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High-Performance Computing Set to Advance Research at Rutgers University-Newark

By Lawrence Lerner

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Rutgers University-Newark is about to add a \$700,000 high-performance computing cluster to its arsenal, which will in turn bolster research efforts in an array of disciplines for years to come.

The cluster, which goes by the name NM3 (for Newark Massive Memory Machine), will be a parallel-computing behemoth running the Linux open-source operating system and containing 1,500 processors (CPUs) and massive amounts of shared random-access memory (RAM) - with all of the CPUs performing complex tasks simultaneously and transmitting data among themselves efficiently. It will also contain significant data-storage capacity.

The net effect: Researchers will increase the scale and speed of their work exponentially.

This will mean better science," says Rutgers University-Newark Chemistry Professor Michele Pavanello, the principal investigator on the grant for NM3. "And that could translate into more grant dollars in the future to help us expand the infrastructure."

The Power of the Cluster

The high-performance computing cluster (HPCC) is funded through the November 2012 state bond referendum. As the principal investigator, Pavanello received input from a group of Rutgers University-Newark science faculty on their research and teaching needs, then came up with a suitable computer architecture to fulfill those needs and incorporated it into the grant proposal.

An assistant professor of theoretical chemistry, Pavanello is an ardent proponent of high-performance computing, which lets researchers perform advanced modeling using complex sets of raw data.

So is Professor Bart Krekelberg, of Rutgers University-Newark's Center for Molecular and Behavioral Neuroscience (CMBN). He studies how the brain sees, and says that to map brain activity, modern techniques require whole arrays of electrodes to record hundreds of neurons at the same time, generating an enormous amount of data.

"The more areas of the brain we can record simultaneously, and the more electrodes we use, the better picture we get of how it works," says Krekelberg. "The technology to record brain activity this way is fairly new, and it requires immense computing power to process it, because even sophisticated desktops no longer cut it. They simply take too long to do the job.

In leveraging the power of the HPCC, regardless of the discipline, the process would be the same, says Pavanello.

"Input raw data. Process it. Output it," he says. "With the cluster, it happens very quickly. The processed data output is much smaller than the original raw data. And that is then ported to a desktop, where researchers can analyze it—or visualize it with a graphical-user-interface."

To understand what Pavanello means by "very quickly," consider this: One of Krekelberg's brain-mapping sessions involving hundreds of electrodes generates about 50GB of data, which takes 12 hours to pre-process on his current servers. NM3 will process that same data in about an hour.

"We can go an order of magnitude larger now and record brain activity with 10 times the number of electrodes," Krekelberg says. "And soon, recording techniques will let us use even more."

Pavanello frames this from a chemist's perspective.

"We'll be able to do much faster and scaled-up simulations, which provide insights that you can't get from single experiments," he says. "The strong simulation side expedites the science."

Build It and They Will Come

The new HPCC will be housed in the current Rutgers University-Newark Data Center, a 1,000-square-foot room in Engelhard Hall that is home to the campus's computer infrastructure. There will be enough space in the facility to triple the new cluster's size as more grant funds come in.

Pavanello is heading up a committee that recently reviewed bids from six HPCC vendors. The hardware will arrive in late April, software uploading and testing will take place in May and June, and NM3 is scheduled to come online in fall 2014.

The psychology, chemistry, and earth & environmental science departments are expected to use the system most intensively, though many other departments across the campus may take interest, including biology, criminal justice and urban planning, to name a few.

Rutgers-Newark faculty and graduate students will have priority access to NM3 initially; researchers at other Rutgers campuses will submit proposals to a formal NM3 leadership committee and be slotted in as time permits.

Pavanello's goal is to expand NM3's size and share the cluster openly and democratically among all three Rutgers campuses. "I'd like us to create a true university community around this so that everyone can have access," he says.

Pictured above: Professors Stephen Hanson (CMBN) & Michele Pavanello, both of whom have played a central role in developing the HPCC at RU-N



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