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UB plans to connect research sites into supercomputer grid

"NYSGrid' could accelerate the discovery of new drugs, aid other data-intensive projects

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Bill Wippert/Buffalo News file photo
Russ Miller, executive director of NYSGrid, inspects UB's HP Computer Storage Area Network.

Scientists use supercomputers to study everything from global climate change to the molecules inside a cancer cell.

Too bad the scarcity of the costly machines has limited scientists' access to them.

But that may be about to change.

Putting enormous computing power into the hands of researchers and students across the state is the aim of "NYSGrid," a project headed by the University at Buffalo, organizers of the effort have announced.

The project, which connects research sites into a grid of shared number-crunching power, could accelerate the discovery of new drugs and other data-intensive projects while raising UB's profile in the world of supercomputer achievements, advocates said.

"The goal is to have cyber infrastructure everywhere," said Russ Miller, executive director of NYSGrid and professor of computer science at UB.

"A scientist or a student can sit in front of a screen and collect data, organize data and analyze data, without worrying about where anything is."

Eight universities across the state share their computing power on NYSGrid, from New York University to the University at Albany and westward to UB, which is the system's hub, Miller said. Connecting over fiber-optic cables, a total of 19 institutions have access to the grid, including research labs like the Hauptman-Woodward Medical Research Institute in Buffalo.

The grid will be a boon for scientists at Hauptman-Woodward who map molecules that hold the keys to health, senior research scientist Charles M. Weeks said.

To map a molecule, researchers use computers to compare X-rays of its structure to theoretical models. Multiple computers working at once can split up the task and reduce what could be a days-long wait into "a matter of minutes," Weeks said.

"If you have to do all these calculations one after the other, you could be waiting a very long time to get your answer," he said. So far, researchers there have mainly tested the grid on known molecules, he added.

NYSGrid is described as analogous to a power grid, where users tap electricity that is generated by far-flung plants over seamless connections.

Similarly, users of a computer grid use mathematical processing power from a number of participating sites, putting idle processors to work.

Not only computers, but also data storage silos, high-end screens or "visualization" devices, and other scientific instruments can connect to the grid.

Getting the simple-sounding idea to work, however, means bridging differences in computer systems, setting priorities of different research tasks, and ensuring security across far-flung sites.

When projects conflict, "you need a human being to decide what's more important," Miller said.

The National Science Foundation awarded $800,000 to UB and other institutions in 2005 to build a regional computer grid in Western New York, a forerunner of NYSGrid.

The statewide grid grew out of discussions at Cornell University this summer, gaining the backing of Cornell's vice president for research, Nobel Prize winner Bob Richardson. The grid's governing board includes representatives from Cornell, SUNY-Albany, Rochester Institute of Technology and Rensselaer Polytechnic Institute as well as UB.

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