Formed in 1999 and supported by the U.S. Department of Energy, the Super Computing Science Consortium is a regional partnership of research and educational institutions in Pennsylvania and West Virginia. (SC)² provides intellectual leadership and advanced computing and communications resources to solve problems in energy and the environment and to stimulate regional high-technology development.

PSC supplies training along with consulting support to (SC)² partners. Training includes workshops in parallel programming and visualization. In September 2005, PSC scientific-visualization specialist Kent Eschenberg presented a tutorial on ParaView, an application for visualization of large data sets, to NETL researchers. ParaView runs on distributed parallel systems such as PSC’s LeMieux and Big Ben.

Since the spring of 2000, a high-speed network — the first fiber-optic service to Morgantown, West Virginia — has linked the National Energy Technology Laboratory (NETL) campuses in Morgantown and Pittsburgh with PSC, facilitating NETL collaborations. Researchers at NETL and WVU have actively used this link to tap PSC computational resources. Since the founding of (SC)², more than 40 (SC)² researchers have used PSC systems for a range of projects, using more than 2.6 million hours of computing time, 840,000 hours within the past year. Along with surface chemistry simulations described here (facing page), this work includes:

- Gas From Black Liquor
- Fluidized-bed Combustion Of Silane
- Lean-fuel Mixes In Next-generation Power-generating Turbines
  [http://www.psc.edu/science/Richards/clean_power.html](http://www.psc.edu/science/Richards/clean_power.html)
- Industrial-scale Technology For Coal Gasification
  [http://www.psc.edu/publicinfo/2002/sc2](http://www.psc.edu/publicinfo/2002/sc2)
- A New Design For A Power-generating Turbine

(SC)² co-chairs: Lynn Layman, PSC, and Bob Romanowsky, NETL. “The (SC)² partnership continues to advance research in both energy and the environment,” says Layman. “Our regional partners are joining together to move forward our nation’s knowledge in these vital areas.”

(SC)² PARTNERS
National Energy Technology Laboratory
Pittsburgh Supercomputing Center
Carnegie Mellon University
Duquesne University
University of Pittsburgh
Waynesburg College
West Virginia University
Institute for Scientific Research
NASA Independent Verification & Validation Facility

[http://www.sc-2.psc.edu](http://www.sc-2.psc.edu)
(SC)² AT SUPERCOMPUTING '04

In November 2004 for the first time, (SC)² sponsored a booth at Supercomputing, the annual International Conference for High Performance Computing, Networking and Storage. The conference, held in Pittsburgh for the second time in eight years, features displays and demonstrations by leading vendors and research organizations around the world. The booth featured posters highlighting research activities from (SC)² partners. In the photo is Barbara Kirby of Waynesburg College, who represents Waynesburg on the (SC)² steering committee and chaired the booth team.

TEAMING TO WIN

(SC)² joined other regional organizations at West Virginia’s Teaming to Win conference June 1-2, at the Stonewall Resort, Walkersville, West Virginia. Sponsored by Congressman Allan B. Mollohan (WV, Dist. 1), the event provides a forum for West Virginia organizations to explore opportunities for collaborative projects. The photo shows Brian Dotson and Steve Zitney of NETL preparing a demonstration of their 3D visualization capability.

HYDROGEN FROM FOSSIL FUELS

The Bush administration’s announcement in 2003 of a hydrogen fuel initiative has spurred interest in hydrogen’s potential to play a major role in U.S. long-term energy planning. Hydrogen is clean, efficient and with hydrogen fuel-cell technology could power cars, airplanes, furnaces and air conditioners. One of the major challenges, however, in harnessing this renewable resource is finding affordable ways to produce fuel-quality hydrogen.

As a member of NETL’s Computational Chemistry Team, NETL scientist Dan Sorescu has used PSC resources for a wide range of studies. In this work, he applies quantum-theory calculations from first principles to gain detailed molecular understanding of the chemistry and physics underlying fossil-fuel related processes. In work this year, he used Ben — PSC’s 64-processor Alphaserver cluster — to explore a catalytic process that offers the potential of recovering hydrogen from hydrogen sulfide (H₂S), one of the principal byproducts from fossil fuel.

Titanium dioxide — a material found in beach sand and widely used as a white pigment — catalyzes the reaction by which hydrogen sulfide dissociates to hydrogen and sulfur. It does this by providing a surface to which H₂S chemically adheres — adsorbs — and from which H₂ subsequently desorbs. As these three frames show, Sorescu’s computations with Ben map the sites on a titanium dioxide (gray & red) surface where H₂S (white & yellow) adsorbs, leading to sulfur formation and desorption of hydrogen. This kind of detailed understanding is essential to optimize the catalytic process.