

National Center for Computational Sciences Snapshot

The Week of January 21, 2008

Simulation Aids Development of First Coal Plants with Near-Zero Emissions

Next-generation plants to produce electricity and hydrogen and sequester carbon dioxide

Department of Energy (DOE) researchers at the National Energy Technology Laboratory (NETL) and Oak Ridge National Laboratory (ORNL) are using supercomputers to improve the industrial design of facilities that tap coal's oxidative potential while trapping its pollutants. The highest-resolution coal-gasification simulation to date should enable faster development of clean coal technology that emits nearly no nitrogen oxide, mercury or sulfur and that sequesters most carbon dioxide.

"An important part of NETL's mission is to supply clean coal technology, and our research group at NETL develops computational tools and applications in support of that mission," says principal investigator Madhava Syamlal of NETL. With Chris Guenther (NETL), Aytakin Gel (Aelous Inc./NETL), Phil Nicoletti (Parsons/NETL), and Sreekanth Pannala (ORNL), he uses the Cray XT4 Jaguar supercomputer at DOE's National Center for Computational Sciences (NCCS) to simulate coal gasification processes.

In gasification, coal is pulverized and partially oxidized to separate fuel-rich hydrocarbons from pollutants. Coal solids are recycled through the system until they are completely gasified to produce "syngas," a mixture of hydrogen and carbon monoxide. The syngas can be used to produce hydrogen or to generate electricity (for example, using gas turbines) in a clean and efficient manner.

"Essentially, we're trying to get the highest-resolution data to date for coal gasification to feed into these test facilities," Guenther says. "Correctly capturing inlet regions is critical in our simulations, not only to understand local conditions in these areas, but also to understand how injection of coal can impact the conversion of coal into syngas."

To examine injection ports in detail, the NETL researchers will run simulation on Jaguar for two weeks in January 2008 that will provide 1 millimeter resolution. Jaguar's high resolution means combustion can be modeled in great detail, enabling simulations that represent reality with unprecedented fidelity. Jaguar's enormous memory and speed produce quicker answers to scientific and engineering questions and accelerate development of the technology.

"There's a move toward modeling instead of building expensive prototypes," says Ramanan Sankaran, an NCCS liaison who optimizes code so researchers can wrest the most science from the supercomputers. Guiding the design process through simulation rather than trial-and error speeds the development of an experimental prototype that works, he says. "Once that prototype is built, researchers can run different experiments and get a new answer every hour."

This work was funded by the DOE Office of Fossil Energy; computer time was provided by the DOE Office of Science.

James J. Hack Named Director of NCCS

Atmospheric scientist to head leadership computing facility at ORNL

James J. ("Jim") Hack has been selected to direct the National Center for Computational Sciences (NCCS), a leadership computing facility at Oak Ridge National Laboratory (ORNL), and to head ORNL's Climate Change Initiative. As director of the NCCS, in partnership with the project director of the Leadership Computing Facility at ORNL, Hack will lead the world's premier high-performance computing facility for open science and advancing scientific discovery. As leader of the Climate Change Initiative, he will develop Laboratory-wide programs in climate change and lead a team of scientists and engineers across ORNL in advancing the state of the art in Earth system discovery and policy through enhanced scientific understanding, Earth system modeling, and advances in computational and observational programs.

Hack joins ORNL from the National Center for Atmospheric Research (NCAR) with a distinguished career in climate science research. He has long collaborated with the international climate community and continues to serve on the Department of Energy's Advanced Scientific Computing Advisory Committee and the Working Group on Numerical Experimentation, which is supported by the Joint Scientific Committee for the World Climate Research Program and the World Meteorological Organization Committee for Atmospheric Sciences, the United Nations' authoritative voices on weather, climate, and water.

Oak Ridge Leads DOE INCITE Effort in 2008

Climate, energy assurance high priorities

Scientific studies on climate change, energy and alternative fuels are among the 30 projects awarded more than 145 million processing hours on supercomputers at Oak Ridge National Laboratory through the Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

Through INCITE, researchers from industry, academia, and government research facilities receive access to computing power at the National Center for Computational Sciences at ORNL for research on climate change, fusion energy, nanoscience, materials, chemistry, astrophysics, and other areas.

"The Department of Energy's Office of Science has two of the top ten most powerful supercomputers, and using them through the INCITE program is having a transformational effect on America's scientific and economic competitiveness," DOE Under Secretary for Science Raymond L. Orbach said. "Once considered the domain of only small groups of researchers, supercomputers today are tools for discovery, driving scientific advancement across a wide range of disciplines. We're proud to provide these

resources to help researchers advance scientific knowledge and understanding and thereby to provide insight into major scientific and industrial issues."

This year's total allotment of processing hours nearly doubles that which ORNL provided in 2007, when the largest allocation was 10 million processor hours. The 2008 program will see six projects with at least 10 million hours, and the largest allocation is 18 million processor hours.

"By providing research access to supercomputing facilities at ORNL, the 2008 INCITE program advances the scientific discovery that is crucial to improving our lives and our understanding of the world we live in," ORNL Director Thom Mason said.

ORNL's 2008 INCITE allocations include energy projects related to biofuels such as ethanol; next-generation fuels such as hydrogen; cleaner-burning, more efficient engines; and research that will contribute to fusion energy projects such as the multinational ITER reactor.

Climate scientists will also have a major presence among the 2008 recipients. Leading researchers from the National Center for Atmospheric Research (NCAR) and other institutions will continue to advance tools that predict climate change with unprecedented accuracy. Other projects are delving into the role of ocean currents in regulating climate, the relationship between carbon dioxide and abrupt climate change, and the feasibility of storing carbon dioxide underground.

"This INCITE grant will allow DOE and its partner National Science Foundation to do three things," said Warren Washington, who heads the NCAR team, "advance the state of climate and earth system models, improve the horizontal and vertical resolution of the models, and explore further the causes of present and future climate change including various future energy policy strategies such as new low-carbon-emission scenarios."

The program will continue to reflect the critical research role played by American industry. "We're extremely happy to be able to pursue our research on ORNL's leadership-class systems," said Jihui Yang, a General Motors researcher whose team is exploring materials at the nanoscale, searching for ways to convert a vehicle's waste heat into usable electricity. "This allocation will greatly advance our efforts to improve vehicle fuel efficiency and promote American energy independence." Besides the General Motors effort, physicists from the Boeing Company will continue using the systems for creating next-generation tools for designing aircraft and physicists from General Atomics will continue their examination of turbulence in fusion reactors.

The 2008 allocations reflect an aggressive program of upgrades to the Cray XT4 Jaguar supercomputer, which is in the midst of the second of two major upgrades in a year. When the current project is complete, Jaguar's 31,000 processing cores will be capable of 275 trillion calculations a second, or 275 teraflops—a fourfold increase over a year ago.

Jaguar's increased processing power is reflected in the size of the allocations being made available to individual projects. Whereas the largest allocation in 2007 was 10 million processor hours, 2008 will see six separate projects with at least 10 million hours, and the largest allocation is 18 million processor hours. The 2008 INCITE program and the large allocations enabled by Oak Ridge's NCCS Leadership Computing Facility will give researchers an invaluable opportunity to continue pushing the boundaries of knowledge, and their efforts promise to improve both our lives and our understanding of the world we live in.

The 2008 INCITE awards adds to the impressive roster of scientific achievements at ORNL made possible by the unique DOE leadership computing capabilities at the NCCS. In 2007, astrophysicists from ORNL and North Carolina State University released the first explanation for the spin of a pulsar that matches observation, publishing their findings in the preeminent journal *Nature*. In that same month, a team of chemists from ORNL and the University of Tennessee released findings that advance our knowledge of adsorption, the molecular process responsible for catalytic converters, chemical sensors, and thousands of other products. Their work appeared as the cover story in the *Journal of Physical Chemistry C*. Later in the year, *National Geographic* featured the work of NCCS users from the University of California–Santa Cruz and the University of Arizona in a discussion of the exploding stars known as supernovas.

Also, a team of fusion researchers from ORNL, the Massachusetts Institute of Technology, Princeton University, and other institutions verified the effectiveness of the heating mechanism that will be used in the multinational ITER reactor. NCCS users are visible throughout the science world and were responsible for well over 300 journal articles and invited presentations in 2007.

To read about all the 2008 INCITE awards, go to the DOE Office of Science home page at: www.science.doe.gov.

For more information on the INCITE program, visit:
<http://www.sc.doe.gov/ascr/incite/index.html>

Knoxville Hosts Dynamics Days

Visiting researchers tour ORNL

Scientists from around the world recently converged on Knoxville, Tennessee to attend the annual Dynamics Days International Conference.

Several researchers from nearby Oak Ridge National Laboratory (ORNL) helped to organize the conference, which focuses on chaos, complex systems, and nonlinear dynamics. ORNL's Yehuda Braiman, Diego del-Castillo-Negrete, Stuart Daw, and Charles Finney all served on the Dynamics Days 2008 organizing committee.

ORNL also gave tours of its various facilities to visiting researchers. The tours included the National Center for Computational Sciences, home to Jaguar, a Cray XT4

supercomputer capable of 119 teraflops; the Center for Nanophase Materials Science; and the Spallation Neutron Source, which, when fully operational, will facilitate the most intense neutron beams in the world for scientific research.

The gathering has become renowned as a forum for researchers in multiple disciplines to share ideas and results in nonlinear dynamical systems. While the audience is primarily made up of physicists and mathematicians, other disciplines have become more prevalent in recent years.

This year the conference emphasized applications of nonlinear science in combustion, plasma physics, materials science and mechanics, to name a few.

The conference was held in downtown Knoxville at the Crowne Plaza Hotel from January 3-6. Two more Dynamics Days conferences are planned for 2008: Dynamics Days Europe will take place August 25-29 in the Netherlands and Dynamics Days Asia Pacific 5 will run from September 9-12 in Nara, Japan.