



Streamlining chemistry with cyberinfrastructure

With the Computational Chemistry Grid, chemists can focus on their science, not the nuts and bolts of their computing.

Led by the University of Kentucky's Center for Computational Sciences in partnership with four supercomputing sites around the nation, the Computational Chemistry Grid is a virtual organization that provides access to high performance computing resources via Web services production infrastructure that includes an intuitive desktop client, user support, and associated services.

"Prior to this, if chemists needed to access the computational chemistry software applications on our systems, they needed to learn how to use UNIX, move input files from their hard drive to our servers, and understand how to run the applications on our high performance computing systems," said Jim Giuliani, Science and Technology Support Group lead, Ohio Supercomputer Center. "But, GridChem, with its desktop client, automates these steps and reduces the effort needed to leverage our resources."

GridChem, a Java-based interface, seamlessly incorporates the hardware, software, and middleware resources computational chemists need to conduct their work, all through a secure Internet portal.

For example, once the scientists click "Run" on the portal interface, GridChem packages up their data, ships it to the target system, configures the job based on established scheduling policies at the remote site and submits the job for execution. The clients have several point-and-click utilities that allow them to monitor the status of their jobs and view a history of all jobs submitted, without having to log into each system. And, once a job has completed, they can browse the remote storage and download results to their desktop.

Giuliani and his colleagues at the Ohio Supercomputer Center lead the education, outreach, and training effort, ensuring that computational chemists have all the tools and training they need to easily submit, monitor, and manage their jobs on supercomputing systems and software around the country—from the convenience of their own computer.

Cyberinfrastructure refers to software that enables scientists to exploit cutting edge technology resources, including computer and data servers, visualization devices, instruments and networks, for advancing research in science and engineering.



OSC Partners:

- University of Kentucky, Center for Computational Sciences
- Louisiana State University, Center for Computation and Technology
- National Center for Supercomputing Applications
- Texas Advanced Computing Center

Research Title:

Computational Chemistry Grid (CCG): Production Cyberinfrastructure for Computational Chemistry

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For more information:

www.gridchem.org