

# The Super Computing Science Consortium

## PENNSYLVANIA-WEST VIRGINIA PARTNERS IN THE DEVELOPMENT OF CLEAN-POWER TECHNOLOGIES

Scientists at the National Energy Technology Laboratory and researchers at West Virginia University use PSC resources to address the critical challenge of developing clean, efficient fossil-fuel combustion. This research involves complex computer modeling in fluid dynamics, chemistry and geology. In recent work, NETL, the newest U.S. Department of Energy national laboratory, has relied on PSC resources to simulate fluidized-bed combustion and the use of lean-fuel mixes to develop clean and efficient next-generation power-generating turbines.

In January 2001, NETL awarded \$2.5 million through the Super Computing Science Consortium to support energy research at PSC. Formed in 1999, the SCS Consortium is a regional partnership of NETL, PSC, Carnegie Mellon University, the University of Pittsburgh, West Virginia University and the West Virginia Governor's Office of Technology. The goal is to provide intellectual leadership and resources to apply high-performance computing and communication to problems in energy and the environment and to stimulate regional high-technology development.

"PSC has been an active partner with NETL in supporting regional initiatives," said Rita A. Bajura, director of NETL. "This agreement will make PSC's computing capabilities available to not only the region but the nation to further research in the efficient production and use of coal, oil, and natural gas — the resources that provide 85 percent of the nation's energy supply."

"We are very excited about the opportunities available through the Super Computing Science Consortium and the Pittsburgh Supercomputing Center," said John Weete, associate provost for research and economic development at West Virginia University. "Through this agreement WVU

researchers will have new and enhanced tools to tackle complex problems requiring high-performance computing resources."

"Working with NETL, we've demonstrated that high-performance computing and communication are powerful tools for solving problems related to fossil-fuel combustion," said PSC scientific directors Michael Levine and Ralph Roskies in a joint statement. "By applying these technologies to the goals of the consortium, we are creating a stronger research and technology base for the region."

Additional resources will be provided through a "supercluster" of computers. Groups of linked computers at NETL, WVU and PSC will connect with each other via a high-performance fiber-optic network. With special software, PSC staff will coordinate and schedule the local clusters to act as a unified supercluster for advanced scientific applications.

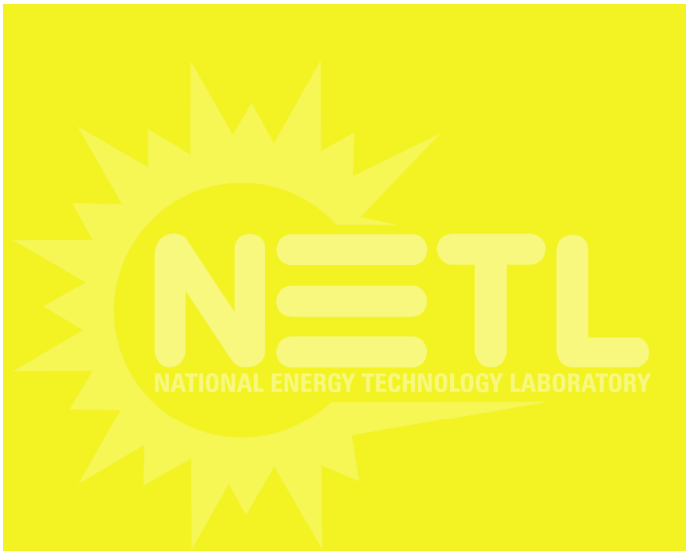
**More information:** <http://www.sc-2.psc.edu>



Jim Kasdorf, PSC director of special projects.



On April 10, the Super Computing Science Consortium consortium broke ground for the EverGreen Technology Park in Waynesburg, Pa. With state and federal funding, this economic development project includes participation of all the school districts in Greene County. PSC has planned data network connections for EverGreen, to provide companies that locate there with access to PSC resources.



“New advances in computer simulation technologies, in revolutionary new concepts for coal and natural gas fueled power plants, in carbon sequestration technologies, and in the production of ultra-clean transportation fuels and chemicals now allow us to envision a future in which the economic advantages of fossil fuel can continue to be enjoyed without environmental concerns.”

— U.S. Secretary of Energy Bill Richardson  
(FROM HIS DEC. 10, 1999 STATEMENT, DESIGNATING THE NATIONAL ENERGY TECHNOLOGY LABORATORY AS DOE'S 15TH NATIONAL LABORATORY)

### SILANE REACTIONS IN A FLUIDIZED BED

An innovative technology with numerous potential applications, fluidized-bed combustion offers a highly efficient means to generate low-cost electricity from coal and other fuels with minimal environmental impact. It promises improved efficiency at substantially less cost to build than conventional non-fluidized bed combustion units used in power generation, and it offers a clean method to rely on coal as a fuel to meet growing energy needs.

Along with coal, fluidized-bed combustion can use waste materials as fuel — such as municipal trash and hospital medical waste — burning them to produce electricity while reducing the need for waste disposal. Because pollutants are incinerated or captured in the bed as they're generated, they aren't released to the air.

NETL carries out extensive programs of research in fluidized-bed combustion. Among the tools it has developed is simulation software called MFIX (Multiphase Flow with Interphase Exchanges). MFIX realistically models the gas-particle dynamics, chemical reactions and heat transfer processes that occur in fluidized-bed combustion.

In a recent MFIX study, NETL researchers used PSC's CRAY T3E to model the chemical reactions of silane, a chemical precursor of silicon, when injected into a fluidized bed. Carried out in collaboration with Dow Corning, this project investigated fluidized-bed technology as a production method for ultra-pure silicon, which deposits on the bed of particles as silane decomposes at high temperature.

This sequence of images, from an animation produced by PSC visualization specialist Greg Foss, depicts some of the simulation results. Color (decreasing from black through red to dark blue) corresponds to the fraction of gas versus solid material visible at a cross-sectional slice through the combustor. These results told the NETL researchers that the reaction occurs rapidly at the bottom of the combustor, where the silane is injected, and that “bubbles” of gas (black) tend to form along the walls of the combustor and migrate toward the center as they rise.

