Rice takes zeolite design Into 21st century using TeraGrid

December 13 2006

A room's design helps define how people interact inside it, and it's much the same in the molecular world. The atomic layout of molecular spaces can provoke very different reactions from chemicals that meet there, in much the way that an intimate bistro and a bustling cafeteria might evoke different interactions among dinners.

One class of substances that chemists often tap for these spatially unique properties are zeolites, silicate minerals with a porous, Swiss-cheese-like structure. For decades, chemists have relied on zeolites to catalyze chemical reactions on an industrial scale. They are used to make everything from gasoline and asphalt to laundry detergent and aquarium filters.

So useful are zeolites that scientists have sought for decades to improve upon Mother Nature's ability to make them. In the past 50 years, the catalog of naturally occurring zeolites – there are about 50 of them – has been bolstered to approximately 180 with the addition of synthetic varieties, minerals whose architecture was found to be, much like a building's, suitable for a particular purpose.

Today, Rice University physicist Michael Deem is taking zeolite design into the 21st Century, using a combination of supercomputers at the University of Texas at Austin and disused computing cycles from more than 4,300 idling desktop PCs at Purdue University to painstakingly calculate many conceivable atomic formulations for zeolites.

Deem's zeolite database contained 3.4 million structures in early December, and it's still growing. By studying the catalog, scientists might find structures that are more efficient, either in terms of energy inputs or in waste byproducts.

"We're working with a major oil company to look at the structures in hopes of finding new catalysts for chemical and petrochemical applications," said Deem, the John W. Cox Professor in Biochemical and Genetic Engineering and professor of physics and astronomy.

In the current project, Deem and former postdoctoral researcher David Earl, now an assistant professor of chemistry at the University of Pittsburgh, worked with experts from the UT's Texas Advanced Computing Center and Purdue's Rosen Center for Advanced Computing to run computer simulations on multiple TeraGrid supercomputing systems, including systems at TACC, Purdue, Argonne National Labs, National Center for Supercomputing Applications and San Diego Supercomputing Center. The NSF-funded TeraGrid is the world's largest, most comprehensive distributed cyberinfrastructure for open scientific research.

Deem and Earl were able to harness the distributed, heterogeneous computing resources on the TeraGrid network into a single virtual environment for their simulations.

"This project could not have been accomplished in a one- to three-year time frame without the TeraGrid," Deem said.

Source: Rice University