NERSC NEWS
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER
Berkeley Lab
Office of Science
U.S. DEPARTMENT OF ENERGY
SUMMER 2008

Orbach Presented Souvenir from Seaborg

As part of his visit to Berkeley Lab on Friday, May 30, DOE Under Secretary of Science Ray Orbach met with representatives of Computing Sciences. ALD Horst Simon and NERSC Director Kathy Yelick opened the meeting by presenting Orbach with a framed memento from the decommissioned IBM supercomputer Seaborg and thanking him for his support of computational science. The Under Secretary quickly showed his knowledge of computing technology and asked if that was the Power 3 machine, and this led to further technical discussions.

The session also included a presentation by John Shalf on "Green Flash," the LBNL research project to design a specialized supercomputer for solving leading-edge scientific problems, using the same design techniques that result in the highly efficient processors of battery-powered consumer electronic devices such as cell phones. In a paper published in the May issue of the International Journal of High Performance Computing Applications, Michael Wehner, Lenny Oliker and John Shalf proposed an innovative architecture for modeling climate change with 1-kilometer resolution.

Sandia Researchers Are Creating Benchmarks for Combustion Strategy

Two Sandia National Laboratories scientists at the Combustion Research Facility are using NERSC resources to create a benchmark data set for modeling combustion physics relevant to the next generation of internal combustion engines, an undertaking that will benefit the development of efficient engines running on alternative fuels.

Ed Richardson and Jackie Chen will develop three-dimensional simulations of combustion representing the stratified conditions that may be useful when developing engines for anticipated fuels and improved fuel consumption. Despite the continuing development of strategies to improve combustion performance, there is still a need to create a benchmark set of fundamental simulation data for understanding this combustion regime.

continued on page 2

NERSC Users Report 6,500 Scientific Publications in Five Years

Over a five-year period, researchers using HPC systems at the U.S. Department of Energy's National Energy Research Scientific Computing Center (NERSC) have reported producing 6,593 scientific publications as a result of running their applications at NERSC.

Beginning in 2003, NERSC staff have asked users to list resulting publications as they request allocations for the coming year. The number of publications has grown steadily in each of the five years in which the data has been collected. In 2003, 936 publications were reported; in 2004, 1,270; in 2005, 1,448; in 2006, 1,437; and in 2007, 1,502.

Links to the publications for each year can be found at: http://www.nersc.gov/news/reports/.

"While there are any number of measures of productivity for a supercomputing center, NERSC prides itself on the scientific productivity of its users," said Kathy Yelick, director of the NERSC Division at Lawrence Berkeley National Laboratory. "The fact that our user community reports nearly 7,000 papers produced thanks to our systems and staff is strong evidence that NERSC is advancing computational science on a grand scale."

NERSC currently has about 3,000 users working on 366 projects. The center supports unclassified research in areas such as climate modeling, fusion energy, combustion, high energy physics, chemistry, life sciences and materials science. NERSC's primary supercomputer is a 19,344-processor Cray XT4 with a theoretical peak performance of 101 teraflops (or trillions of calculations per second).

"Supercomputers such as ours are powerful tools for scientific discovery, but many announcements about such systems focus on the potential, not the actual results," said Horst Simon, Associate Lab Director for Computing Sciences at Berkeley Lab. "We are committed to providing the systems and services that help our users harness the potential to produce verifiable, peer-reviewed scientific results."

SPOTLIGHT

GRID CONFERENCE

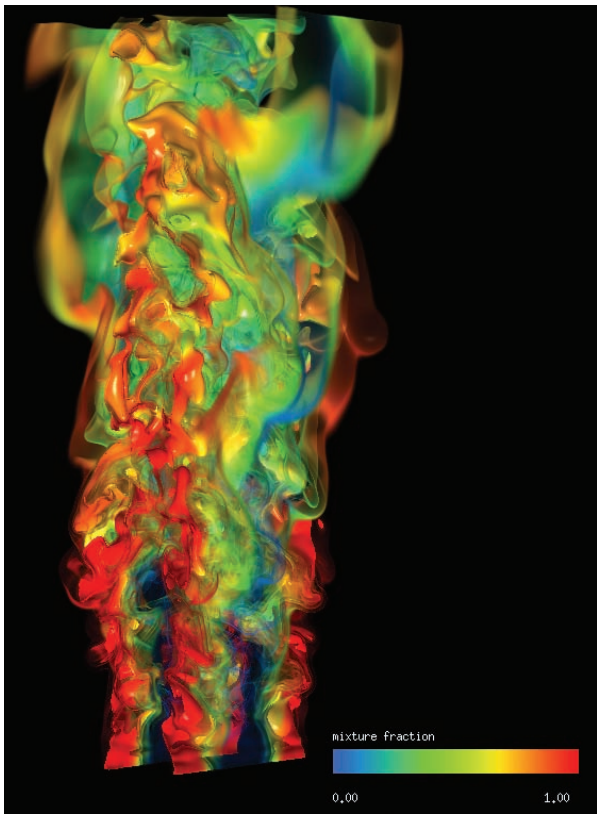
NERSC staff presented their work at the Open Source Grid & Cluster Conference, which showcased the latest grid and cluster software, including Globus, Grid Engine, Rocks, Ganglia and UniCluster Express. The conference took place May 12-16 in Oakland.

Shreyas Cholia, who has worked on connecting NERSC systems to the Open Science Grid, gave a talk about NERSC's certification authority service. He, along with Dan Gunter and Brian Tierney from the Computational Research Division (CRD) at Berkeley Lab, also presented a talk on trouble-shooting grid applications and middleware.

Arie Shoshani, head of the Scientific Data Management group in the Computational Research Division at Berkeley Lab, discussed storage management issues such as allocation and access. Eric Roman, also from CRD, talked about checkpoint and restart, a mechanism for saving files that can be restarted in an event of a system crash or other computer problems.

Combustion Research

continued from page 1



Complementary to experimental measurements, direct numerical simulation is a valuable tool for isolating and revealing the interactions among reactants and turbulent mixing in the stratified combustion regime, Richardson said.

"Probing the smallest scales of highly turbulent flames tests our computational limits. With the NERSC resources, we are gaining highly detailed data that currently is unobtainable experimentally."

Modern combustion devices have been highly optimized for the range of fossil fuels currently available. However, the proposed use of hydrogen, biomatter or synthetic fuels requires different conditions for effective and clean burning. Stratified combustion is a leading strategy for control of the combustion process in applications ranging from internal combustion engines to the largest power plants.

In stratified combustion, the fuel and the oxidizer are not completely mixed or separated prior to combustion. As a result, conventional combustion models that assume a premixed or non-premixed

continued on page 3

NERSC Helps STAR Researchers Find Evidence of Elusive Phenomena in Mountains of Experimental Data

With help from NERSC's Parallel Distributed Systems Facility (PDSF) and High Performance Storage System (HPSS), the STAR collaboration is analyzing evidence for some of the most elusive phenomena in high energy physics — quarks, gluons, and proton spin.

The STAR collaboration, 600 scientists from 52 institutions in 12 countries, studies the QCD phase diagram of nuclear matter and the origins of proton spin at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL).

In collisions of highly energetic gold nuclei, hot and dense matter is created that is observed with the Solenoid Tracker at RHIC (STAR), an advanced particle detector. Scientists scrutinize the data from millions of collisions to look for evidence of a new state of matter, the Quark Gluon Plasma (QGP). In a QGP, protons and neutrons are "melted" into a liquid of quarks and gluons. Such a state is believed to have existed in the early universe.

Scientists also study highly energetic collisions of polarized protons in search of the origin of proton spin, a fundamental property resembling internal rotation. The proton consists of quarks and gluons, and hence its spin is carried by quarks and gluons. Recent STAR results refute the view that the contribution from gluon spins compensates for the puzzlingly small sum of quark spins, observed in earlier experiments. The measurements will thus continue to challenge our understanding of the proton, one of the building blocks of nature.

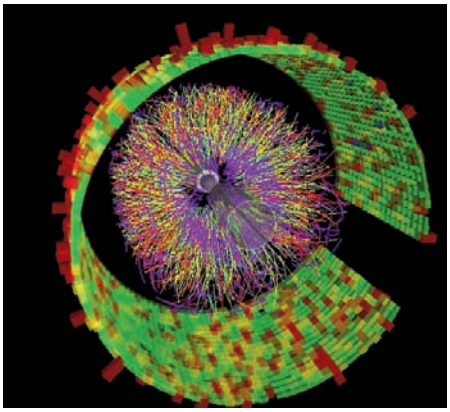
In their research, STAR scientists process hundreds of terabytes of data. With technological advances in the accelerator and detector systems increasing the data rates, their need for large-scale computing resources is increasing every year. In concert with the computing resources available at RHIC, NERSC's PDSF and HPSS address this need.

continued on page 3

STAR Data *continued from page 2*

HPSS, a massive tape robot system and front-end disk cache, allows the researchers to access the half a petabyte of STAR data and simulations reliably and efficiently. Concurrent and continual access to the data is essential to timely analyses of and comparisons between data sets. HPSS reliably provides such access, even across a data sample of this magnitude. The STAR data analysis at NERSC is accomplished on PDSF, a facility that seeks to exploit the economy of scale in computing to process the data from many STAR collision events simultaneously.

Software tools developed by DOE's SciDAC project called the Particle Physics Data Grid, a member of the Open Science Grid, have enabled STAR researchers to efficiently transfer the many terabytes of data between the RHIC and NERSC computing sites, as well as to coordinate simulation studies between the main facilities and other satellite clusters. NERSC has been a vital part of the development of the



software tools necessary for this effort.

Last year, simulations carried out at PDSF were used as the basis of standard corrections for analyses throughout STAR's scientific program. Such simulation studies focus primarily on providing a detailed understanding of the detector by embedding a few simulated particles into real data from the experiment. Reconstruction of this data provides an understanding of the performance of the detector and software systems. Also, pure simulation studies of new detector technologies and proposed implementations play a key role in planning the future development of the experiment as a whole.

STAR scientists will continue to acquire new data sets of ever increasing size and complexity. The production of extremely rare particles containing very heavy quarks will be of particular interest for future studies. Massive hadrons are unique probes that will give new insights in the characteristics of the hot and dense matter formed at RHIC.

To date STAR scientists have published over 110 papers in peer-reviewed journals, and presented more than 250 conference talks. More than 100 Ph.D. and Master's students have written their theses on STAR data. Learn more about the STAR experiment research program at the STAR website (http://www.star.bnl.gov).

Combustion Research *continued from page 2*

mode don't apply. Models for partially premixed modes still require considerable development and validation.

Because of the high computational expense, Richardson and Chen are looking specifically at laboratory-scale flows of several centimeters in scale, which exhibit underlying turbulence–flame interactions also found in combustion engines. The micro-scale mixing and reaction coupling are uniquely captured in high-fidelity direct simulations which resolve all turbulence and flame scales. The researchers' goal is to determine the combustion efficiency and emissions of compounds, such as carbon monoxide and nitrogen monoxide, that result from the stratified distribution of fuel and oxidizer.

"The flame structures and burning velocity under stratified conditions will be compared to the equivalent uniformly premixed case," Richardson. "The benchmark simulation data resulting from this study will provide a unique testbed for predictive engineering models in the challenging partially premixed regime."

The scientists are building on previous research for the current study. A three-dimensional, direct numerical simulation they already have constructed includes a reduced methane and nitrogen chemistry component developed by Tianfeng Lu and C.K. Law at Princeton University. The simulation, a stratified turbulent Bunsen flame, allows for intense turbulence to interact with the flame in a computationally efficient manner.

Richardson and Chen will carry out further calculations by setting different parameters, such as the range of fuel-air ratios, in order to analyze the flame regime.

The researchers have enlisted the help of Kwan-Lui Ma and Hongfeng Yu at the SciDAC Institute of Ultra-Scale Visualization to render their calculations into images for better data analyses.

WHAT IS NERSC NEWS?

NERSC News publishes every other month and highlights the cutting-edge research performed using the National Energy Research Scientific Computing Center, the flagship supercomputer facility for DOE's Office of Science. NERSC News editor Jon Bashor can be reached at 510 486-5849 or JBashor@lbl.gov. Find previous NERSC News articles at http://www.nersc.gov/news/nerscnews.