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Buffalo Gateway "Rocks" the TeraGrid

SUNY-Buffalo's Center for Computational Research (CCR, www.ccr.buffalo.edu) was created in 1998 to serve a dozen or so projects in science and engineering that required high-end computing. It has since grown to one of the leading supercomputing sites in the world, supporting high-end computing, data storage, networking, and visualization. Currently, CCR supports approximately 140 projects in 40 departments across campus. In addition, it also supports more than a dozen local companies and institutions. Key areas of support include visualization, urban planning, science, engineering, media, finance, animation, medicine, and management, to name a few. Outreach and economic development include projects with the city, state, K-12, local law firms, local animation companies, and local companies working in urban planning. CCR's efforts can be seen in places ranging from 30+ videos on MTV to local public planning efforts.

CCR has had a tradition of naming all of its devices, be they supercomputers, workstations, printers, visualization devices, storage devices, and so forth, after members of the Rock and Roll Hall of Fame (www.rockhall.com). For example, CCR's most recent 1600-processor 10TF Dell Cluster was named "U2" after the Irish supergroup. Other highly-visible machines are named after music legends Janis Joplin, Ray Charles, and John Lennon, to name a few.

CCR has long been involved in a variety of grid efforts. CCR Director, Dr. Russ Miller, and his associate, grid computational scientist Dr. Mark L. Green, are leading the effort to integrate advances made in CCR with the Open Science Grid.

Therefore, CCR felt like it had just won a "Grammy" when TeraGrid was integrated into CCR's grid environment this past summer. In fact, the integration occurred in "record" time.

According to TeraGrid Director Charlie Catlett, "Mark Green contacted me on a Friday afternoon via email, asking if it would be possible to connect his Advanced Computing Data Center (ACDC) Grid Portal to the TeraGrid so that jobs could be run for his user communities in bioinformatics, biomedical, hydrodynamics, physics, and other disciplines. By Monday, he had obtained the information needed to apply for an initial allocation, and by Wednesday he had logins on several TeraGrid machines. By the following Monday, July 18, he had integrated the TeraGrid resources into his portal, and test jobs were running by Wednesday—less than two weeks after we first made contact."

The public perception of grid computing has been that it is fraught with difficulties—hardly a "plug and play" affair. "That was true for a long time," Mark Green says, "but it certainly isn't the case today. Grids are more complicated because of the variety of platforms, the various network connections, and the need to move a lot more data from here to there. But the software to make all that easier has been written, and it really works."

As Green reported to his Open Science Grid collaborators on July 19, "We have successfully run batch job submissions, deployed our volatile storage elements, deployed the ACDC Grid Dashboard, and are obtaining intermediate job status from all submitted jobs."

While CCR is only seven-years-old, it has been leveraged enormously, bringing nearly $500M into Western New York. One of the most visible projects is the New York State Center of Excellence in Bioinformatics, which includes SUNY-Buffalo, the Roswell Park Cancer Institute, and the Hauptman-Woodward Medical Research Institute.

While much of CCR?s grid development was supported by an NSF/ITR grant, a new CRI grant from NSF has enabled the formation of a Western New York Grid consisting of CCR, Hauptman-Woodward Institute (HWI), Niagara University, and SUNY-Geneseo. This effort enables CCR to harden areas of its "grass roots" New York State grid effort, which includes four SUNY campuses (Albany, Binghamton, Buffalo, and Geneseo), Columbia University,

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Niagara University, Canisius College, and the Hauptman-Woodward institute. "We're going to add the Rochester Institute of Technology, the University of Rochester, and Cornell," Green says, "via the Western New York Grid for Engineering and Science."

With 10 major cross-institutional research groups, CCR formed the Grid Resources for Advanced Science and Engineering (GRASE) Virtual Organization. The GRASE VO concentrates on structural biology, groundwater modeling, earthquake engineering, computational chemistry, and the integration of geographic information systems with biohazard research. The connections among the grass-roots grid institutions and these groups all run over New York's NYSERnet 32-lambda backbone.

"The 10 major collaborations are driving our grid efforts," Green notes. "Each group has an application manager who uses an API to port their applications to our ACDC Grid Portal and Grid and Operations Dashboards." The applications include SnB (Shake-and-Bake) and BnP (Buffalo-'n'-Pittsburgh) for molecular structure determination and phasing; a suite of codes for groundwater modeling; a major earthquake engineering code; Q-Chem for quantum chemistry, and a code called Titan for modeling hazardous geophysical mass flows.

Miller and Green are particularly pleased to have added the TeraGrid capabilities to the mix available at CCR. "Having access to these kinds of computational resources really changes the way scientists think about their projects," Green says. "They can ask more challenging questions and ask them more often. As models and simulations become more realistic, their predictive power grows, and their value to society changes."
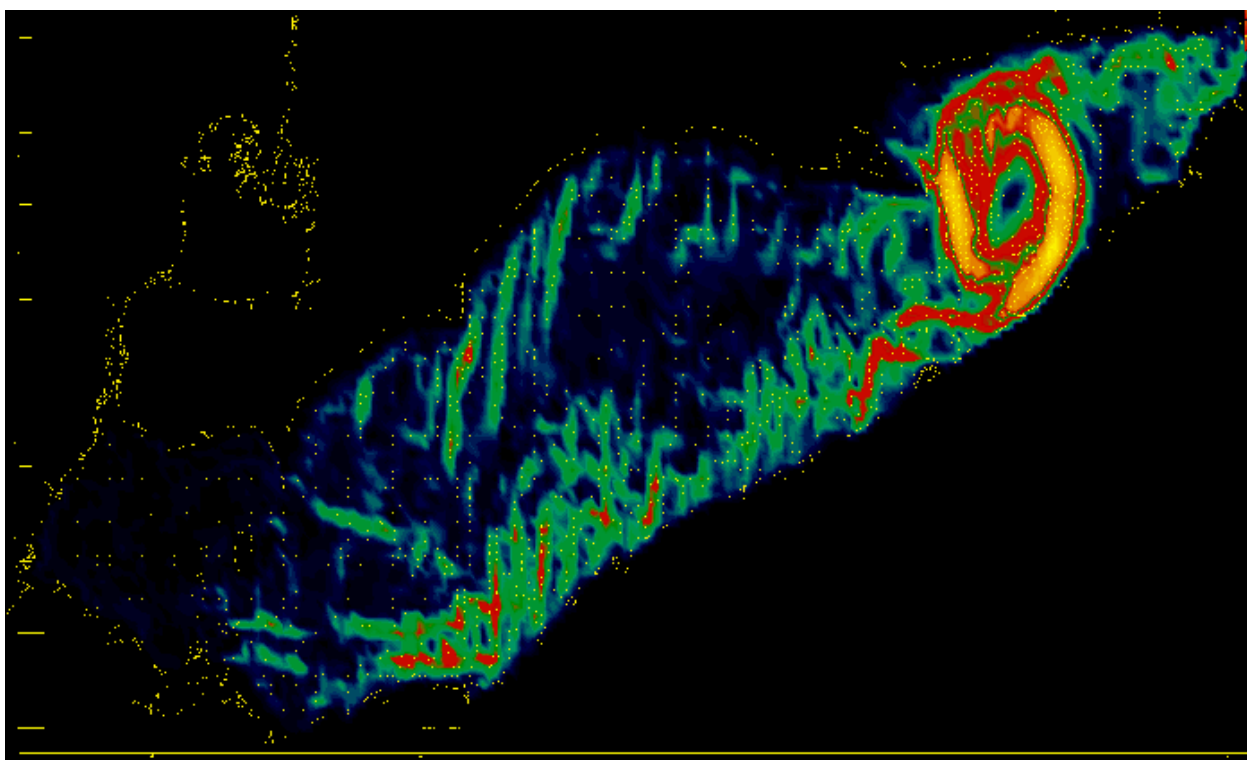

IMAGE DESCRIPTION AND CREDIT:
Princeton Ocean Model Great Lakes version surface water velocity vectors for Lake Erie produced from computational and data grid jobs run through the ACDC Grid Portal on TeraGrid, ACDC and Open Science Grid resources. Credit: Mark L. Green, grid computational scientist, Center for Computational Research and Joseph F. Atkinson, director, Great Lakes Program.

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