CCR staff plans to meet with departments throughout UB and the Center of Excellence to understand better how the center can respond to their needs.

Also planned is a series of workshops describing CCR's capabilities, infrastructure and ways that CCR resources can be used.

Liang, who is director of Roswell Park's newly established Bioinformatics Core Facility, had used CCR when it was housed on the North Campus.

"Having CCR move into the Center of Excellence definitely has improved our interactions with their staff," he says. "Considering the nature of the research we do at Roswell, I envision that we and other biomedical researchers will become major users and beneficiaries of CCR in the near future."

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Mark Halfon, PhD, right, assistant professor of biochemistry and biological sciences, studies gene-regulatory elements in DNA sequences, which are critical to understandng diseases.

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