Power to the people
Scientific discovery used to rely on what could be observed under microscopes and through telescopes and what could be learned through experiments in the laboratory. But over the past two decades, computational simulation has emerged as a third powerful technique and is now integral to the scientific process. High-performance computers enable researchers to explore phenomena too big, too small, too fast, too slow, or simply too complex to be observed or contained within an experimental framework.

A national cyberinfrastructure of powerful computers and fast networks exists and is ever expanding to meet the needs of computational researchers. Thousands of scientists consume thousands of hours of compute time on systems across the country, many of which are linked through the National Science Foundation’s TeraGrid.

To get a slice of the computing pie, investigators submit proposals, which are peer-reviewed. This process works well for researchers who want time in the tens or hundreds of thousands of hours, but for researchers, educators, and students who may use just a handful of hours the barriers to entry are daunting—not just the need to write a proposal and wait for it to be reviewed, but the learning curve involved in tapping computing resources and the delays as submitted calculations await their turn on busy computers.

University of Utah chemistry professor Thanh Truong wants to break down those barriers to entry, making access to computational resources as simple as logging on to a website. In collaboration with NCSA, Truong’s team recently released a new version of CSE-Online (Computational Science and Engineering Online), a web-based framework for science and engineering disciplines as well as a science gateway that connects users with some of the computational resources of the TeraGrid.

Breaking down barriers
Prior to collaborating with NCSA, Truong’s Utah team spent three years developing CSE-Online with support from the National Science Foundation. From the outset, the goal has been to provide integrated, user-friendly access to a wide range of remote data stores, computational tools, and modeling and visualization resources for both research and education.

“We’re removing all of the hurdles, all of the technical difficulties, all of the barriers to entry,” Truong says. “The benefits of CSE-Online to the user are similar to the improvements offered by the Windows operating system over DOS.”

Supported in part by a summer fellowship with NCSA, Truong began work with NCSA in 2006, aiming to make it easier for researchers, educators, and students to access the TeraGrid’s powerful computing resources.

Previous versions of CSE-Online enabled users with their own TeraGrid allocations to run computational jobs on TeraGrid resources.
using their personal credentials for authentication. The version released in spring 2007 provides the same capability for users who have asked to become part of the community. These community users are authenticated and given access to TeraGrid resources by a community credential, which maps to a TeraGrid account that everyone in the community shares. Because an individual allocation isn’t needed, the TeraGrid is accessible to more research and education users.

To increase security, NCSA developed a restricted shell capability that limits the actions community users can take; this prevents malicious users from posing as legitimate community users in order to gain access to TeraGrid.

“Since creating the CSE-Online community we have doubled the number of registered users on the gateway,” Truong says. There are currently more than 600 registered users from countries around the globe, and nearly 4,000 jobs have been submitted to the TeraGrid. “People are using it every day.”

One of those users is Timothy Lippa, a research scientist at the Johns Hopkins University Applied Physics Laboratory. A part of his research looks at the fundamental physical properties of materials, and he has used CSE-Online to branch out into computational chemistry.

“I’m an experimentalist by training, but I’ve started to get interested in computation so CSE-Online has been a great tool for me,” he says.

As he dipped his toe into the computational waters, Lippa found the integration of multiple features and programs into a single platform particularly helpful.

“The way it’s all tied together really increases its usability” he says.

**Computation in the classroom**

Looking at the data on CSE-Online over the past several months, Truong believes that many of the thousands of often small jobs submitted may be coming from teachers and students. And that means his plan to broaden access to computational tools is working.

“These high-performance infrastructures are mainly used for research but can also be used for education,” he says. Truong points out that educating tomorrow’s scientists and engineers is a key first step in ensuring continued competitiveness and innovation.

Small institutions “don’t have the resources, they don’t have their own clusters, they can’t afford the software or IT professional to maintain the system,” he says. But with CSE-Online, “people can use it to learn computational chemistry. They can use it to teach undergraduates.” And they don’t need to invest in hardware, software, and the expertise required to keep both in operation.

NCSA provided CSE-Online users with a dedicated queue to the center’s Mercury cluster. This type of access enables educators
who use CSE-Online in the classroom to submit jobs and receive results in minutes, making it practical for instructors to introduce their students to high-performance computational science in the classroom.

**Beta and beyond**

NSF funding for the development of CSE-Online has ended, so now Truong’s team is courting support from industry and is focusing on meeting users’ needs for domain-specialized sets of integrated computational resources.

“Sustainability requires you to continually focus development on what is most relevant,” Truong says.

Work continues on refining CSE-Online, with the latest version—featuring a more user-friendly interface—planned for beta release by the end of the year. Truong intends to release an initial production version early in 2008.

“Although the environment that we have developed so far is extremely innovative, there are still some barriers to overcome,” he says. “But toward the end of the year when we release our beta version we are confident we'll have removed those barriers.”

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**Access Online:** [www.ncsa.uiuc.edu/News/Stories/CSEonline](http://www.ncsa.uiuc.edu/News/Stories/CSEonline)

**More information:** [http://cse-online.net](http://cse-online.net)

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