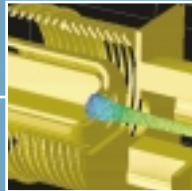
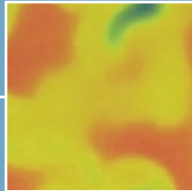
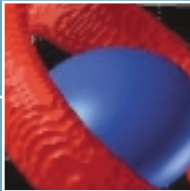


NERSC Annual Report 2002







# National Energy Research Scientific Computing Center

## 2002 ANNUAL REPORT

This work was supported by the Director, Office of Science, Office of Advanced Scientific Computing Research of the U.S. Department of Energy under Contract No. DE-AC 03-76SF00098.

LBNL-51979, January 2003



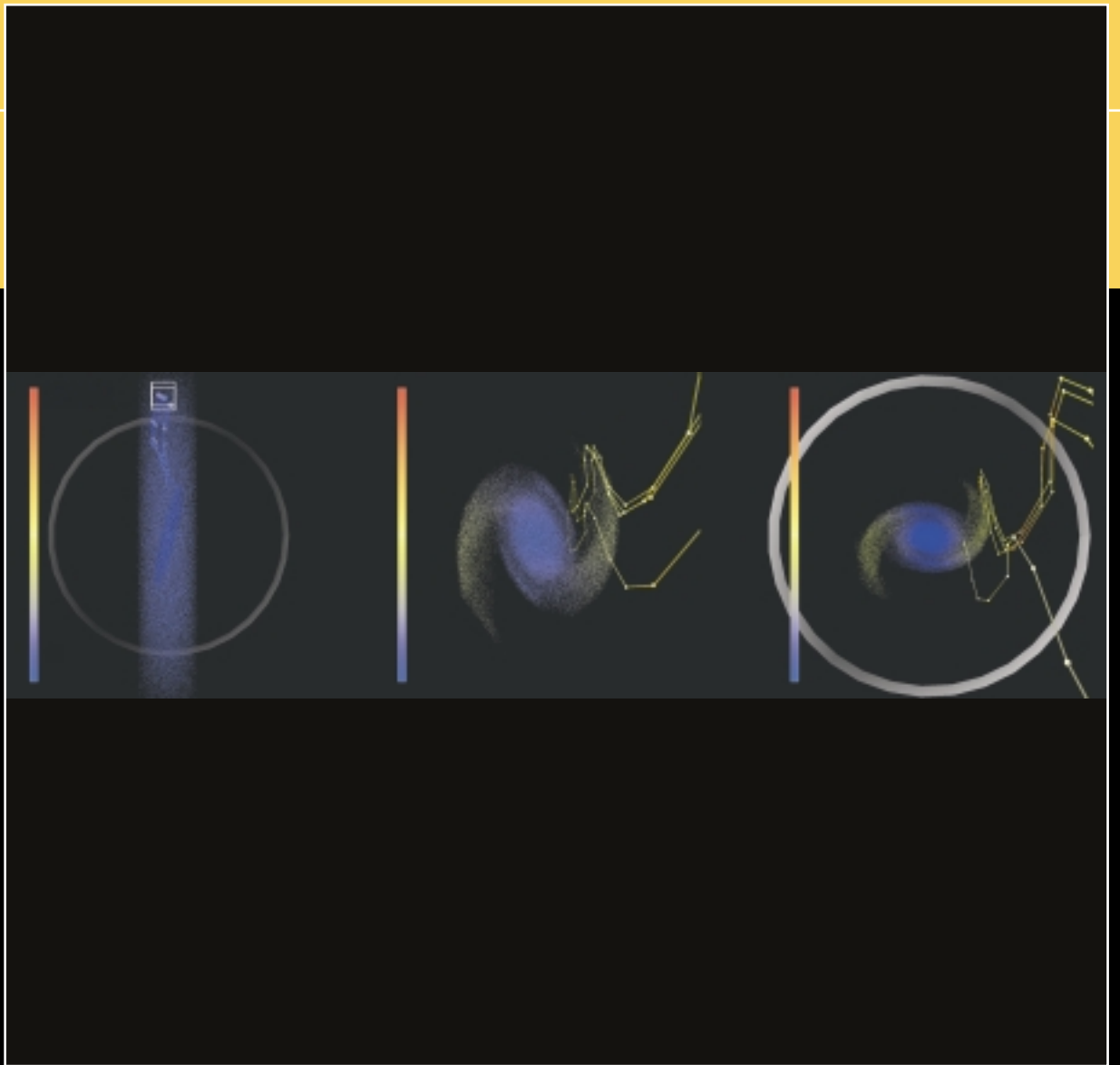


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# Director's Perspective



The year 2002 has brought very significant changes in high performance computing whose impact will be felt for years to come. At NERSC the biggest visible change was the decision to upgrade our current Seaborg platform from 5 to 10 teraflop/s peak performance. This will create one of the largest systems in the U.S. dedicated to basic computa-

tional science. It will give NERSC users routine access to an unprecedented 6,556 processors, coupled with one of the largest memory systems anywhere. DOE-supported computational scientists again will have access to one of best possible resources to further the DOE mission in basic sciences.

It is clear to me that resources of this scale are required if simulations are to make the scientific impact that we all expect. In 2002 NERSC dedicated a large share of its resources to a small number of projects that require the full NERSC capability or special services. This strategy has paid off with a number of scientific accomplishments that are discussed in this report.

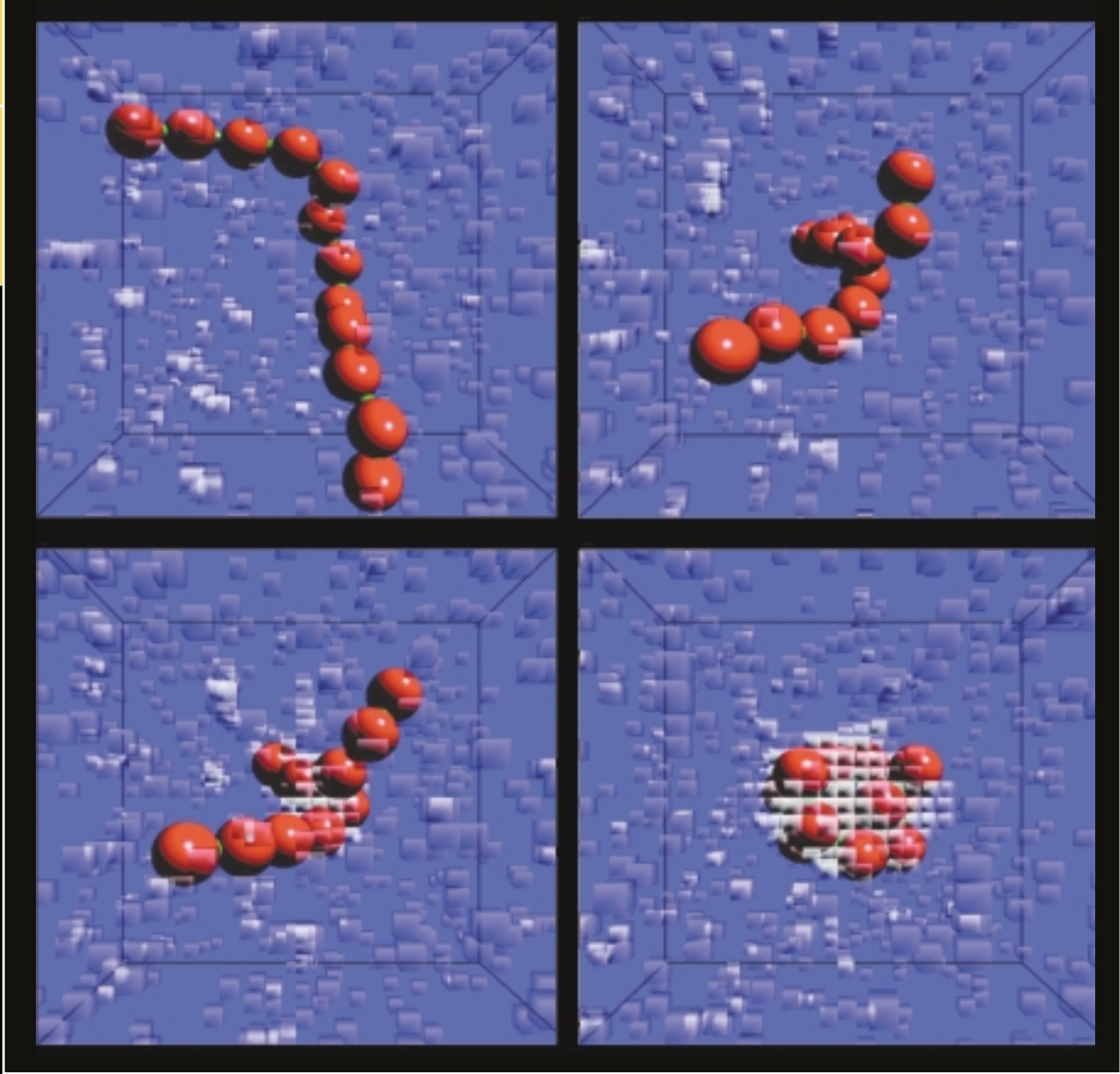
One of the signposts of change was the arrival of the Earth Simulator system in Japan. After only a few months of operation, this system has already made a profound impact on computational science and high performance computing in the U.S. This system broadened our horizon and gave us a glimpse of what kinds of simulations are possible at sustained

speeds in the range of tens of teraflop/s. During the summer and fall of 2002, our computational scientists held a series of town hall meetings using the Access Grid and defined their needs for future simulation capabilities. The Earth Simulator made us suddenly “think big” again in supercomputing, and I am thrilled that the DOE computational science community, in particular our NERSC users, are ready to lead the way to the next level of computational science.

The Earth Simulator also challenged our dependence in the U.S. on hardware platforms that are designed primarily for commercial applications. It exposed the “divergence problem,” the fact that scientific applications obtain only a small fraction of the peak performance of current platforms, and that this ratio seems to be getting even smaller. One of the highlights of 2002 at NERSC was a workshop with IBM and Argonne National Laboratory that produced a proposal on how to change this situation. In particular the workshop defined the “Blue Planet” system, and more fundamentally it was able to produce a whole new strategy for creating science-driven computer architecture that may change the future of high performance computing in the U.S.

This workshop also brought out what is for me the best of NERSC: a great team of dedicated staff who within a few weeks are able to rise to the challenge and produce a new way of thinking about a problem. My special thanks and congratulations, as always, go to the NERSC staff for their skill, dedication, and tireless efforts to make NERSC the best scientific computing resource in the world.

Horst D. Simon  
NERSC Center Division Director



## SCIENCE HIGHLIGHTS

*NERSC is the principal provider of high performance computing services to laboratory and university researchers whose work advances the mission of DOE's Office of Science (DOE SC). Our mission is to accelerate the pace of scientific discovery by providing high performance computing tools to tackle science's biggest and most challenging problems, and to play a major role in advancing large-scale computational science and computing and networking technology.*

*This section of the Annual Report presents some of the scientific advances achieved with NERSC's support during the past year, from the demanding science-of-scale projects, to research affiliated with the Scientific Discovery through Advanced Computing (SciDAC) program, to a representative selection of research funded by DOE SC's five offices—Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy and Nuclear Physics, and Advanced Scientific Computing Research. This year, rather than giving overviews of entire projects as we have in the past, we focus in most cases on publications whose results demonstrate the contributions of computation to the advancement of science. Investigators listed include the NERSC and SciDAC project leaders.*



# Science-of-Scale Projects

To promote the productivity of cutting-edge science, NERSC adapts its systems to provide the resources needed by data-intensive applications and provides "Red Carpet" support to large-scale strategic projects so that they can make rapid progress. These projects typically need support such as very large computing allocations, very large scratch disk, terabytes of usable memory and support for 64-bit computing, large-scale visualization, consulting support to make effective use of these resources, good bandwidth between the resources, and large archival storage.

The projects described below show how the unique resources of the IBM SP combined with excellent consulting support have produced scientific breakthroughs. They also demonstrate the size of the resources needed for rapidly growing, data-intensive projects. Three of these projects could have used all of NERSC's resources in FY 2002.

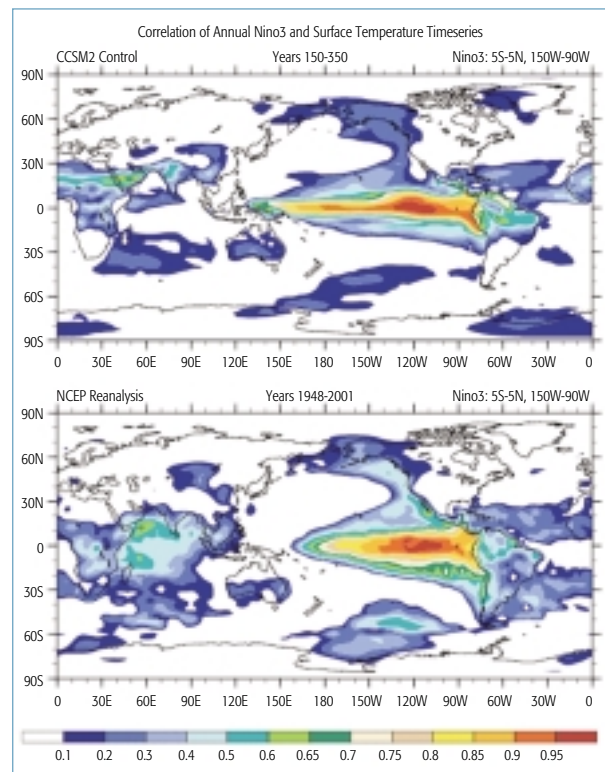
## DOE Climate Change Prediction Program

Scientists in the DOE Climate Change Prediction Program recently completed a 1,000-year run of a powerful new climate system model on a supercomputer at NERSC. The millennium-long simulation of the new Community Climate System Model (CCSM2) ran for more than 200 uninterrupted days on the IBM SP supercomputer at NERSC. The lengthy run served as a kind of "shakedown cruise" for the new version of the climate model and demonstrated that its variability is stable, even when run for century-after-century simulations. The 1,000-year CCSM2 run had a total drift of just one-half of one degree Celsius, compared to older versions with two to three times as much variance.

A 1,000-year simulation demonstrates the ability of CCSM2 to produce a long-term, stable representation of the earth's climate (Figure 1). Few if any climate models in the world can

make this claim, since all previous simulations contained drifts too large to allow complete, uncorrected simulations to 1,000 years. In addition, the simulation provides scientists with a database to analyze the variability of weather and climate on time scales ranging from interannual to interdecadal to intercentennial. Few datasets exist which are as comprehensive as the one produced during this simulation.

CCSM2 tightly couples four complex models, including atmosphere and land modeling codes developed at the National Center for Atmospheric Research (NCAR) and ocean and sea ice models developed at Los Alamos National Laboratory. Computationally, the full CCSM2 code consists of five binaries which are organized to execute concurrently within a single job. The models exchange data at various frequencies appropriate to the physical, large-scale processes being simulated. CCSM2



**FIGURE 1** Two hundred years of modeling El Niño events and surface temperatures on the Community Climate System Model (CCSM2) closely correlate with 50 years of actual climate data.

requires 4.5 wall-clock hours on 144 1.5-Gflops CPUs of the NERSC IBM SP to complete one simulated year. NERSC gave CCSM2 special queue priority to complete this project in a timely fashion. Preliminary results of 800 model years were presented to 250 participants at the Seventh Annual CCSM Workshop held in Breckenridge, Colorado, on June 25–27, 2002.

**INVESTIGATORS** W. Washington, P. Gent, J. Hack, J. Kiehl, G. Meehl, and P. Rasch, National Center for Atmospheric Research; B. Semtner, Naval Postgraduate School; J. Weatherly, U.S. Army Cold Regions Research and Engineering Lab Laboratory.

**PUBLICATION** J. T. Kiehl and P. Gent, "The Control Climate Simulation from the Community Climate System Model (CCSM2)" (in preparation).

**URL** <http://www.cesm.ucar.edu/index.html>

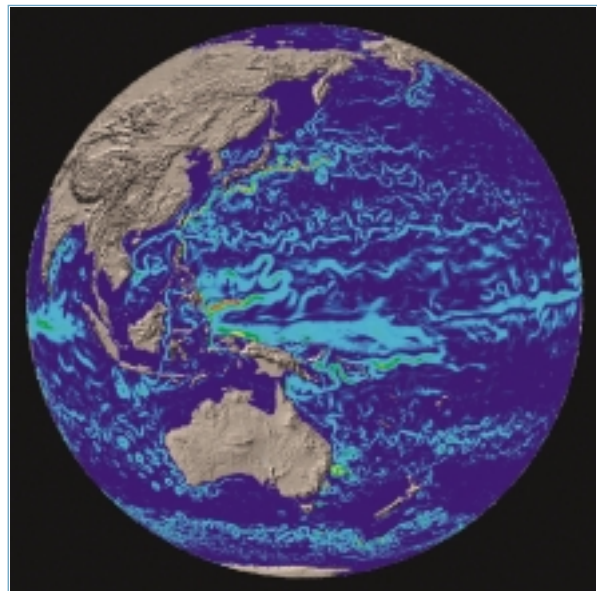
## High-Resolution Global Coupled Ocean/Sea Ice Modeling

The objective of this project is to couple a high-resolution ocean general circulation model with a high-resolution dynamic-thermodynamic sea ice model in a global context. Currently, such simulations are typically performed with a horizontal grid resolution of about 1 degree. At this resolution (about 30 to 50 km in the polar regions), the ocean model cannot resolve very narrow current systems (including fronts and turbulent eddies) that play a crucial role in the transport of heat and salt in the global ocean. Similarly, lower-resolution sea ice models cannot resolve important dynamics that occur in regions of complicated topography (such as the Canadian Archipelago).

This project is running a global ocean circulation model with horizontal resolution of approximately 1/10th degree—between 11 km and 2.5 km (Figure 2). This is the highest-resolution simulation even attempted with a such a realistic model. This configuration has dimensions of  $3600 \times 2400 \times 40$ , resulting in 177 million active ocean grid points (some grid points are on land). The code being used is the Parallel Ocean Program (POP), developed at LANL under the Department of Energy's CHAMMP program. At NERSC, 448 processors are used to run the model. One year can be simulated in about eight wall-clock days (86,000 processor hours), generating over 500 GB of output. Eight model years have been run to date,

with a goal of 30–50 years. After the ocean simulation has run for 10–15 model years, it will be coupled with a sea ice model to more accurately simulate the polar circulation.

The interaction of the ocean and overlying sea ice in global coupled numerical models is poorly understood, though very important. When ocean water freezes into sea ice, salt is released into the upper ocean, making it more dense. Conversely, when the ice melts, it creates a layer of fresh water that is less dense than the underlying ocean. This delicate balance between melting and freezing is very difficult to simulate with coarse grids. In particular, high vertical resolution is needed near the surface to simulate this salinity balance correctly. High horizontal resolution is required to properly simulate the current systems that advect these salinity anomalies into the open ocean. Inaccuracies in the surface ocean properties due to poor representation of ocean-ice interaction can have wide-ranging global consequences. Most notable is the possibility that too much fresh surface water can inhibit vertical convection in the northern seas (since it is less dense than the salty water beneath it), which then disrupts the entire global heat budget. Coarse-resolution simulations have found that the circulation and heat budget are extremely sensitive to the way sea ice is prescribed in ocean-only runs. The best tool for simulating the global circulation accurately is a high-resolution, fully coupled ocean-sea ice model.



**FIGURE 2** High-resolution (1/10 degree) POP ocean model currents at 50m depth. Blue = 0; red > 150 cm/s.



**INVESTIGATORS** M. E. Maltrud and E. C. Hunke, Los Alamos National Laboratory; J. L. McClean, Naval Postgraduate School.

**PUBLICATION** In preparation.

**URL** <http://www.lanl.gov/orgs/t/t3/codes/pop.shtml>

## Supernova Explosions and Cosmology

This collaboration brings together the SciDAC Supernova Science Center and the members of the PHOENIX/SYNPOL collaboration. The goal is a better understanding of supernovae of all types through simulation and model validation. Specific objectives are to clarify the physics of supernova explosions, to improve the reliability of such explosions as calibrated standard candles, and to measure fundamental cosmological parameters. Despite decades of research and modeling, no one understands in detail how supernovae work. The problem persists largely because, until recently, computer resources have been inadequate to carry out credible multi-dimensional calculations.

On June 4, 2002, at the American Astronomical Society meeting in Albuquerque, N.M., Michael Warren and Chris Fryer from Los Alamos National Laboratory presented the results of one of several projects in this collaboration, the first 3D supernova explosion simulation, based on computation at NERSC (Figure 3). This research eliminates some of the doubts about earlier 2D modeling and paves the way for rapid advances on other questions about supernovae.

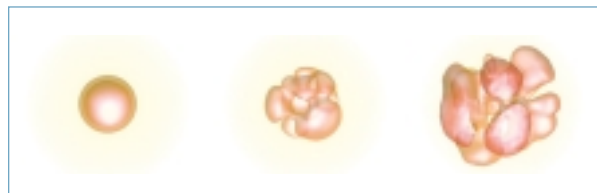
Earlier one-dimensional simulations of core-collapse supernovae almost always failed to explode. Two-dimensional simulations were qualitatively different from 1D, leading to a robust explosion without fine-tuning of the star's physical properties. They showed that the explosion process is critically dependent on convection, the mixing of the matter surrounding the iron core of the collapsing star. It was believed that the results could again be changed radically by adding a third dimension, but the 3D simulations turned out to be similar to the 2D results. The explosion energy, explosion time scale, and remnant neutron star mass do not differ by more than 10 percent between the 2D and 3D models. With these 3D results, researchers are ready to attack more exotic problems that involve rotation and non-symmetric accretion.

The 3D simulation used a parallel smooth particle hydrodynamics (SPH) code coupled with a flux-limited diffusion radiation transport. Supernova calculations are computationally demanding because many processes, involving all

four fundamental forces of physics, must be modeled and followed for more than 100,000 time steps. Typical simulations (1 million particles) took about three months on the IBM SP at NERSC.

In the next five years, the Supernova Cosmology Project and the Nearby Supernova Factory experiments will increase both the quality and quantity of observational supernova data at low and high redshift by several orders of magnitude. The purpose of these experiments is to improve the use of supernovae as tools for cosmology by determining the underlying physics behind these catastrophic events and to utilize these tools to help us understand the dark energy that drives the acceleration of the universe. The only way to fully exploit the power of this amazing data set is to make a similar order-of-magnitude improvement in computational studies of supernovae, via spectrum synthesis and radiation hydrodynamics. The focus of the PHOENIX/SYNPOL collaboration's portion of this project is to start the process of creating 3D spectrum synthesis models of supernovae (Figure 4) in order to constrain the observations and place limits on the explosion models and progenitors of supernovae using the full-physics 1D models as a guide.

Currently two sets of spectrum synthesis codes, PHOENIX and SYNPOL, are used at NERSC to study the model atmospheres of supernovae. PHOENIX models astrophysical plasmas in one dimension under a variety of conditions, including differential expansion at relativistic velocities found in supernovae. The current version solves the fully relativistic radiative transport equation for a variety of spatial boundary conditions in both spherical and plane-parallel geometries for both continuum and line radiation simultaneously and self-consistently using an operator splitting technique. PHOENIX also solves the



**FIGURE 3** Computer visualization shows (left to right) three stages of a simulated supernova explosion over a period of 50 milliseconds, starting about 400 milliseconds after the core begins to collapse. The surfaces show the material which is flowing outward at a speed of 1,000 kilometers/second. Left is the initial spherical implosion. Center, as in-falling gas approaches the core, it is exposed to a higher and higher influx of neutrinos that heat the gas and make it buoyant. Right, as more cold gas sinks in, it is heated and rises, resulting in enough convective energy transfer to create an explosion.

full multi-level non-local thermodynamic equilibrium (NLTE) transfer and rate equations for a large number of atomic species (with a total of more than 10,000 energy levels and more than 100,000 primary NLTE lines), including non-thermal processes. PHOENIX accurately solves the fully relativistic radiation transport equation along with the non-LTE rate equations (currently for ~150 ions) while ensuring radiative equilibrium (energy conservation).

SYNPOL is a 3D radiative transfer code to study the spectropolarimetry of supernovae. It is based on a Monte Carlo treatment of line formation via the Sobolev approximation and includes electron scattering. Because SYNPOL does not solve rate equations and does not do continuum transfer, it is not used for quantitative abundance determinations or for absolute flux calculations. Rather its value lies in establishing line identifications (the intervals of ejection velocity within which the presence of particular ions is detected) and in probing the geometry of the supernova and its ejecta. For a full 3D run, with signal-to-noise and resolution an order of magnitude greater than the observational data, approximately  $10^{12}$  photons are generated within a Cartesian grid of 300 per side. Due to the size of the atomic data—over 42 million lines whose strengths can vary at each cube in the grid—the memory requirements and the time it takes to process the scattering of such a large number of photons are quite large: 1 million CPU hours for a 3D simulation with simplified physics, and 10 GB input and 1 GB

output per iteration, with 20 iterations per star model for 20 to 30 models.

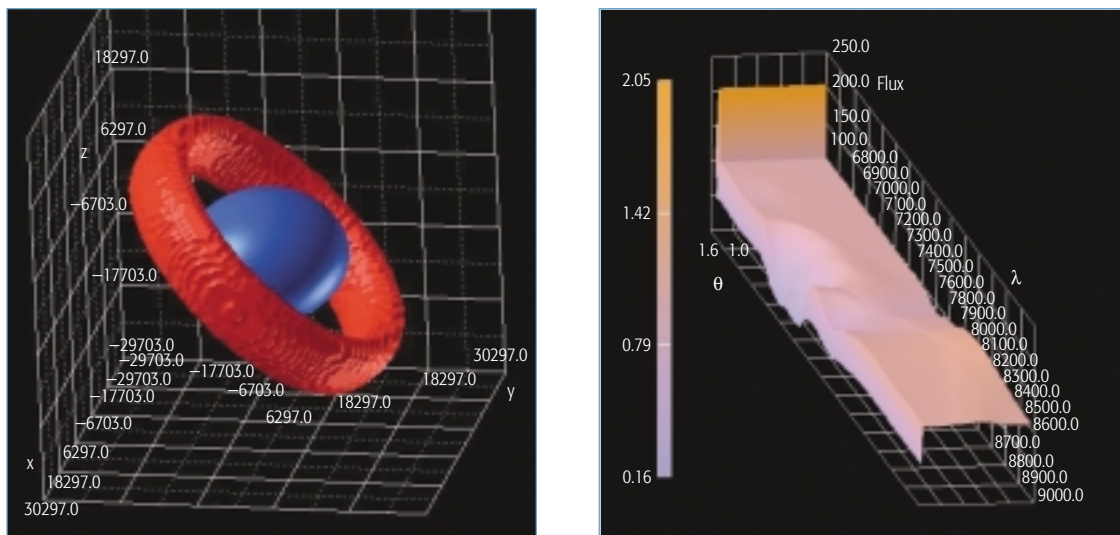
NERSC provided a new 24-hour run queue to accommodate this simulation. Within the next two or three years, 100 times more CPUs will be needed to run 3D simulations with complex physics if there are no algorithmic improvements.

**INVESTIGATORS** P. Nugent, D. Kasen, and S. Perlmutter, Lawrence Berkeley National Laboratory; S. Woosley and G. Glatzmaier, University of California, Santa Cruz; P. Hauschildt, J. Aufdenberg, C. Shore, A. Schweitz, and T. Barman, University of Georgia; E. Baron, University of Oklahoma; T. Clune, Goddard Space Flight Center; A. Burrows, S. Hariri, A. Hungerford, P. Pinto, H. Sarjoughian, and B. Ziegler, University of Arizona; T. Evans, C. Fryer, M. Gray, W. Miller, and M. Warren, Los Alamos National Laboratory; F. Dietrich and R. Hoffman, Lawrence Livermore National Laboratory.

**PUBLICATIONS** C. L. Fryer and M. S. Warren, "Modeling core-collapse supernovae in three dimensions," *Astrophysical Journal* **574**, L65 (2002).  
C. L. Fryer, D. E. Holz, and S. A. Hughes, "Gravitational wave emission from core collapse of massive stars," *Astrophysical Journal* **565**, 430 (2002).

D. N. Kasen, P. E. Nugent, L. Wang, and D. A. Howell, "Interpreting supernova polarization spectra," *Bulletin of the American Astronomical Society* **33**, 8409.

**URLS** <http://www.supersci.org/>  
<http://www.lbl.gov/~nugent>



**FIGURE 4** A spectrum synthesis calculation of a supernova atmosphere surrounded by a toroid. The layout of the atmosphere is presented on the left, while at the right is a graph of the flux vs. wavelength vs. viewing angle. As the viewing angle shifts towards the toroid, the strength of the absorption increases dramatically. Data that confirm such a model would for the first time put strong constraints on the progenitors of Type Ia supernovae. Such flux features are seen in the spectrum of SN 2001el.



## Black Hole Merger Simulations

Physicists at the Max Planck Institute for Gravitational Physics are performing simulations of the spiraling coalescence of two black holes, a problem of particular importance for interpreting the gravitational wave signatures that will soon be seen by new laser interferometric detectors around the world. Detection of the first gravitational waves (or failure to do so) will strongly test Einstein's Theory of General Relativity, the results of which will have ramifications that extend throughout the world of physics. The Cactus simulation code is being used to perform the calculations. This is the first time ever that a spiraling merger of this type has been accurately simulated (Figure 5). The results so far indicate that the Meudon model for coalescence seems to match the simulation data more accurately than the competing Cook-Baumgarte model.

Collisions between black holes should theoretically create propagating gravitational waves, similar to the electromagnetic waves given off by distant stars. These ripples in space-time should be seen as subtle variations in the length of objects as they move through space. Recently built laser interferometric detectors such as LIGO and VIRGO are capable of measuring these subtle ripples in space. However, the gravitational wave signal that can be detected by these interferometers is so faint that it is very close to the level of noise in these devices. So simulations of the kinds of events that might produce gravitational waves can provide important insights into the gravitational wave signature produced by these events, potentially making the instruments more productive.

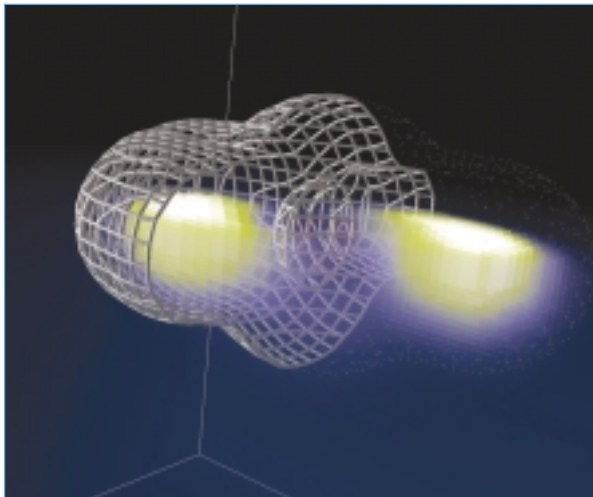


FIGURE 5 Visualization of binary black hole inspiral.

The Cactus code performs a direct evolution of Einstein's equations, which are a system of coupled nonlinear elliptic hyperbolic equations that contain thousands of terms if fully expanded. Consequently, the simulation resource requirements are enormous just to do the most basic of simulations. The simulations have been limited by both the memory and CPU performance of supercomputers as they attempt to move from calibrating against analytic black hole solutions to non-analytic astrophysically relevant cases in full 3D. The spiraling merger is just such a non-analytic case.

These simulations must use more than one-third of the NERSC IBM SP's available aggregate memory of 4.3 TB in order to achieve the resolution required to accurately simulate these phenomena. This simulation uses 1.5 TB of memory and more than 2 TB of disk space for each run. These runs typically consume 64 of the large-memory nodes of the SP (a total of 1,024 processors) for 48 wall-clock hours at a stretch. The simulation can use all 184 nodes, but this would only allow simulations that are fractionally larger than using the large-memory nodes due to memory/load-balancing issues.

NERSC provided access to a special queue to improve turnaround, opened ports to allow remote steering and Grid access, and provided consulting support for 64-bit integration and code debugging. In the space of two months, this simulation consumed 700,000 CPU hours, simulating three-fourths of a full orbit before coalescence. In the near future, this project could use 10 TB of disk for each run, 5 TB of uniform, user-available memory, and 15 million CPU hours.

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**INVESTIGATORS** E. Seidel, M. Alcubierre, G. Allen, B. Brügmann, P. Diener, D. Pollney, T. Radke, and R. Takahashi, Max Planck Institute for Gravitational Physics; J. Shalf, Lawrence Berkeley National Laboratory.

**PUBLICATIONS** M. Alcubierre, B. Brügmann, P. Diener, M. Koppitz, D. Pollney, E. Seidel, and R. Takahashi, "Gauge conditions for long-term numerical black hole evolutions without excision," *Phys. Rev. D* (in press). M. Alcubierre, B. Brügmann, P. Diener, F. Guzman, S. Hawley, M. Koppitz, D. Pollney, and E. Seidel, "Dynamical evolution of binary black hole data," in preparation (2002).

**URL** <http://www.aei-potsdam.mpg.de/>



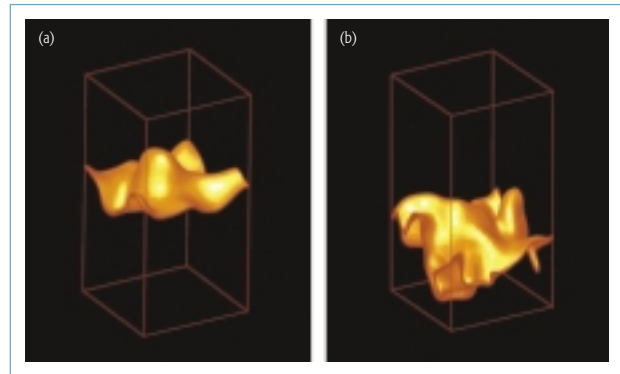
The DOE Office of Science (SC) initiated the Scientific Discovery through Advanced Computing (SciDAC) program in 2001 to achieve three goals: (1) create a new generation of **scientific challenge codes** for terascale computers that can address the most critical scientific problems in SC's research programs; (2) create the **mathematical and computing systems software** to enable the scientific challenge codes to take full advantage of the extraordinary capabilities of terascale computers; and (3) create the **laboratory software infrastructure** to enable geographically separated scientists to effectively work together as a team as well as provide electronic access to both facilities and data.

In addition to computing resources, NERSC is providing specialized consulting and algorithmic support (see page 61 below) for many SciDAC projects, including several Integrated Software Infrastructure Centers (ISICs). This section highlights some of the initial accomplishments of these SciDAC projects as well as closely related research by SciDAC investigators conducted on NERSC systems.

## Applied Partial Differential Equations

The Applied Partial Differential Equations Center (APDEC) is an ISIC that aims to develop a high-performance algorithmic and software framework for solving partial differential equations arising from problems in three important mission areas for the DOE Office of Science: magnetic fusion, accelerator design, and combustion. This framework will provide a new set of simulation capabilities based on locally structured grid methods.

APDEC's major accomplishment in 2002 was the first fully resolved direct numerical simulation of turbulent methane combustion with comprehensive chemistry and transport (19 reacting species, 84 reactions). These simulations allowed researchers from Berkeley Lab's Center for Computational



**FIGURE 1** Volume-rendered image showing surface of maximum heat release for the weak (a) and strong (b) turbulence cases.

Sciences and Engineering (CCSE) to examine the basic structure of the flame, including turbulent flame speed and flame surface area, and to investigate the effect of turbulence-flame interaction on the flame chemistry. The results indicate that flame wrinkling is the dominant factor leading to the increased turbulent flame speed (Figure 1). Future work will include a broader range of turbulence scales, more detailed methane mechanisms, and a range of configurations relevant to lean premixed combustion experiments, such as turbulent jets and swirl burners.

**INVESTIGATORS** P. Colella and J. Bell, Lawrence Berkeley National Laboratory; D. Brown, Lawrence Livermore National Laboratory; M. Berger, New York University; R. Leveque, University of Washington; M. Minion, University of North Carolina; G. Puckett, University of California, Davis; C. Rutland, University of Wisconsin.

**PUBLICATION** J. B. Bell, M. S. Day, and J. F. Grcar, "Numerical simulation of premixed turbulent methane combustion," Proceedings of the Combustion Institute (in press); Berkeley Lab report LBNL-49331 (2002).

**URL** <http://davis.lbl.gov/APDEC/>

## DOE Science Grid

This SciDAC collaboration is working to define, integrate, deploy, support, evaluate, refine, and develop the persistent Grid services needed for a scalable, robust, high-performance DOE Science Grid. It will create the underpinnings of the software

environment that the SciDAC applications need to enable innovative approaches to scientific computing through secure remote access to online facilities, distance collaboration, shared petabyte datasets, and large-scale distributed computation.

In its first year, the project has focused on one of the biggest problems in large-scale collaborations: a common authentication and security approach that allows researchers from all over the world to securely collaborate and share resources. The DOE Science Grid and ESnet have developed a formal approach to issuing and managing identity certificates in order to support worldwide science collaborations. This process has been put into place for several DOE science collaborations, including several international high energy physics collaborations involving European Union Data Grid sites. As a result, high energy physicists in the U.S. and Europe are now securely collaborating and sharing science resources.

In a related issue, many scientific institutions use firewalls to protect their internal networks and resources. The Science Grid is developing procedures for establishing the trust that is necessary to open up firewalls to Grid applications. These procedures have been tested and accepted by the DOE Science Grid sites (Lawrence Berkeley, Argonne, Oak Ridge, and Pacific Northwest national laboratories and NERSC) and are being formalized so that they may be used with other collaborating institutions.

Several applications are being prototyped on Science Grid compute resources, including a regional air quality model and a supernova cosmology data analysis application. Several Grid

R&D technology integration projects are also making good progress, including the Python-wrapped Globus services toolkit, which is being used to build some experimental Grid system administration tools. A Grid Portal Developers Workshop was held in Berkeley on June 4–5, 2002, allowing 24 developers from across the U.S. and Europe to share their latest ideas and accomplishments.

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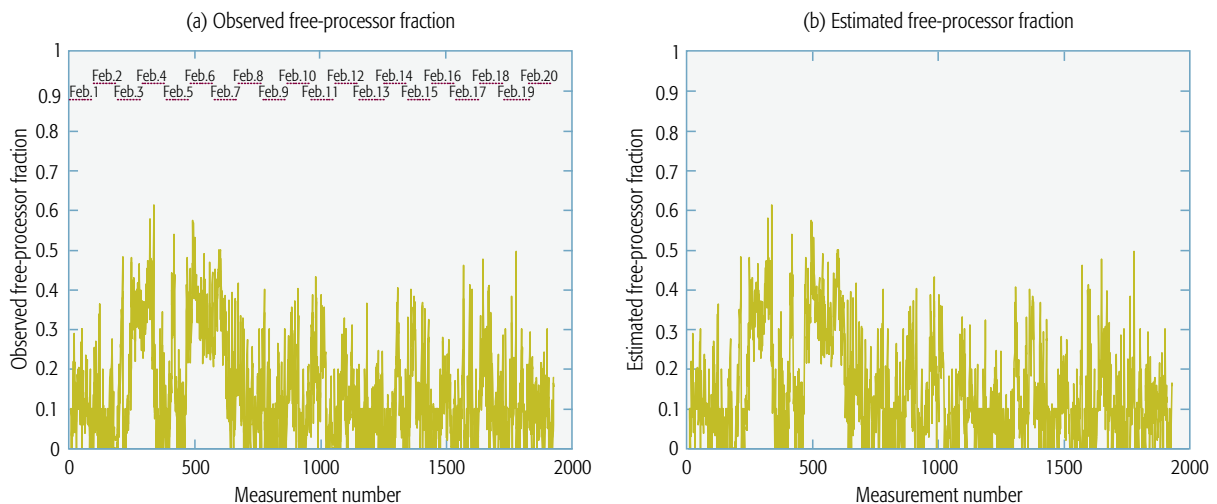
**INVESTIGATORS** W. E. Johnston, Lawrence Berkeley National Laboratory and NASA Ames Research Center; R. A. Bair, Pacific Northwest National Laboratory; I. T. Foster, Argonne National Laboratory; A. Geist, Oak Ridge National Laboratory; W. T. C. Kramer, Lawrence Berkeley National Laboratory/NERSC.

**PUBLICATION** W. E. Johnston, "Using computing and data grids for large-scale science and engineering," *Internatl. J. High Perf. Computing* Apps. 15, 223 (2001).

**URL** <http://doesciencegrid.org/>

## Performance Evaluation Research Center

The Performance Evaluation Research Center (PERC) is an ISIC whose goals are to develop a science for understanding performance of scientific applications on high-end computer systems, and to develop engineering strategies for improving performance on these systems.



**FIGURE 2** Estimation results for NERSC's IBM SP (Seaborg) with variable sample size: (a) observed free-processor fraction, (b) estimated free-processor fraction. Among the total 1,920 measurements, the estimation was within the required 8% accuracy 1,747 times, corresponding to an estimation success rate of 91%. The average sample size obtained was 46 processors, or 1.5% of the machine size.

One of PERC's first milestones was installation of the Hockney development platform at NERSC, one frame of an SP system donated by IBM and dedicated to the PERC effort. Named in honor of the late British computer scientist Roger Hockney, this system will be used for software testing and development. Other PERC accomplishments included analyzing the key codes EVH1, AORSA3D, PCTM, CCSM2.0, MILC, and pVarDen, identifying changes to improve performance in many cases; developing a highly effective tool for modeling performance of large-scale codes; developing a data-dependent memory tracing tool; and developing a Fortran interface for a performance assertion prototype.

A joint PERC/Los Alamos Computer Science Institute/NSF project addressed the growing problem of monitoring systems with thousands of components. In the resulting publication, Mendes and Reed proposed a new technique for monitoring large systems based on statistical sampling. Instead of checking every system component individually, they select a statistically valid subset of components, inspect this subset in detail, and derive estimates for the whole system based on the properties found in the subset. Their experiments demonstrated the effectiveness of these techniques for estimating the fraction of available processors in parallel machines (Figure 2), the fraction of network sites reachable from a certain point, and the mean latency expected from that point to the rest of the network. These results show that one can reliably estimate the state of a large system at a small fraction of the cost required by traditional monitoring schemes. This cost reduction, in turn, can enable measurements that would be impractical by regular means, and can also enable the use of more powerful algorithms for system management and for optimized resource utilization.

**INVESTIGATORS** D. H. Bailey and E. Strohmaier, Lawrence Berkeley National Laboratory; J. Dongarra, University of Tennessee; D. A. Reed, University of Illinois; D. Quinlan, B. de Supinski, and J. Vetter, Lawrence Livermore National Laboratory; P. Worley and T. Dunigan, Oak Ridge National Laboratory; P. Hovland and B. Norris, Argonne National Laboratory; J. Hollingsworth, University of Maryland; A. Snively, San Diego Supercomputer Center.

**PUBLICATION** C. L. Mendes and D. A. Reed, "Monitoring large systems via statistical sampling," *Proc. of LACSI Symposium 2002*, Santa Fe, NM, October 2002.

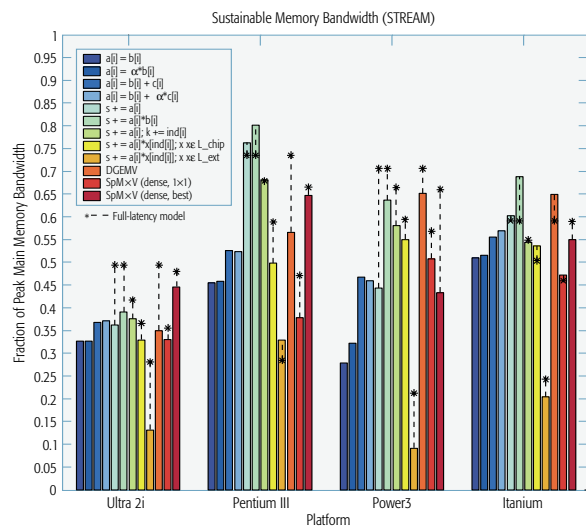
**URL** <http://perc.nersc.gov/>

## Terascale Optimal PDE Simulations

The Terascale Optimal PDE Simulations (TOPS) ISIC is researching and developing and will deploy a toolkit of open-source solvers for the nonlinear partial differential equations (PDEs) that arise in many application areas, including fusion, accelerator design, global climate change, and the collapse of supernovae. These algorithms aim to reduce computational bottlenecks by one or more orders of magnitude on terascale computers, enabling scientific simulation on a scale heretofore impossible.

One of the major TOPS activities in 2002 involved the magnetohydrodynamics (MHD) code M3D (see below, page 18). A Hypr algebraic multigrid solver was ported into M3D underneath the existing PETSc interface, and scalability studies were done on M3D production runs. PETSc itself, a suite of data structures and routines for solving PDEs, is undergoing performance tuning and testing on terascale applications.

The Berkeley Benchmarking and Optimization Group (BeBOP) successfully achieved over 80% of the modeled peak Mflop/s for performance-tuned models of sparse matrix-vector products and sparse triangular solutions on the IBM SP Power 3 processor nodes at NERSC (Figure 3). The model estimates the best possible performance for a computer's memory system. This translates to 15–20% of the processor's peak performance, a good gain over previous codes.



**FIGURE 3** Memory bandwidth benchmark results. Asterisks show the model bandwidth computed for each of the last eight bars (non-standard STREAM kernels).

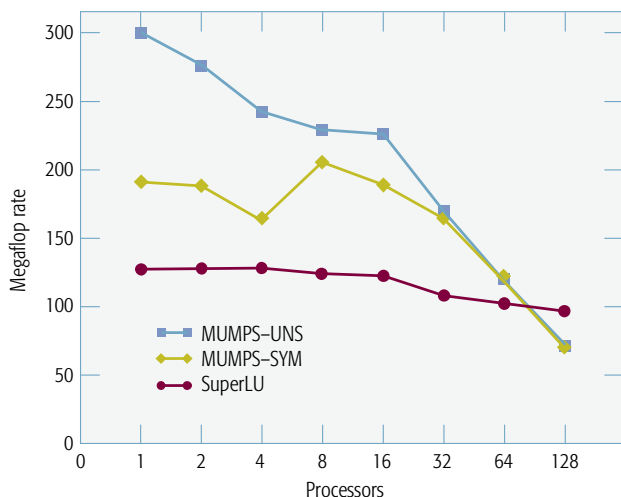


FIGURE 4 Megaflop rate per processor (cubic grids, nested dissection).

Amestoy et al. conducted a comprehensive study and comparison of two state-of-the-art direct solvers for large sparse sets of linear equations on large-scale distributed-memory computers. One is a multifrontal solver called MUMPS, the other is a supernodal solver called SuperLU. The authors described the main algorithmic features of the two solvers and compared their performance characteristics with respect to uniprocessor speed, interprocessor communication, memory requirements, and scalability (Figure 4). They found that both solvers have strengths and weaknesses.

**INVESTIGATORS** D. Keyes, Old Dominion University; B. Smith and J. More, Argonne National Laboratory; E. G. Ng, Lawrence Berkeley National Laboratory; R. Falgout, Lawrence Livermore National Laboratory; J. W. Demmel, University of California, Berkeley; O. Ghattas, Carnegie Mellon University; O. Widlund, New York University; S. McCormick, University of Colorado, Boulder; J. Dongarra, University of Tennessee.

**PUBLICATIONS** R. Vuduc, J. W. Demmel, K. A. Yelick, S. Kamil, R. Nishtala, and B. Lee, "Performance optimizations and bounds for sparse matrix-vector multiply," *Proc. of the IEEE/ACM Conference on Supercomputing*, 2002.

P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li, "Analysis and comparison of two general sparse solvers for distributed memory computers," *ACM Transactions on Mathematical Software* 27, 388 (2001).

URL <http://www.mcs.anl.gov/scidac-tops>

## Advanced Methods for Electronic Structure

This project is working to advance the capabilities of quantum chemical methods to describe efficiently and with controllable accuracy the electronic structure, statistical mechanics, and dynamics of atoms, molecules, and clusters.

One example of molecular dynamics being studied is hydrophobic interactions. For nearly a half century, hydrophobic interactions have been considered the primary cause for self-assembly in soft matter and a major source of stability in biophysical assembly. Studying these interactions in perhaps their most basic form, ten Wolde and Chandler used computer simulation to demonstrate the mechanism for the collapse of a hydrophobic polymer in water (Figure 5). They found that the mechanism of collapse is much like that of a first-order phase transition. The evaporation of water in the vicinity of the polymer provides the driving force for collapse, and the rate limiting step is the nucleation of a sufficiently large vapor bubble. This study suggests that the kinetic effects of changing pressure may play an important role in the hydrophobic interactions of protein folding.

This simulation was made possible by transition path sampling and a coarse-grained treatment of liquid water. The use

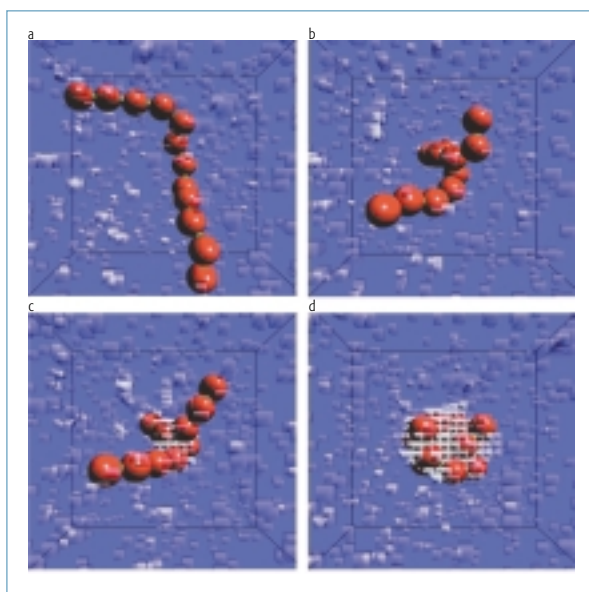


FIGURE 5 Four configurations from a 1.5 ns trajectory in which a 12-unit hydrophobic chain in water collapses from an extended coil to a compact globule. Transparent cubes denote vapor cells.



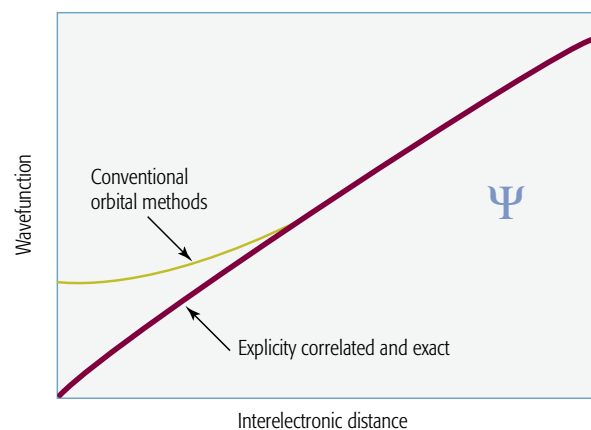
of a statistical field model of water allows the simulation of solvent dynamics over large length and time scales that would be impractical to study with purely atomistic simulation. Spatially complex small length-scale fluctuations were analytically integrated out, thus removing the most computationally costly features from the simulation.

**INVESTIGATORS** R. J. Harrison, Oak Ridge National Laboratory; M. Head-Gordon, University of California, Berkeley, and Lawrence Berkeley National Laboratory; W. D. Allen and H. F. Schaefer III, University of Georgia; W. C. Ermler, University of Memphis; J. W. Evans, M. S. Gordon, R. A. Kendall, K. Ruedenberg, and M. W. Schmidt, Iowa State University/Ames Laboratory; W. S. Gray, Old Dominion University; M. Minkoff, R. Shepard, and A. F. Wagner, Argonne National Laboratory; D. L. Thompson, Oklahoma State University.

**PUBLICATION** P. R. ten Wolde and D. Chandler, "Drying-induced hydrophobic polymer collapse," *PNAS* **99**, 6539 (2002).

## Explicitly Correlated Methods for Computations of Properties to Chemical Accuracy

The goal of this project is to develop efficient methods for incorporating dynamical electron correlation effects into molecular quantum mechanics by using basis sets that depend explicitly on the interelectronic distance ( $R_{12}$ ). This will allow extremely high accuracy in calculating the electronic



**FIGURE 6** Achieving the full promise of molecular quantum mechanics through next-generation, explicitly correlated electronic structure methods.

## ROBERT HARRISON RECEIVES 2002 SIDNEY FERNBACH AWARD

Robert J. Harrison, an internationally recognized quantum chemist who is the principal architect of the Northwest Computational Chemistry Software (NWChem), has received the IEEE Computer Society's 2002 Sidney Fernbach Award. The Fernbach Award recognizes outstanding contributions in the application of high performance computers using innovative approaches.



In his nomination of Harrison for the award, NERSC Director Horst Simon noted that NWChem, the first computational quantum chemistry software with algorithms specifically designed for massively parallel computers, "has the potential to revolutionize the discipline." Harrison, co-PI of the Advanced Methods for Electronic Structure SciDAC project, worked at Pacific Northwest National Laboratory before joining the staff at Oak Ridge National Laboratory this past summer. He is a member of NERSC's Computational Review Panel.

structure of atoms, molecules, and clusters (Figure 6) while dramatically reducing the number of basis functions needed to describe the electron-electron correlation cusp, thus dramatically reducing the computational costs.

The first application of the MP2-R12/A code was published in a study of the second-order Møller-Plesset limit for the barrier to linearity of water. Here, the basis set limit to the barrier of linearity of water was computed and found to match well with the most recent empirical value. The authors found that basis functions with orbital quantum number higher than 3 (i.e.,  $g$  and higher) are essential for spectroscopic accuracy. This finding differs from previous claims that computations saturated only to the  $f$  level were all that is necessary for spectroscopic accuracy with explicitly correlated approaches. Ongoing research seeks to approach the basis set limit via

plane wave expansions (that is, basis sets are constructed so as to saturate each angular momentum level sequentially) in order to explore more fully the contribution of each level.

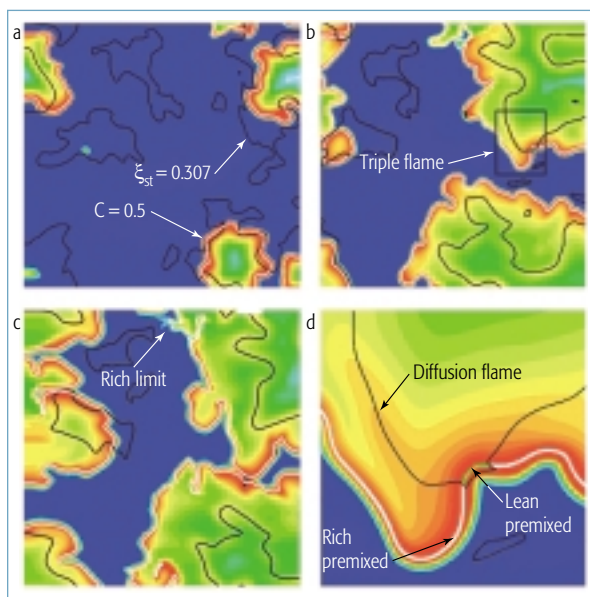
**INVESTIGATORS** H. F. Schaefer III, W. D. Allen, J. Kenny, N. Richardson, K. Sattelmeyer, and M. Schuurman, University of Georgia.

**PUBLICATION** E. F. Valeev, W. D. Allen, H. F. Schaefer III, and A. G. Császár, "The second-order Møller-Plesset limit for the barrier to linearity of water," *J. Chem. Phys.* **114**, 2875 (2001).

**URL** <http://zopyros.ccqc.uga.edu/scidac/scidac-intro.html>

## Terascale High-Fidelity Simulations of Turbulent Combustion with Detailed Chemistry

The objective of this program is to develop a high fidelity direct numerical simulation (DNS) software package for the



**FIGURE 7** Isocontours of the heat-release rates (log of heat release is presented to highlight both premixed and diffusion modes of combustion) at three time sequences of tile evolution of flame kernels (a–c) corresponding to times 0.061, 0.08, and 0.10 ms. Panel d is an inset of the second time frame to illustrate a triple flame structure. Also shown are isocontours of the stoichiometric mixture fraction (black lines) and isocontours of progress variable at 0.5 (to highlight the premixed flame fronts) (white lines for panels a–c). In panel d, lean and rich premixed flames are distinguished at the progress variable isocontour of 0.5 by white (for rich flames) and green (for lean flames) lines.

simulation of turbulent reactive flows. This capability is essential for realistic modeling of systems such as internal combustion engines and gas turbines. The focus is on including extensive new developments in an existing software package at Sandia National Laboratories named S3D to address more realistic combustion features and geometries while exploiting terascale computational possibilities.

In a DNS study of autoigniting non-homogeneous mixtures of hydrogen in heated air, Echehki and Chen found that high-temperature combustion follows an initial autoignition stage in fuel-lean, low-dissipation kernels. These kernels propagate initially as lean premixed fronts. As they expand into richer mixtures, diffusion flames develop in the wake of rich premixed flames along stoichiometric isocontours (Figure 7). These flames are initially stabilized by diffusion of radicals (H) and excess fuel from the rich premixed flames' side against excess radicals (O and OH) and oxidizer from the earlier passage of lean premixed fronts. In time, diffusion flames detach from the rich premixed flames, and their burning intensity is reduced accordingly. Triple flames also form at the interfaces of the rich and lean premixed flames with the stoichiometric mixture isocontours, but their contribution to the stabilization and burning intensity of the diffusion branches is insignificant.

Analysis of the simulations shows that the dominant contribution to the volumetric heat release is attributed to the lean and rich premixed flames, while the dominant contribution to NO formation is attributed to diffusion flames. The results also show that the relative contribution of the different burning modes is strongly dependent on the mixture distribution and the scalar dissipation rate field. The authors believe that these parameters affect the diffusion flames' structures and their rates of detachment from the rich premixed flames.

**INVESTIGATORS** A. Trouvé, University of Maryland; J. H. Chen, Sandia National Laboratories; H. G. Im, University of Michigan; C. J. Rutland, University of Wisconsin; S. Sanilevici and R. Reddy, Pittsburgh Supercomputing Center.

**PUBLICATION** T. Echehki and J. H. Chen, "High-temperature combustion in autoigniting non-homogeneous hydrogen/air mixtures," *Proc. Combustion Inst.* (in press).

**URL** <http://scidac.psc.edu/>

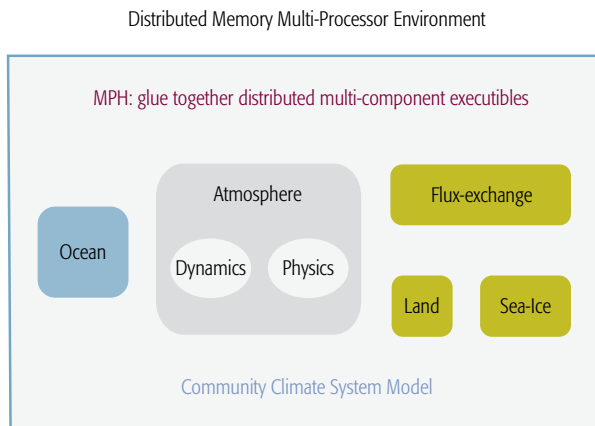


## Collaborative Design and Development of the Community Climate System Model for Terascale Computers

The multi-institutional team will develop, validate, document, and optimize the performance of a coupled climate model, the Community Climate System Model (CCSM), using the latest software engineering approaches, computational technology, and scientific knowledge. The portion of the research being conducted at NERSC involves optimizing the input/output, parallel communications and efficiency, and numerical reproducibility and stability of the code.

Coupled climate systems include atmosphere, ocean, land, and sea ice models coupled through the flux coupler (Figure 8). The component models are usually independently developed by different groups and remain as independent executables on parallel supercomputers. MPH, a multi-component handshaking library for climate and other applications, allows component models to recognize and talk to each other in a convenient and consistent way.

MPH provides component name registration, resource allocation, inter-component communication, inquiries on the multi-component environment, and other functions. It supports three integration mechanisms: multi-component multi-executable, multi-component single executable, and multi-component executable hierarchy. MPH is being used in CCSM and in Argonne National Laboratory's Model Coupling Toolkit.



**FIGURE 8** MPH integrates the components of CCSM to run efficiently on distributed-memory parallel computers.

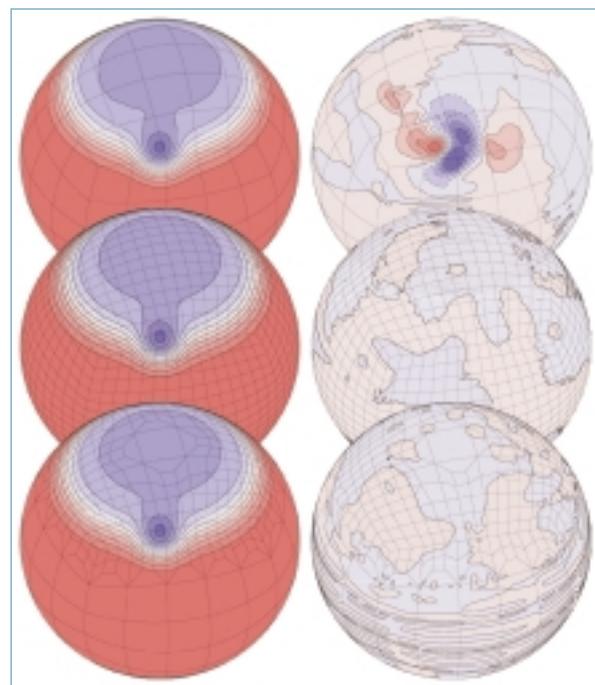
**INVESTIGATORS** R. C. Malone, Los Alamos National Laboratory; J. B. Drake, Oak Ridge National Laboratory; C. Ding, Lawrence Berkeley National Laboratory; I. Foster, Argonne National Laboratory; D. Rotman, Lawrence Livermore National Laboratory; M. Blackmon and W. Washington, National Center for Atmospheric Research.

**PUBLICATION** C. Ding and Y. He, "MPH: A library for distributed multi-component environment," *Proc. of the IEEE/ACM Conference on Supercomputing, 2001*; Berkeley Lab report LBNL-47930.

**URL** <http://www.scidac.org/CCSM/>

## Multi-Resolution Climate Modeling

This project will further develop and apply a spectral element model of the atmospheric general circulation for use as a component in a coupled climate model. The spectral element method allows higher resolution over a limited region within a global model. This method could improve climate and turbulence simulations by allowing increased resolution in a few dynamically significant areas, such as fronts or vortex filaments, while modeling the interaction between coarse- and fine-scale phenomena. Regional climate simulations may be



**FIGURE 9** Mesh refinement in the northern hemisphere: two uniform meshes (top and middle) and a locally refined mesh (bottom).

improved by allowing regional resolution to be incorporated within a global model in a two-way interactive fashion.

The advantages of the Spectral Element Atmosphere Model (SEAM) include its high-resolution accuracy, flexibility, and efficiency on parallel computers. Fournier et al. showed how local mesh refinement in SEAM can be used to study regional dynamics within a global model, without the usual recourse to interpolation, boundary value or flux fixing (Figure 9). By locally refining the element mesh, nearly the same-accuracy solution as a high-resolution computation can be computed with only 1/22 the number of elements and 3/4 of the time steps—a 94% saving of computational cost.

**INVESTIGATORS** F. Baer, A. Fournier, and H. Wang, University of Maryland; M. A. Taylor, Los Alamos National Laboratory; J. J. Tribbia, National Center for Atmospheric Research.

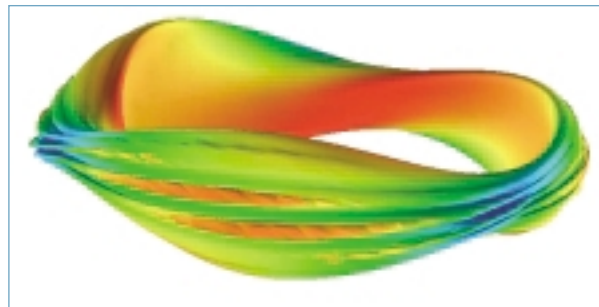
**PUBLICATION** A. Fournier, M. A. Taylor, and J. J. Tribbia, "The Spectral Element Atmosphere Model (SEAM): High-resolution parallel computation and localized resolution of regional dynamics" (in preparation).

**URL** <http://www.cgd.ucar.edu/gds/fournier/>

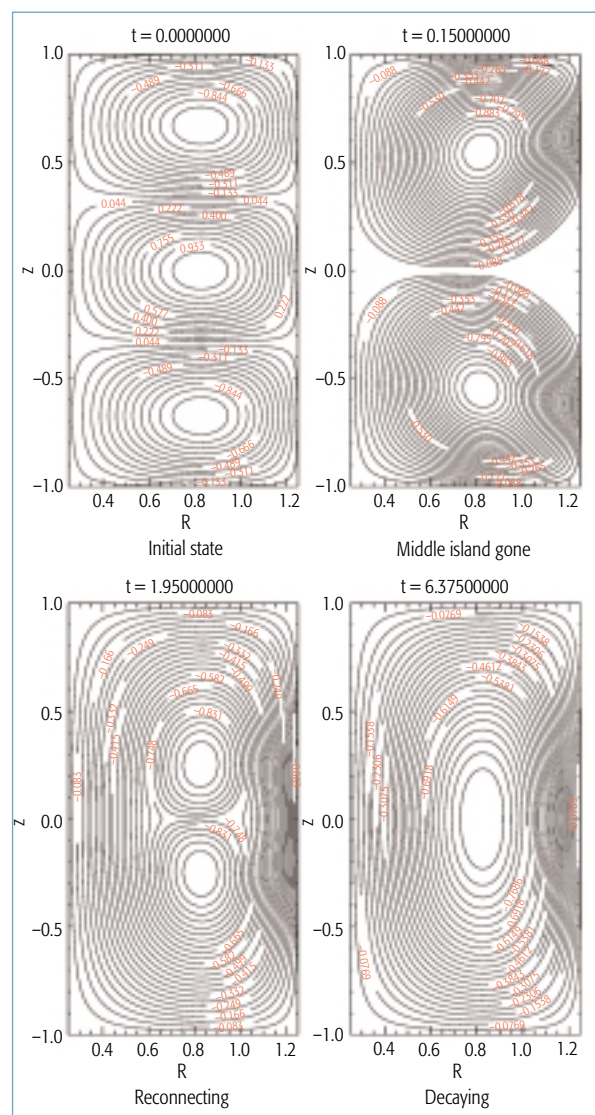
## Center for Extended Magnetohydrodynamic Modeling

The Center for Extended Magnetohydrodynamic Modeling (CEMM) will extend and apply computer codes (M3D and NIMROD) that will enable a realistic assessment of the mechanisms leading to disruptive and other stability limits in the present and next generation of fusion devices. With an improvement in the efficiency of codes and with the extension of the leading 3D nonlinear magneto-fluid models of hot, magnetized fusion plasmas, this research will pioneer new plasma simulations of unprecedented realism and resolution.

The Multi-Level 3D (M3D) project simulates plasmas using multiple levels of physics, geometry, and grid models in one code package. The M3D code has been extended to fundamentally non-axisymmetric and small aspect ratio,  $R/a \geq 1$ , configurations. Applications include the non-linear stability of the NSTX spherical torus and of the spherical pinch, as well as the relaxation of stellarator equilibria (Figure 10). The fluid level physics model has been extended to evolve the anisotropic pressures  $p_{j\parallel}$  and  $p_{j\perp}$  for the ion and electron species and has



**FIGURE 10** M3D simulation of the proposed compact quasi-axisymmetric (QAS) stellarator. Equi-pressure surface of the li383 case with  $\beta$  exceeding the design limit shows the nonlinear ballooning mode steepening to form a ribbon-like structure.



**FIGURE 11** Poloidal flux contours during successive phases of co-helicity reconnection, computed with MRC.

been applied to magnetic island evolution. Further development of the M3D code is being done in collaboration with the TOPS Center (page 13 above).

The CEMM and APDEC (page 11 above) centers are collaborating to apply the CHOMBO adaptive mesh refinement framework to MHD problems of importance to fusion energy. They are targeting two primary applications: magnetic reconnection including Hall physics, and pellet injection and ablation. The Magnetic Reconnection Code (MRC) uses a fixed, non-uniform rectangular mesh to resolve the different spatial scales in the reconnection problem. The resistive MHD version uses an implicit/explicit hybrid method, while the two-fluid version uses an alternating-direction implicit (ADI) method with high-order artificial dissipation. MRC has proven useful for comparing several different theories of collisional and collisionless reconnection (Figure 11).

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**INVESTIGATORS** S. C. Jardin, J. A. Breslau, J. Chen, G. Fu, S. Klasky, W. Park, and R. Samteney, Princeton Plasma Physics Laboratory; J. Callen, C. Hegna, and C. Sovinec, University of Wisconsin; E. Held, Utah State University; C. Kim and S. Parker, University of Colorado; S. Kruger and D. Schnack, Science Applications International Corp.; R. Nebel, Los Alamos National Laboratory; D. Schissel, General Atomics; L. E. Sugiyama, Massachusetts Institute of Technology; H. R. Strauss, New York University; F. Waelbroeck, University of Texas.

**PUBLICATIONS** L. E. Sugiyama, W. Park, H. R. Strauss, S. R. Hudson, D. Stutman, and X.-Z. Tang, "Studies of spherical tori, stellarators and anisotropic pressure with the M3D code," *Nuclear Fusion* **41**, 739 (2001).

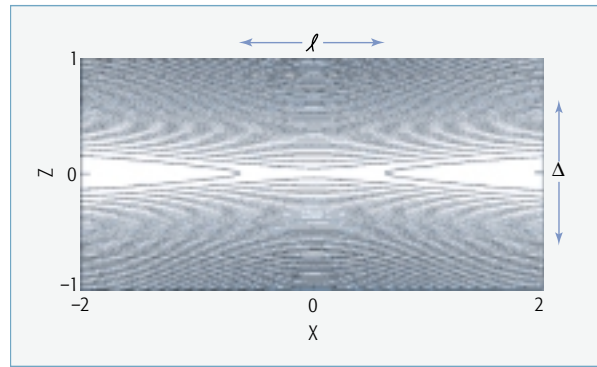
J. A. Breslau and S. C. Jardin, "A parallel algorithm for global magnetic reconnection studies," *Computer Physics Communications* (in press).

**URL** <http://w3.pppl.gov/CEMM/>

## Center for Magnetic Reconnection Studies

The goal of this project is the development of high-performance computing tools that will elucidate the physics of magnetic reconnection, and apply these tools to the solution of outstanding problems in fusion and astrophysical plasma physics.

During the last four decades, two models of steady-state reconnection—Sweet-Parker and Petschek—have been the



**FIGURE 12** Flux surface plot on the  $(x, z)$  plane from a Hall MHD simulation indicating schematically the width  $\Delta$  and length  $\ell$  of the reconnection layer.

focal points of discussions on nonlinear reconnection dynamics. Both models are based on resistive magnetohydrodynamics (MHD). Computer simulations of high- $S$  plasmas have revealed strengths and weaknesses in both models. A possible resolution of this quandary may be found by going beyond the resistive MHD model and including collisionless effects via the generalized Ohm's law.

In a nonlinear Hall MHD simulation under quasisteady conditions, with a reconnection layer of length  $\ell$  and width  $\Delta$  (Figure 12), no current theory calculates the important length parameter  $\ell$  from first principles. Wang et al. recently attempted to settle this question by determining analytically the dependency of the parameter  $\ell$  on local and global parameters for a model of forced reconnection. They obtained an explicit analytical expression for  $\ell$ , which is much smaller than the system size, and identified its dependencies on local plasma parameters as well as global parameters determined by boundary conditions. They also tested the analytical scaling by simulations using the University of Iowa (UI) Hall MHD code.

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**INVESTIGATORS** A. Bhattacharjee, N. Bessho, B. Chandran, K. Germaschewski, Z. W. Ma, C. S. Ng, and P. Zhu, University of Iowa; F. Cattaneo, T. Linde, R. Rosner, and A. Siegel, University of Chicago; R. Fitzpatrick and P. Watson, University of Texas, Austin.

**PUBLICATION** X. Wang, A. Bhattacharjee, and Z. W. Ma, "Scaling of collisionless forced reconnection," *Phys. Rev. Lett.* **87**, 265003 (2001).

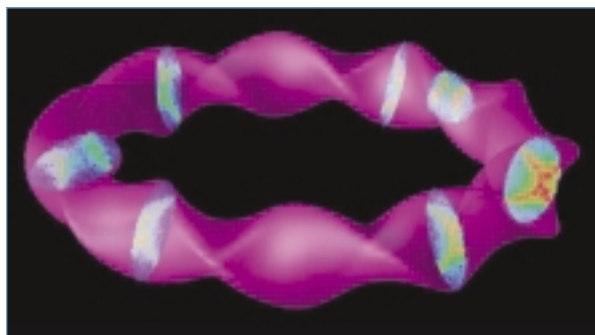
**URL** <http://www.physics.uiowa.edu/cmrs/>

## Numerical Computation of Wave-Plasma Interactions in Multi-Dimensional Systems

The goal of this research is to use advanced terascale computing to obtain quantitatively accurate predictive understanding of electromagnetic wave processes, which support important heating, current drive, and stability and transport applications in fusion plasmas.

Recently developed all-orders spectral algorithms (AORSA) take advantage of new computational routines in ScaLAPACK to solve the integral form of the wave equation in multiple dimensions without any restriction on wavelength relative to orbit size, and with no limit on the number of cyclotron harmonics retained. These new models give high-resolution, 2D solutions for mode conversion and high harmonic fast wave heating in tokamak geometry. In addition, they have been extended to give fully 3D solutions of the integral wave equation for minority ion cyclotron heating in stellarator geometry (Figure 13). By combining multiple periodic solutions for individual helical field periods, it is possible to obtain complete wave solutions valid over the entire volume of the stellarator for arbitrary antenna geometry. This work is an initial step toward multidimensional modeling of wave processes.

**INVESTIGATORS** D. B. Batchelor, L. A. Berry, J. A. Carlsson, M. D. Carter, E. F. Jaeger, and D. A. Spong, Oak Ridge National Laboratory; C. K. Phillips, Princeton Plasma Physics Laboratory; P. T. Bonoli, Massachusetts Institute of Technology; D. N. Smithe, Mission Research Corp.; R. W. Harvey, CompX; D. A. D'ippolito, Lodestar Research Corp.



**FIGURE 13** AORSA calculation of minority ion cyclotron heating for all ten field periods of the LHD (Large Helical Device) stellarator with a single antenna located at the far right. Individual cross sections show the logarithm of the minority ion power absorption at various toroidal angles.

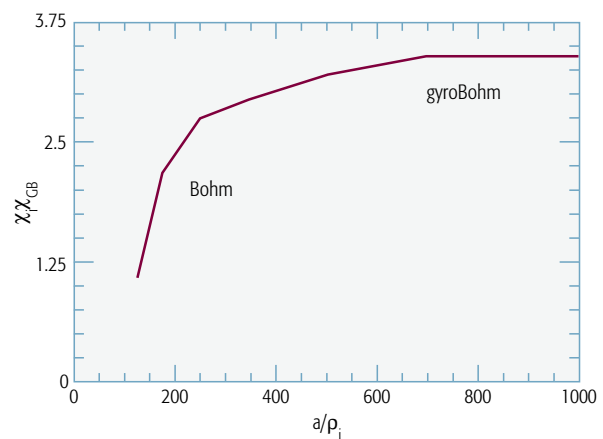
**PUBLICATION** E. F. Jaeger, L. A. Berry, E. D'Azevedo, D. B. Batchelor, M. D. Carter, K. F. White, and H. Weitzner, "Advances in full-wave modeling of radio frequency heated, multidimensional plasmas," *Phys. Plasmas* 9, 1873 (2002).

**URL** <http://www.ornl.gov/fed/scidacr/>

## Plasma Microturbulence Project

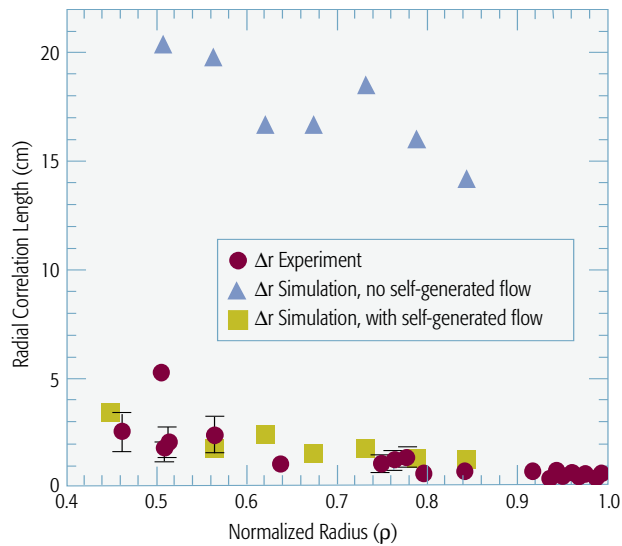
The goal of this research is to develop computational tools that will advance the understanding of microturbulence and its role in the confinement of fusion plasmas. The development of tools in this project will advance the interpretation of experimental confinement data and will be used to test theoretical ideas about electrostatic and electromagnetic turbulence.

Accurate prediction of the heat and particle transport level is critical for the design of fusion reactors. Current reactor design studies rely on extrapolations of turbulent transport properties from present-day tokamak experiments to larger devices. However, simulations of full-size reactors, only recently made possible by efficient algorithms and terascale computers, have found that these extrapolations can be unreliable. Simulation results reported by Lin et al. show that the ion-temperature-gradient turbulence fluctuation scale length is microscopic and independent of device size, that test particle transport is diffusive, and that the local transport coefficient exhibits a gradual transition from a Bohm-like scaling for today's tokamak sizes to a gyro-Bohm scaling for future larger devices (Figure 14). The device size where this transition occurs is much larger than that expected from linear theory based on pressure gradient profile variations.



**FIGURE 14** Ion heat conductivity vs tokamak minor radius.





**FIGURE 15** Correlation lengths  $\Delta r$  from a set of L-mode discharges and numerical simulations from the UCAN code. Numerical values are with and without self-induced or zonal flows.

An alternative approach to more accurate prediction of microturbulence is to benchmark and validate plasma simulations through detailed comparison with experimental measurements. This comparison relies on implementation of numerical diagnostics that simulate real-world experimental measurements and analysis techniques. Rhodes et al. have begun making such comparisons between simulations and experimental results from the DIII-D tokamak. One of their findings is that simulations must include self-induced or zonal flows for agreement with experimental  $\Delta r$  (Figure 15). Although much work remains, the closeness of the simulation results to experimental measurements so far is encouraging.

**INVESTIGATORS** W. M. Nevins, B. I. Cohen, A. Dimits, and D. Shumaker, Lawrence Livermore National Laboratory; J. Candy and R. Waltz, General Atomics; Y. Chen, C. Kim, and S. Parker, University of Colorado, Boulder; W. Dorland and S. Novakovski, University of Maryland; W. W. Lee, D. Ernst, G. Hammett, S. Klasky, and J. Lewandowski, Princeton Plasma Physics Laboratory; Z. Lin, University of California, Irvine; V. Decyk and J.-N. Leboeuf, University of California, Los Angeles; V. Lynch, Oak Ridge National Laboratory; D. Ross, University of Texas; D. Ernst, Massachusetts Institute of Technology; F. Jenko, IPP Garching.

**PUBLICATIONS** Z. Lin, S. Ethier, T. S. Hahm, and W. M. Tang, "Size scaling of turbulent transport in magnetically confined plasmas," Phys. Rev. Lett. **88**, 195004 (2002).

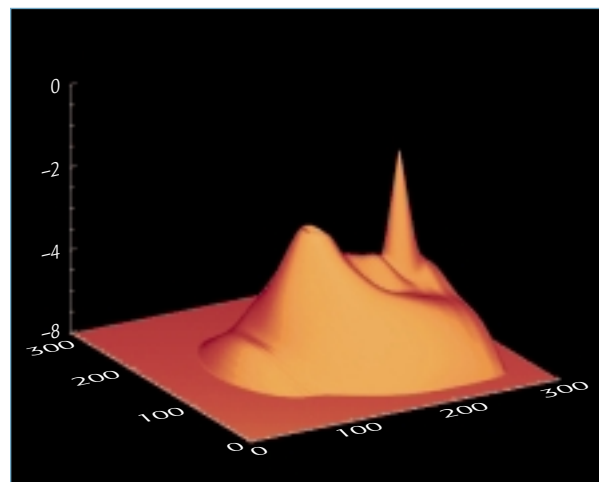
T. L. Rhodes, J.-N. Leboeuf, R. D. Sydora, R. J. Groebner, E. J. Doyle, G. R. McKee, W. A. Peebles, C. L. Rettig, L. Zeng, and G. Wang, "Comparison of turbulence measurements from DIII-D low-mode and high-performance plasmas to turbulence simulations and models," Phys. Plasmas **9**, 2141 (2000).

**URL** <http://fusion.gat.com/theory/pmp/>

## Terascale Atomic Physics for Controlled Fusion Energy

Modeling the electron-impact ionization of atomic and molecular constituents is a key to understanding many astrophysical and laboratory plasmas. The goal of this collaboration is to implement state-of-the-art atomic collision codes on the newest generation of terascale computing facilities. Studies will then ensue on a wide range of atomic collision processes present in the edge region of controlled fusion plasmas. Computational research advances will be applied to other general science areas, including laser interactions with atoms and molecules, atomic physics near compact stars, and the dynamics of cold atom gases.

Colgan et al. have conducted three independent nonperturbative calculations for the electron-impact ionization of both the ground and first excited states of the neutral lithium atom (Figure 16). The time-dependent close-coupling, the  $R$



**FIGURE 16** Electron probability cloud following a head-on collision between a proton and a lithium atom at 15 keV incident energy. The large peak at the center represents excitation of the lithium target, the narrow peak at right center represents charge transfer to the proton projectile, while the many plains and valleys represent ionization of the lithium target.

matrix with pseudostates, and the converged close-coupling methods yield total integral cross sections that are in very good agreement with each other, while perturbative distorted-wave calculations yield cross sections that are substantially higher. These nonperturbative calculations provide a benchmark for the continued development of electron-atom experimental methods designed to measure both ground and excited state ionization.

**INVESTIGATORS** M. S. Pindzola and F. J. Robicheaux, Auburn University; D. R. Schultz, Oak Ridge National Laboratory; D. C. Griffin, Rollins College, Winter Park, Florida; N. R. Badnell and H. P. Summers, University of Strathclyde, Glasgow; P. G. Burke, Queen's University of Belfast; C. J. Noble, Daresbury Laboratory, Warrington, England.

**PUBLICATION** J. Colgan, M. S. Pindzola, D. M. Mitnik, D. C. Griffin, and I. Bray, "Benchmark nonperturbative calculations for the electron-impact ionization of Li(2s) and Li(2p)," *Phys. Rev. Lett.* **87**, 213201 (2001).

**URL** <http://www.physics.auburn.edu/~scidac/>

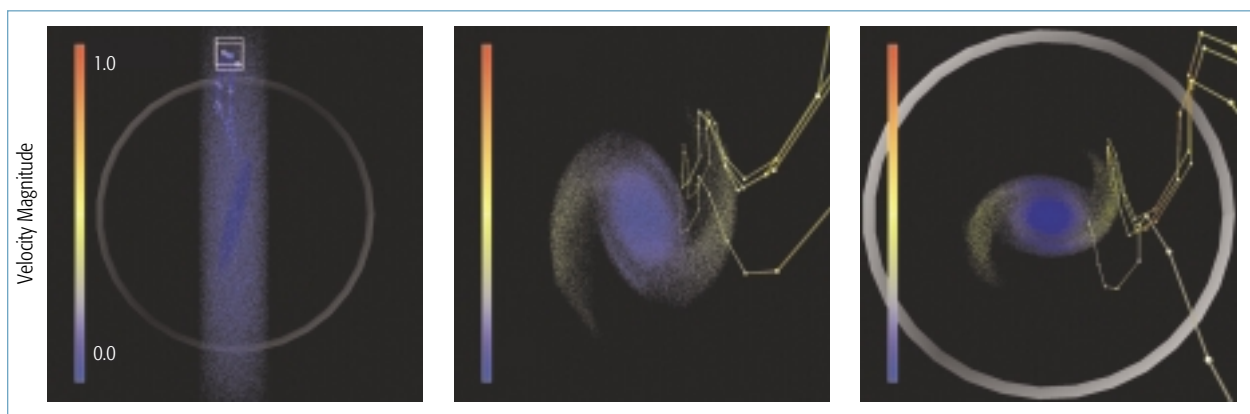
## Advanced Computing for 21st Century Accelerator Science and Technology

This project is working on simulating particle accelerators, some of the largest and most complex scientific instruments. A new generation of accelerator simulation codes will promote more efficient use of existing accelerators and will strongly impact the design, technology, and cost of future accelerators.

Macroparticle simulation plays an important role in modern accelerator design and operation. Most linear rf accelerators have been designed based on macroparticle simulations using longitudinal position as the independent variable. The choice of an independent variable affects the accuracy of the simulation with regard to the calculation of the space-charge forces and hence the accuracy of the particle trajectories. This leads to changes in the prediction of the evolution of the beam distribution, both in the core and in the halo (Figure 17).

Qiang et al. have done a systematic comparison between using longitudinal position as the independent variable and using time as the independent variable in macroparticle simulations. They found that, for an rms-matched beam, the maximum relative moment difference for second and fourth moments and for beam maximum amplitudes between these two types of simulations is 0.25% in a 10 m reference transport system with physical parameters similar to the Spallation Neutron Source linac design. The maximum  $z$ -to- $t$  transform error in the space-charge force calculation of the position dependent simulation is about 0.1% in such a system. This might cause a several percent error in a complete simulation of a linac with a length of hundreds of meters. The error may be several times larger in simulations of mismatched beams. New algorithms, such as a particle advance method based on the use of multiple reference particles, are being studied in order to improve the accuracy of position-dependent simulations of high-intensity beams.

**INVESTIGATORS** K. Ko, Stanford Linear Accelerator Center; R. D. Ryne and E. G. Ng, Lawrence Berkeley National Laboratory; A. Dragt,



**FIGURE 17** Simulation showing halo particles being tracked backward in an accelerator to their starting points. Such simulations and associated visualizations provide insight into the halo formation mechanism in high intensity beams.

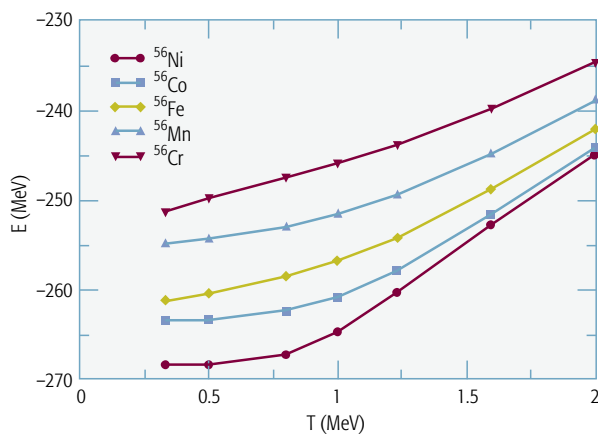
University of Maryland; G. H. Golub, Stanford University; K.-L. Ma, University of California, Davis; W. Mori, University of California, Los Angeles.

**PUBLICATION** J. Qiang, R. D. Ryne, and R. W. Garnett, "Systematic comparison of position and time dependent macroparticle simulations in beam dynamics studies," *Phys. Rev. ST Accel. Beams* **5**, 064201 (2002).

**URL** <http://scidac.nersc.gov/accelerator/>

## Terascale Supernova Initiative

The Terascale Supernova Initiative is a multidisciplinary collaboration to develop models for core-collapse supernovae and enabling technologies in radiation transport, radiation



**FIGURE 18** Energy expectation value  $E = \langle H \rangle$  as a function of temperature  $T$  for selected  $A = 56$  isobars.

hydrodynamics, nuclear structure, linear systems and eigenvalue solution, and collaborative visualization. (See also the SciDAC Supernova Science Center, page 7 above.)

An essential part of the nuclear equation of state in computer simulations of core-collapse supernovae is the symmetry energy, which describes the energy needed to separate protons and neutrons. Symmetry energy is important because the dynamical evolution of the collapse is strongly influenced by electron captures on nuclei and free protons. Dean et al. performed large-scale shell model Monte Carlo calculations for many nuclei in the mass range  $A = 56$ – $65$  using an effective quadrupole–quadrupole+pairing residual interaction. Their main focus was the temperature dependence of the symmetry energy, which they determined from the energy differences between various isobaric pairs with the same pairing structure and at different temperatures (Figure 18). They found that the symmetry energy increases slightly when the temperature is increased from 0.33 MeV to 1.23 MeV.

**INVESTIGATORS** A. Mezzacappa, D. J. Dean, M. Strayer, and R. Toedte, Oak Ridge National Laboratory; J. Dongarra and V. Eijkhout, University of Tennessee, Knoxville; D. Swesty, J. Lattimer, and M. Prakash, State University of New York, Stony Brook; P. Saylor, F. Saied, and P. Baker, University of Illinois; J. Hayes and G. Fuller, University of California, San Diego; W. Haxton, University of Washington; J. Blondin, North Carolina State University; B. Meyer, Clemson University; S. Bruenn, Florida Atlantic University.

**PUBLICATION** D. J. Dean, K. Langanke, and J. M. Sampaio, "Temperature dependence of the symmetry energy," *Phys. Rev. C* **66**, 045802 (2002).

**URL** <http://www.phy.ornl.gov/tsi/>





# Basic Energy Sciences

NERSC provides computational support for a large number of materials sciences and chemical sciences projects sponsored by DOE's Office of Basic Energy Sciences. Highlights this year include the first complete explanation of the unusual superconducting properties of magnesium diboride; the first comparison with experimental measurements of a fully detailed simulation of fluid viscosity; the first determination of the magnetic structure of a superconductor from first-principles calculations; the first ab initio molecular dynamics simulation of low-energy deposition of metal clusters on a solid surface; and an important contribution to the study of the relationship between microstructure and magnetism in nanosystems.

## The Origin of the Anomalous Superconducting Properties of MgB<sub>2</sub>

The quest for high-temperature superconductors is one of the grand challenges of materials science. Magnesium diboride (MgB<sub>2</sub>) differs from ordinary metallic superconductors in several important ways, including its high transition temperature,  $T_c = 39$  °K, and its multiple superconducting energy gaps. Understanding why MgB<sub>2</sub> behaves as it does opens the possibility of creating new superconducting materials with analogous electronic structure.

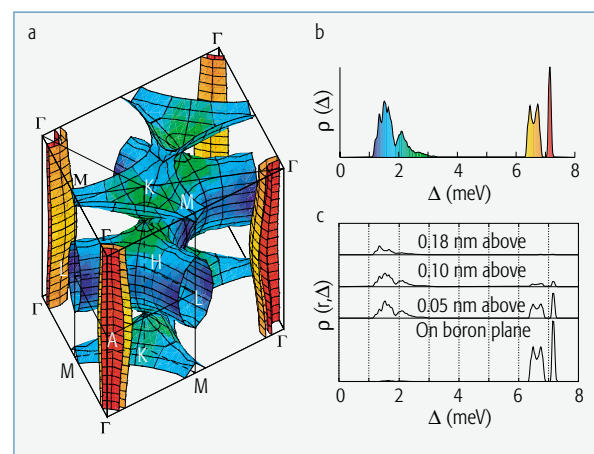
Choi et al. are the first researchers to successfully explain the superconducting transition temperature and energy gaps (Figure 1) of MgB<sub>2</sub>, along with its isotope effects, quasiparticle density of states, specific heat, and temperature dependencies. Using first principles pseudopotential density-functional method coupled with a fully anisotropic Eliashberg formalism, they found that the momentum-dependent electron-phonon interactions and the anharmonicity of phonons in MgB<sub>2</sub> are the most important material properties that determine the superconducting properties. Their calculated superconducting properties are all in agreement with corresponding experiments.

Their analysis suggests that layered materials based on boron, carbon, and nitrogen may exhibit comparable or higher transition temperatures.

**INVESTIGATORS** M. L. Cohen, S. G. Louie, and D. Roundy, University of California, Berkeley, and Lawrence Berkeley National Laboratory; H. J. Choi and H. Sun, University of California, Berkeley.

**PUBLICATION** H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, "The origin of the anomalous superconducting properties of MgB<sub>2</sub>," *Nature* **418**, 758 (2002).

**URL** <http://civet.berkeley.edu>

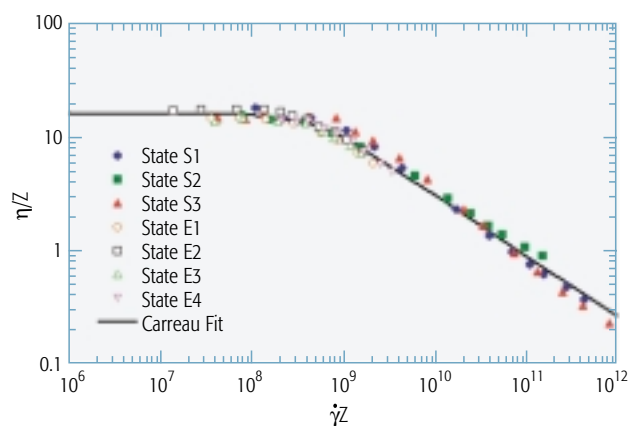


**FIGURE 1** The superconducting energy gap of MgB<sub>2</sub>. (a, b) The superconducting energy gap on the Fermi surface at 4 K given using a color scale (a), and the distribution of gap values at 4 K (b). The Fermi surface of MgB<sub>2</sub> consists of four distinctive sheets. Two  $\sigma$  sheets ("cylinders"), derived from the  $\sigma$ -bonding  $p_{x,y}$  orbitals of boron, are shown split into eight pieces around the four vertical  $\Gamma$ - $\Gamma$  lines. Two  $\pi$  sheets ("webbed tunnels"), derived from the  $\pi$ -bonding  $p_z$  orbitals of boron, are shown around K-M and H-L lines (upper and lower K-M lines are equivalent). The superconducting energy gap is  $\sim 7.2$  meV on the narrower  $\sigma$  cylindrical sheet, shown in red, with variations of less than 0.1 meV. On the wider  $\sigma$  cylindrical sheet, shown in orange, the energy gap ranges from 6.4 to 6.8 meV, having a maximum near  $\Gamma$  and a minimum near A. On the  $\pi$  sheets, shown in green and blue, the energy gap ranges from 1.2 to 3.7 meV. The density of states at the Fermi energy is 0.12 states per (eV atom spin), 44% of which comes from the  $\sigma$  sheets and the other 56% comes from the  $\pi$  sheets. (c) Local distribution of the superconducting energy gap on a boron plane and on planes at 0.05, 0.10, and 0.18 nm above a boron plane, respectively.

## Comparison of Nonequilibrium Molecular Dynamics Simulations with Experimental Measurements of Viscosity

A better understanding of the viscous properties of lubricants can lead to the design of improved lubricants in automobile engines, resulting in better energy efficiency. Nonequilibrium molecular dynamics (NEMD) is a particularly useful technique for studying rheological properties, since the key algorithm is a direct implementation of the experimental method for measuring viscosity. While NEMD has been around for 30 years, and for a decade has been used to predict viscosity in systems ranging from carbon dioxide and its mixtures to short polymers, it was not until this year that, for the first time, a fully detailed simulation was compared with experimental measurements of a real fluid.

Bair et al. compared a NEMD simulation of squalane (a low-molecular-weight fluid) with experimental measurements in both the linear (Newtonian) and nonlinear (non-Newtonian) regimes—the first comparison of the nonlinear rheology predicted by NEMD with experiment. Although it is not possible with today's computers to perform NEMD simulations on the same state conditions as the experiments, and thus the experiments and simulations cannot be directly compared, the results can be put in comparable form using the standard rheological analysis technique of temperature-time superposition. Temperature-time superposition is a theoretically and experimentally well-established technique in polymer rheology for collapsing



**FIGURE 2** Plot of reduced viscosity versus reduced strain rate for the experimental and simulation data.

experimental data for a given polymer at different temperatures, densities, and strain rates onto a single curve characteristic of that polymer.

When Bair et al. used this technique and placed all of the simulation and experimental results for squalane on a single plot (Figure 2), their remarkable finding was that all of the data followed the same master curve, leading to the conclusion that the behavior of squalane predicted by NEMD in the non-Newtonian region is in good agreement with experiment.

**INVESTIGATORS** P. T. Cummings and C. McCabe, University of Tennessee, Knoxville, and Oak Ridge National Laboratory; S. Bair, Georgia Institute of Technology.

**PUBLICATION** S. Bair, C. McCabe, and P. T. Cummings, "Comparison of nonequilibrium molecular dynamics with experimental measurements in the nonlinear shear-thinning regime," *Phys. Rev. Lett.* **88**, 058302 (2002).

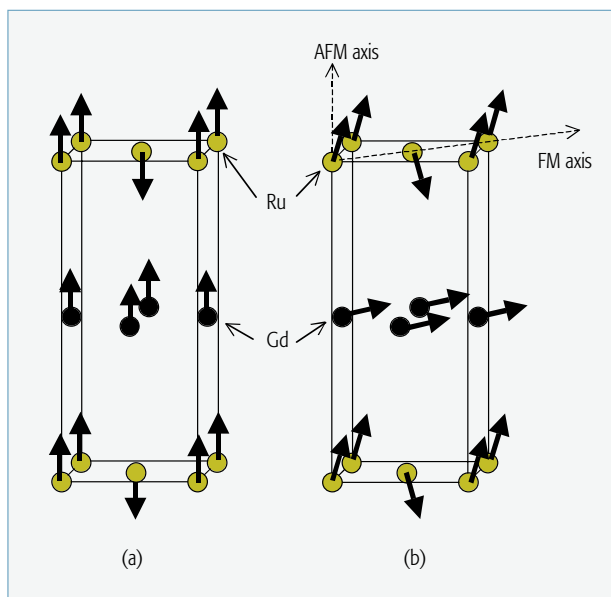
**URL** <http://flory.engr.utk.edu>

## Determining the Magnetic Structure of a Superconductor

Superconducting materials are the subject of widespread research because of their potential contributions to improved magnetic energy-storage systems, motors, generators, transformers, computer parts, medical imaging devices, and other types of instrumentation. Computational simulations are necessary for understanding the properties of these materials and improving their design. For the first time, the complex nature of the coexistence of magnetism and superconductivity on a microscopic scale has been determined from first-principles calculations.

Nakamura and Freeman have determined the magnetic structures of the ruthenocuprate compound  $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ —a ferromagnetic superconductor—from first principles by using the highly precise full-potential linearized augmented plane-wave (FLAPW) method. FLAPW includes a newly developed intra-atomic noncollinear magnetism capability that can describe the canting of Ru moments.

The researchers found that the magnetism of  $\text{RuSr}_2\text{GdCu}_2\text{O}_8$  arises from the  $\text{RuO}_6$  octahedra, where the moments on neighboring Ru sites order antiferromagnetically but cant perpendicular to the antiferromagnetic (AFM) axis, and so induce a weak ferromagnetism (Figure 3). From the canting of the Ru moments, a double exchange interaction is exerted via itinerant



**FIGURE 3** Schematic magnetic ordering of Ru and Gd moments in (a) collinear AFM and (b) noncollinear AFM structures of  $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ , where the Cu,  $\text{O}_{\text{Ru}}$ ,  $\text{O}_{\text{Cu}}$ , and  $\text{O}_{\text{apical}}$  atoms are not given. The ordering of the Ru moments in (b) is similar to a C-type AFM ordering in (a), but the moments cant perpendicular to the AFM axis, i.e., along the FM axis direction. Note that the moment directions are defined in a spin space, since spin-orbit coupling is not taken into account.

$t_{2g}$  electrons which can travel through the neighboring O p states. The projected Ru moments along the AFM and FM axes result in magnetic moments of 1.16 and  $0.99\mu_B$ , respectively. The results are consistent with the possible coexistence of canted ferromagnetism and superconductivity in  $\text{RuSr}_2\text{GdCu}_2\text{O}_8$  as inferred from experiments.

**INVESTIGATORS** A. J. Freeman, Northwestern University, and K. Nakamura, Mie University, Japan.

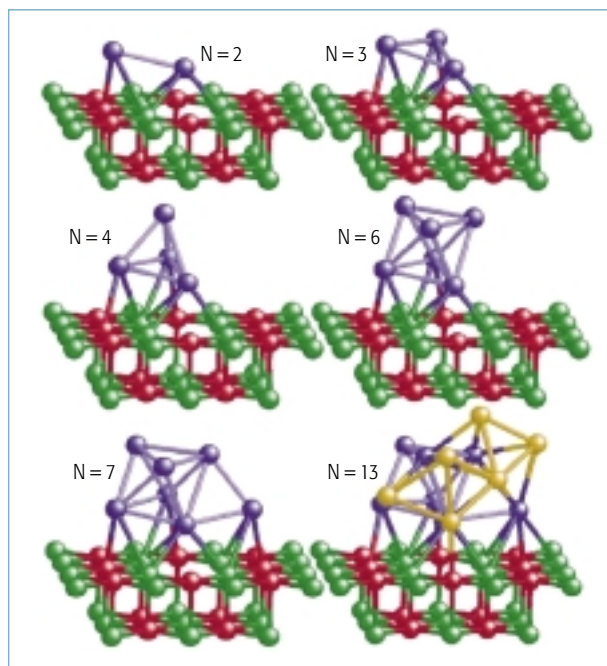
**PUBLICATION** K. Nakamura and A. J. Freeman, "Canted ferromagnetism in  $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ ," *Phys. Rev. B* **66**, 140405(R) (2002).

## Simulating the Deposition of Atomic Clusters of Palladium on a Magnesium Oxide Surface

Deposition of atomic clusters onto solid surfaces is a versatile surface-processing tool, with applications ranging from micromachining and surface smoothing to thin-film growth and fabrication of model nanocatalysts. Theoretical investigations,

most often employing molecular dynamics (MD) simulations with semiempirical interatomic potentials, provide valuable insights into the microscopic mechanisms of the deposition process. However, when cluster-surface interaction involves surface chemistry (that is, the creation or breaking of chemical bonds), spin-dependent (magnetic) processes, or surface defects of electronic origin (e.g., F center on an ionic surface), a full quantum description of the cluster deposition process is necessary.

Moseler et al. have performed the first *ab initio* molecular dynamics simulation of low-energy deposition of metal clusters on a solid surface (Figure 4). The simulation (based on the density functional formalism) provided insights into the electronic mechanisms that govern the deposition process. It was found that palladium clusters larger than a trimer remain magnetic when deposited in the vicinity of surface F-center defects of  $\text{MgO}(001)$ . This suggests that the soft-landing of magnetic clusters on purposefully patterned surfaces may allow preparation of ordered arrays of magnetic quantum dots. These results are important for understanding the activity of Pd/MgO nanocatalysts as well as for future investigations of supported magnetic nanoclusters.



**FIGURE 4** Structural evolution of  $\text{Pd}_N$  supported clusters ( $N = 2, 3, 4, 6, 7,$  and  $13$ ). Pd atoms are depicted as blue, Mg as green, and O as red spheres, except for  $\text{Pd}_{13}$ , where a subset of the Pd atoms is colored in yellow in order to highlight the  $\text{Pd}_7$  subunit (blue).

The simulations show that an F center creates an attractive funnel for the approaching metal cluster, resulting in preferred binding configurations with one Pd atom atop the F center. For adsorbed Pd<sub>2</sub>-Pd<sub>6</sub> the gas-phase geometry is retained, while Pd<sub>7</sub> and Pd<sub>13</sub> adapt to the underlying MgO structure. Although the surface tends to reduce the spin of the adsorbed cluster, clusters larger than Pd<sub>3</sub> remain magnetic at the surface, exhibiting several low-lying structural and spin isomers. These results provide the impetus for further investigations regarding the interplay of structural and magnetic states of supported metal clusters and their catalytic properties.

**INVESTIGATORS** U. Landman, R. N. Barnett, C. L. Cleveland, H. Häkkinen, and W. D. Luedtke, Georgia Institute of Technology; M. Moseler, University of Freiburg, Germany.

**PUBLICATION** M. Moseler, H. Häkkinen, and U. Landman, "Supported magnetic nanoclusters: Soft landing of Pd clusters on a MgO surface," *Phys. Rev. Lett.* **89**, 176103 (2002).

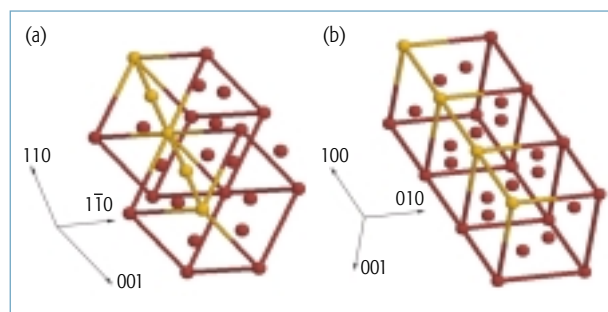
## Magnetic Anisotropy of Iron Nano-Chains Embedded in Copper

As the size of magneto-electronic devices (such as recording media) continues to shrink, magnetic nanosystems are the focus of intensive experimental research. Nanosystems also provide a unique opportunity for theory and simulation to contribute to the understanding and prediction of magnetic properties. Understanding the relationship between microstructures and magnetism will be one of the keys to designing new magnetic materials with precisely engineered properties. Recent calculations have made important contributions to this understanding.

Using first-principles relativistic density functional calculations, Eisenbach et al. have studied monoatomic iron chains embedded in copper, focusing on chains of atoms aligned along different directions in the copper matrix (Figure 5). They found that the magnetocrystalline anisotropy energy favored orientations of the magnetic moments perpendicular to the chain, while the magnetostatic energy was lowest when the moments were aligned parallel to the chain. Due to the delicate balance of these competing effects, the ground state orientation of the magnetic moments on

the iron sites can be either parallel or perpendicular to the chain, depending on whether the chains are embedded in the copper along the 100 or 110 directions.

Due to the lower symmetry of these embedded chain systems (as compared to a bulk iron system with its cubic symmetry), the contribution of the spin-orbit coupling was significantly increased. The reduced symmetry led to a noticeably larger crystalline anisotropy energy, which favored the perpendicular orientation of the iron moments. The competing magnetic dipolar interaction preferred the parallel orientation. As it turned out, the nearest neighbor chains exhibited such a close balance between the magnetocrystalline and shape contributions to the total anisotropy that the preferred orientation in the system depended on the direction in which the iron chain was embedded in the copper.



**FIGURE 5** The orientations of the iron chains in the copper matrix. (a) Chain along the copper 110 direction. Here two of the nearest neighbors of each iron atom are also iron atoms. (b) Chain along the 100 direction. All nearest neighbors to iron atoms are copper, and the closest iron atom is in the next nearest neighbor position.

**INVESTIGATORS** G. M. Stocks and B. Újfalussy, Oak Ridge National Laboratory; B. N. Harmon, Ames Laboratory; M. Weinert, University of Wisconsin, Milwaukee; D. P. Landau, University of Georgia; M. Eisenbach and B. L. Györfy, University of Bristol, U.K.

**PUBLICATIONS** M. Eisenbach, B. L. Györfy, G. M. Stocks, and B. Újfalussy, "Magnetic anisotropy of monoatomic iron chains embedded in copper," *Phys. Rev. B* **65**, 144424 (2002).

M. Eisenbach, G. M. Stocks, B. Újfalussy, and B. L. Györfy, "Magnetic anisotropy of iron chains embedded in copper," *J. Appl. Phys.* **91**, 6878 (2002).

**URL** <http://theory.ms.ornl.gov/~gms/M4home.html>

# Biological and Environmental Research

DOE's Office of Biological and Environmental Research is a major supporter of computational biological research and global climate studies using NERSC resources. This year's accomplishments include the first report on the structure of a carcinogenic heterocyclic amine, in a study combining nuclear magnetic resonance (NMR) imaging and molecular mechanics computation. A poster presentation of this study at the Pasteur Institute in Paris in February 2002 received a Certificate of Merit Award from the Sixth International Symposium on Predictive Oncology and Intervention Strategies.

In other studies, comparison of the Fugu and human genomes enabled researchers to discover almost 1,000 human putative genes that have so far not been described in public annotation databases. And computational studies are increasing our understanding of how an enzyme called TIM speeds up the breakdown of carbohydrates. Climate research highlights include the first study of tropopause height as an indicator of climate change, and an analysis of the complex effects of aerosols on clouds.

## Determining the Structure of a Carcinogenic Heterocyclic Amine

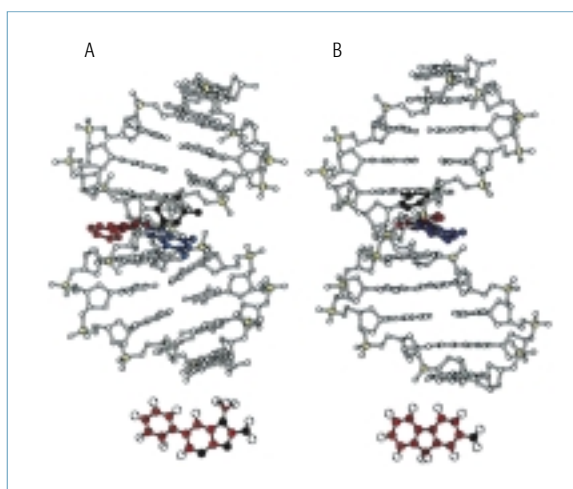
Consumption of foods containing heterocyclic amines (HA) has been implicated in the etiology of human cancers, including cancer of the colon, lung, and breast. The mutagen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) is the most abundant of the HAs, which are formed in meat and fish during cooking. PhIP has been shown to induce tumors in several organs in rodents and to form DNA adducts, which are considered initiating events in chemical carcinogenesis.

Because of difficulties in synthesizing the large quantities of highly purified samples needed, no structural studies of HA-DNA adducts had been reported until the work of Brown et al.,

who optimized the synthesis of the C8-dG-PhIP adduct in an 11-mer DNA sequence and determined its structure through a combination of NMR imaging and molecular mechanics computation. Restrained conformational searches were carried out with DUPLEX, a molecular mechanics program for nucleic acids that performs potential energy minimization in the reduced variable domain of torsional angle space.

The covalent binding of bulky carcinogens such as PhIP to DNA can alter biological processing of the DNA by cellular proteins governing replication, transcription, and repair, and thereby cause mutations and ultimately cancer, especially if the lesion is located in an oncogene or tumor-suppressor gene. Consequently, considerable efforts are being made to understand how adduct conformation affects cellular responses to DNA damage.

This study shows that the [PhIP]dGzdC 11-mer adduct duplex undergoes a conformational exchange between a major base-displaced intercalative structure and a minor external groove-binding structure. The subtle differences in the structural details and in the population ratios of each conformer of the C8-dG-PhIP-DNA adduct reveal the importance of the chemical structure of the PhIP molecule in governing its



**FIGURE 1** Comparison of the [PhIP]dG-dC and [AF]dG-dC 11-mer adduct duplexes with [PhIP]dG6 in blue, dC17 in green, and PhIP and AF ligands in red. The PhIP and AF structures are shown at the bottom.

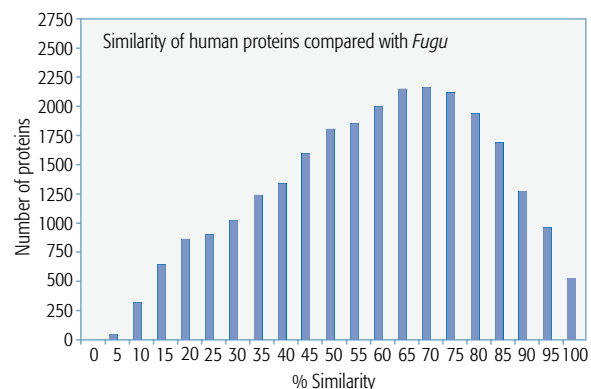


DNA adduct conformation. A comparison of the structures of the major conformers of the C8-dG-PhIP and C8-dG-AF (31) 11mer duplexes (Figure 1) shows that although both DNA adducts adopt overall similar structural motifs, several important differences are observed that would directly influence how cellular proteins interact with this type of damaged DNA substrate. Determination of the structure of this adduct is an important first step in elucidating the mechanisms by which DNA damage by PhIP can lead to cancer.

**INVESTIGATORS** B. E. Hingerty, Oak Ridge National Laboratory; S. Broyde, New York University; K. Brown, M. Cosman, E. A. Guenther, V. V. Krishnan, and K. W. Turteltaub, Lawrence Livermore National Laboratory; L. Wang, New York University; M. Minkoff, Argonne National Laboratory; R. Wagner, Duke University.  
**PUBLICATION** K. Brown, B. E. Hingerty, E. A. Guenther, V. V. Krishnan, S. Broyde, K. W. Turteltaub, and M. Cosman, "Solution structure of the 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine C8-deoxyguanosine adduct in duplex DNA," *PNAS* **98**, 8507 (2001).  
**URL** <http://bio.lsd.ornl.gov/gst/newresearch/r1.html>

## Whole-Genome Shotgun Assembly and Analysis of the *Fugu rubripes* Genome

The genome of the pufferfish *Fugu rubripes* is unusually small for a vertebrate, at about one-eighth the length of the human genome, but it contains a comparable complement of protein-coding genes. When sequencing of the *Fugu* genome was proposed a decade ago, it was expected that direct comparison of the two genomes would be useful for identifying human genes. The analysis performed by Aparicio et al. shows



**FIGURE 2** Distribution of protein similarities between *Fugu* and human proteomes.

that this expectation has been fulfilled.

The similar numbers of gene loci in both *Fugu* and human (between 30,000 and 40,000) led the researchers to conclude that the core set of vertebrate gene loci is unlikely to exceed 40,000. Examination of the similarities and differences between the human and *Fugu* proteomes (Figure 2) revealed two features: first, the majority of peptides have some degree of match in *Fugu*; second, ~25% of predicted human proteins (8,109) do not appear to have homologs in the *Fugu* genome.

The comparison of the two genomes enabled researchers to discover almost 1,000 human putative genes that have so far not been described in public annotation databases. Examination of the conservation of synteny (location of genes on the same chromosome, whether or not there is demonstrable linkage between them) reveals that about one-eighth of the *Fugu* genome—more than 900 segments of two or more genes—shows conserved linkages of two or more genes with the human genome. Enumeration of conserved segments between *Fugu* and human may be an important starting point for detecting conserved regulatory elements. Tracing the fate of such segments in other species may allow us to reconstruct some of the evolutionary history of vertebrate chromosomes.

**INVESTIGATORS** D. Rokhsar, J. Chapman, N. Putnam, P. Dehal, S. Rash, M. D. S. Gelpke, I. Y. Ho, C. Detter, P. Predki, S. Lucas, P. Richardson, and T. Hawkins, DOE Joint Genome Institute; S. Aparicio, Cambridge University; E. Stupka, J.-M. Chia, A. Christoffels, S. Hoon, T. Oh, M. Wong, F. Verhoef, A. Tay, Y. H. Tan, B. Venkatesh, and S. Brenner, Institute of Molecular and Cell Biology, Singapore; A. Smit, J. Roach, G. Glusman, L. Rowen, and L. Hood, Institute for Systems Biology, Seattle; S. F. Smith, M. S. Clark, Y. J. K. Edwards, and G. Elgar, UK Human Genome Mapping Project Resource Centre; N. Doggett, Los Alamos National Laboratory; A. Zharkikh, S. V. Tavtigian, and D. Pruss, Myriad Genetics Inc.; M. Barnstead, C. Evans, and H. Baden, Celera Genomics; J. Powell, Paradigm Therapeutics Ltd.  
**PUBLICATION** S. Aparicio, J. Chapman, E. Stupka, N. Putnam, J.-M. Chia, P. Dehal, A. Christoffels, S. Rash, S. Hoon, A. Smit, M. D. S. Gelpke, J. Roach, T. Oh, I. Y. Ho, M. Wong, C. Detter, F. Verhoef, P. Predki, A. Tay, S. Lucas, P. Richardson, S. F. Smith, M. S. Clark, Y. J. K. Edwards, N. Doggett, A. Zharkikh, S. V. Tavtigian, D. Pruss, M. Barnstead, C. Evans, H. Baden, J. Powell, G. Glusman, L. Rowen, L. Hood, Y. H. Tan, G. Elgar, T. Hawkins, B. Venkatesh, D. Rokhsar, and S. Brenner, "Whole-genome shotgun assembly and analysis of the genome of *Fugu rubripes*," *Science* **297**, 1301 (2002).  
**URL** <http://www.jgi.doe.gov/>

## QM/MM Studies of the Triosephosphate Isomerase-Catalyzed Reaction

Triosephosphate isomerase (TIM) is a dimeric enzyme that catalyzes the conversion between dihydroxyacetone phosphate (DHAP) and R-glyceraldehyde 3-phosphate (GAP), which is an important step in glycolysis (the enzymatic breakdown of carbohydrates). TIM increases the reaction rate by more than  $10^9$  times, and has thus been referred to as a “perfect” enzyme. Many experimental techniques have been used to study the enzyme, supplemented by a number of theoretical calculations, but the complex catalytic mechanisms are not yet fully understood. However, detailed calculations by Cui and Karplus are providing a wealth of information and bringing us closer to a complete solution.

Three possible mechanisms for the second step of TIM-catalyzed reactions, which involves a proton transfer, have been studied by the combined quantum mechanical/molecular mechanical (QM/MM) approach at a number of QM levels (Figure 3). Cui and Karplus compared the various QM levels to verify the adequacy of their recent MM analysis of the reaction mechanism, which ruled out one of the proposed

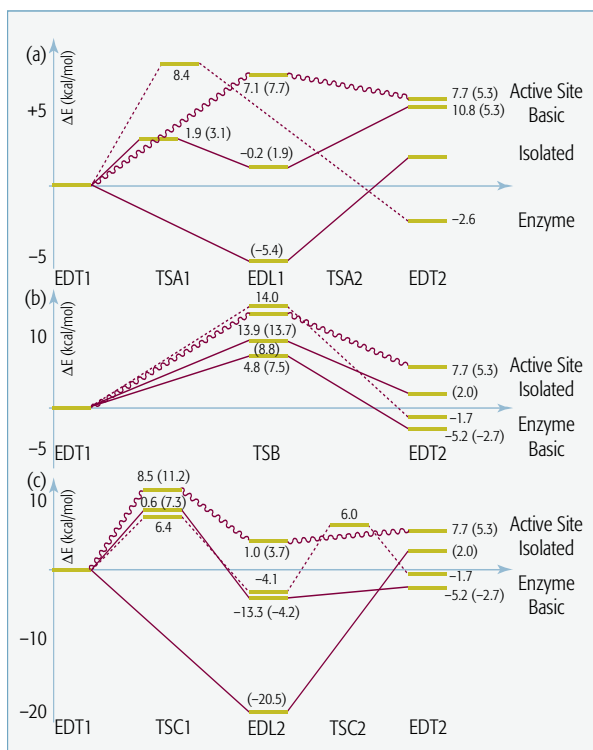
pathways. The relative contributions from the two other proposed pathways, however, are difficult to determine at the present level of theory, and both pathways are consistent with available experiments.

Density functional calculations were conducted for model systems in the gas phase and in solution, and selected models were also studied with *ab initio* calculations. The QM model calculations in solution and a QM/MM perturbation analysis showed that a number of factors combine to yield the factor of  $10^9$  reaction rate enhancement by TIM. These include orienting catalytic groups in good positions for the proton transfers, employing charged and polar groups that stabilize the reaction intermediates, and permitting flexibility of the catalytic groups. Some residues far from the active site as well as certain water molecules also make significant contributions. For the electrostatic interaction and polarization to function effectively, the active site of TIM has a relatively low effective dielectric constant, which reflects the structural integrity of the enzyme active site as compared with solution. Short hydrogen bonds occur during the reaction, but the calculated energetics indicate that they do not have a specific role in catalysis.

**INVESTIGATORS** M. Karplus and Q. Cui, Harvard University.

**PUBLICATION** Q. Cui and M. Karplus, “Quantum mechanical/molecular mechanical studies of the triosephosphate isomerase-catalyzed reaction: Verification of methodology and analysis of reaction mechanisms,” *J. Phys. Chem. B* **106**, 1768 (2002).

**URL** <http://www.chem.harvard.edu/faculty/karplus.html>



**FIGURE 3** Relative energies for three different models along the alternative proton-transfer steps.

## Tropopause Height As an Indicator of Climate Change

Studies of human influence on global climate change have focused mostly on changes in surface or atmospheric temperatures. But climate change should be manifest in a variety of climate variables, not just temperature. One variable that has just been examined for the first time from a climate-change standpoint is the height of the tropopause—the transition zone between the turbulently mixed troposphere and the more stably stratified stratosphere.

Santer et al. have examined changes in tropopause height, diagnosing the pressure of the lapse rate tropopause ( $p_{LRT}$ ) from reanalyses of observational data and from integration of simulations performed with coupled and uncoupled climate models

(Figure 4). (Lapse rate is the rapidity with which temperature decreases with altitude.) Simulated  $p_{LRT}$  trends over the past several decades are consistent with reanalysis results. The increase in tropopause height seems to be driven by the warming of the troposphere by greenhouse gases and the cooling of the stratosphere by ozone depletion. Changes in tropopause height deserve further attention because they may be a useful “fingerprint” of human effects on climate.

**INVESTIGATORS** M. F. Wehner, Lawrence Berkeley National Laboratory; B. D. Santer, J. S. Boyle, K. AchutaRao, C. Doutriaux, and K. E. Taylor, Lawrence Livermore National Laboratory; G. A. Meehl, W. Washington, and T. M. L. Wigley, National Center for Atmospheric Research; R. Sausen, German Aerospace Center; J. E. Hansen, R. Ruedy, and G. Schmidt, NASA Goddard Institute for Space Studies; E. Roeckner, Max Planck Institute for Meteorology.

**PUBLICATION** B. D. Santer, R. Sausen, T. M. L. Wigley, J. S. Boyle, K. AchutaRao, C. Doutriaux, J. E. Hansen, G. A. Meehl, E. Roeckner, R. Ruedy, G. Schmidt, and K. E. Taylor, "Behavior of Tropopause Height and Atmospheric Temperature in Models, Reanalyses, and Observations: Decadal Changes," *J. Geophys. Res.* **108**, 10.1029/2002JD002258 (2003).

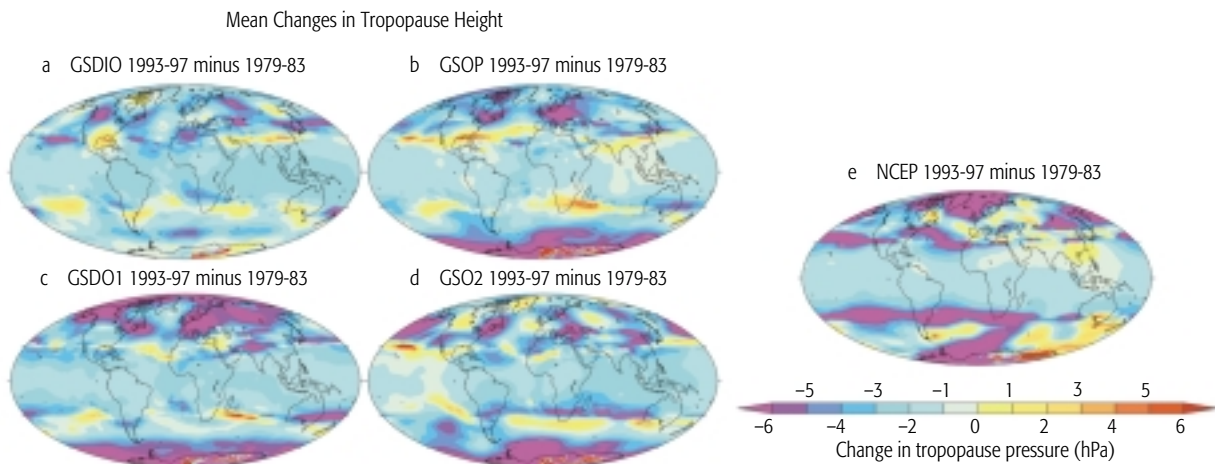
**URL** <http://www-pcmdi.llnl.gov/>

## BENJAMIN SANTER RECEIVES 2002 E. O. LAWRENCE AWARD

On September 26, Secretary of Energy Spencer Abraham named Benjamin D. Santer of Lawrence Livermore National Laboratory as one of the seven winners of the 2002 Ernest Orlando Lawrence Award. Each winner received a gold medal, a citation, and \$25,000. Santer, a physicist, was honored in the Environmental Science and Technology category and is the first Lawrence awardee to be honored for research in climate modeling. The award cited "his seminal and continuing contributions to our understanding of the effects of human activities and natural phenomena on the Earth's climate system."



Santer runs sophisticated computer models at NERSC and elsewhere to understand the nature and causes of global climate change. In 1998 Santer was named a MacArthur Fellow in recognition of his "originality, creativity, self-direction, and capacity to contribute importantly to society particularly in atmospheric science."



**FIGURE 4** Changes in annual-mean  $p_{LRT}$  patterns in four ECHAM climate-change experiments (panels a–d) and in the NCEP reanalysis (panel e). Changes are defined as the average over 1993–1997 minus the average over 1979–1983.



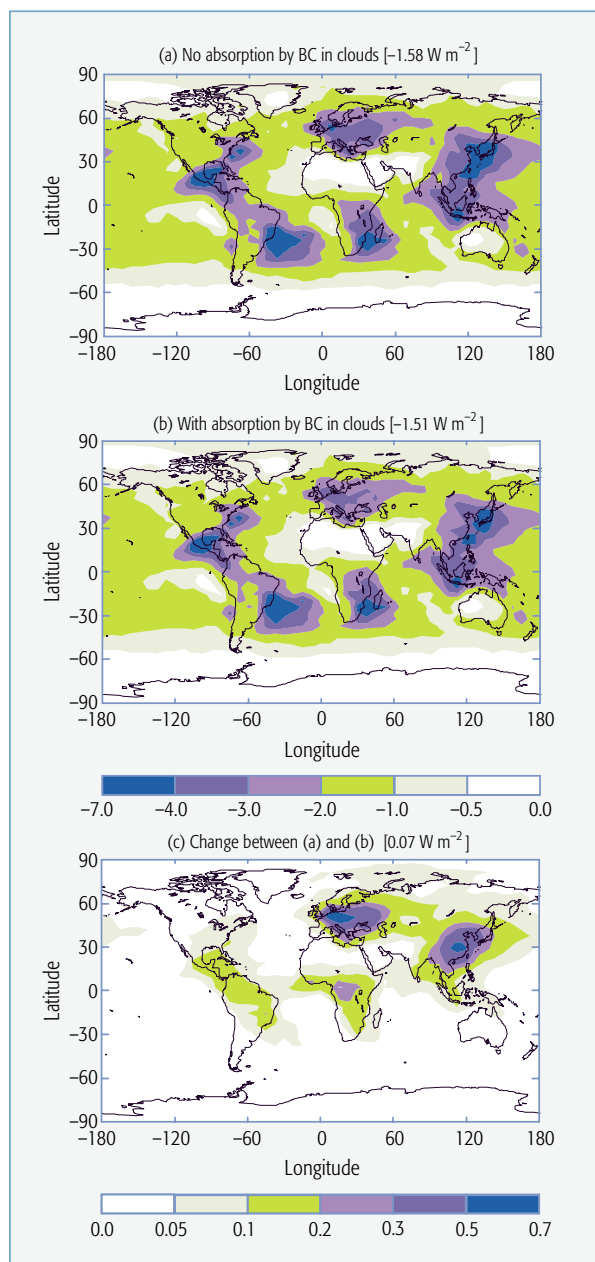
## Cloud Sensitivity to Black Carbon and Aerosol Concentrations

While greenhouse gases get most of the attention in studies of global climate change, aerosols—suspensions of small particles in the air, such as dust, sea salt, and soot—can also affect climate in two ways: (1) they scatter and absorb radiation (the *direct effect*), and (2) they change the microphysical structure of clouds (the *indirect effect*). Aerosols can act as cloud condensation nuclei, increasing the number and decreasing the size of cloud droplets, a process called the *first*

*indirect forcing* or *Twomey effect*; they can also affect the initial size distribution of precipitation drops, thereby influencing the cloud lifetime and liquid water content (the *second indirect effect*). Human activity, especially fossil fuel and biomass combustion, has greatly increased the amount of aerosols in the atmosphere. Whether these aerosols contribute to climate warming or cooling depends on many factors, and including those factors in global climate models can increase their accuracy.

Chuang et al. have simulated and quantified the first indirect effect of aerosols, its sensitivity to natural and anthropogenic emissions, and the role of absorption by black carbon in clouds. The first indirect effect is generally thought to contribute to cooling by increasing cloud albedo (reflectivity). The sensitivity of cloud albedo to changes in drop number concentration is referred to as *cloud susceptibility*. But black carbon from combustion counteracts this effect by absorbing radiation and decreasing albedo.

The simulated contribution of anthropogenic aerosols to cloud susceptibility is consistent with satellite data and confirms previous findings that marine stratus clouds are more sensitive to changes in drop concentration than continental clouds. However, if the effect of black carbon absorption in clouds is not included, the first indirect forcing by anthropogenic aerosols may be overestimated by 15–25% in regions where black carbon emissions are pronounced (Figure 5). The first indirect forcing is also highly sensitive to the abundance of natural aerosols; without accounting for natural dust and sea salt particles, it could be overestimated by at least a factor of 2. If half of dust emissions are due to human activities, these might be responsible for additional forcing. The researchers concluded that to quantify the first indirect effect on the radiation budget with a higher level of certainty, we need further understanding of the interactions between anthropogenic components and natural particles, together with a more thorough investigation of aerosol–cloud interactions.



**FIGURE 5** Annual average of the simulated first indirect forcing ( $\text{W m}^{-2}$ ) by anthropogenic carbonaceous aerosols (a) without absorption by black carbon in clouds and (b) with absorption. (c) Increases in the magnitude of forcing if the effect of black carbon is not taken into account. Values shown in brackets are global averages.

**INVESTIGATORS** J. E. Penner, University of Michigan; C. C. Chuang and K. E. Grant, Lawrence Livermore National Laboratory; J. M. Prospero, University of Miami; G. H. Rau, University of California, Santa Cruz; K. Kawamoto, Virginia Polytechnic Institute and NASA Langley Research Center.

**PUBLICATION** C. C. Chuang, J. E. Penner, J. M. Prospero, K. E. Grant, G. H. Rau, and K. Kawamoto, "Cloud susceptibility and the first aerosol indirect forcing: Sensitivity to black carbon and aerosol concentrations," *J. Geophys. Res.* (in press).

**URL** <http://aoss.engin.umich.edu/Penner/>

# Fusion Energy Sciences

NERSC has historically been the leading computer center for fusion energy research. Insights resulting from computational studies at NERSC have contributed to the progress of both the magnetic confinement (tokamak and stellarator) and the inertial confinement (heavy ion) fusion programs.

A major contribution to magnetic confinement research this year was a numerical study of tokamak plasmas that cleared up a discrepancy between theory and experimental results by showing that toroidal flows have a stabilizing effect on sawtooth instability. Another study comparing magnetohydrodynamics (MHD) stability code calculations with high-resolution diagnostic measurements from the DIII-D tokamak experiment showed close quantitative agreement in many cases, demonstrating the maturity of the codes. And the NIMROD code was used for detailed exploration of the onset mechanisms of instabilities in the DIII-D on multiple time scales.

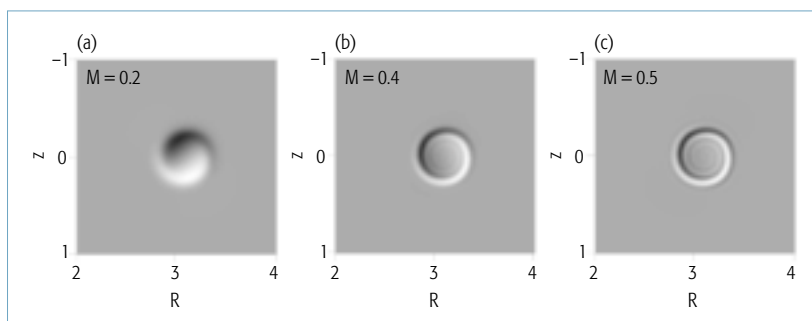
In heavy ion fusion research, simulations of alternative beam transport schemes revealed the strengths and weaknesses of each approach, contributing valuable information to assist in the design of both the accelerator and the fusion target. And to improve the accuracy of heavy ion fusion simulations, researchers are developing algorithms to synthesize the 4D phase space distribution of ion beams from the reduced 2D experimental data.

## Stabilization of Sawteeth in Tokamaks with Toroidal Flows

The maximum temperature in tokamak experiments is often limited by the occurrence of sawteeth. During a discharge with sawteeth, there is a rapid, fractional drop in the central temperature, followed by a slower increase as the temperature recovers. This process then repeats periodically. The resulting time trace of the central temperature resembles sawteeth.

MHD theory predicts that tokamak plasmas are unstable to sawteeth when the safety factor  $q$  is less than unity. But experiments on tokamaks have demonstrated that tokamaks can be free of sawteeth even when  $q < 1$ . Kleva and Guzdar have used NERSC computers to numerically study the stability of tokamak plasmas with  $q < 1$ , including the effect of a sheared toroidal flow in the plasma.

Their numerical results demonstrate that when the magnitude of a sheared toroidal flow approaches the speed of sound, the resulting centrifugal force becomes large enough to impact the toroidal equilibrium (Figure 1); a toroidal flow can completely stabilize the  $n = 1$  mode in tokamaks with  $q_0 < 1$ . In the absence of flows, the growth rate of the  $n = 1$  mode rises as  $\beta$  increases because of the increasing pressure gradient. However, the addition of a toroidal flow to the equilibrium has a stabilizing effect. As the magnitude of the flow approaches the speed of sound, the  $n = 1$  mode can be completely stabilized, eliminating sawteeth. The simulations demonstrate that, in addition to the current and pressure profiles, the toroidal velocity profile must be included in sawtooth stability analyses of tokamaks.



**FIGURE 1** Mode structure with increasing flow speed. The real part of the pressure perturbation of the  $n = 1$  mode is plotted in the poloidal plane  $(R, z)$  for Mach number  $M =$  (a) 0.2, (b) 0.4, and (c) 0.5. The light area is the region where the pressure perturbation is positive, while the region of negative perturbed pressure is dark.

**INVESTIGATORS** P. N. Guzdar, W. Dorland, J. Drake, A. Hassam, and R. G. Kleva, University of Maryland.

**PUBLICATION** R. G. Kleva and P. N. Guzdar, "Stabilization of sawteeth in tokamaks with toroidal flows," *Phys. Plasmas* 9, 3013 (2002).

**URL** <http://www.ireap.umd.edu/Theory/research.htm>

## Predictive Capability of MHD Stability Limits in Tokamak Discharges

Development of a fully predictive capability for the MHD stability limits in high performance tokamak discharges is critical to the success of the Advanced Tokamak program. The theory and experimental diagnostic capabilities have now been developed to the point where detailed predictions can be productively tested so that competing effects can be isolated and either eliminated or confirmed. Turnbull et al. have tested discharge equilibrium reconstruction simulations against observations for the principal limiting phenomena in the DIII-D experiment: L-mode negative central shear (NCS) disruptions, H-mode NCS edge instabilities, and tearing and resistive wall modes (RWMs) in long pulse discharges.

In the case of predominantly ideal MHD instabilities, agreement between the predictions and experimentally

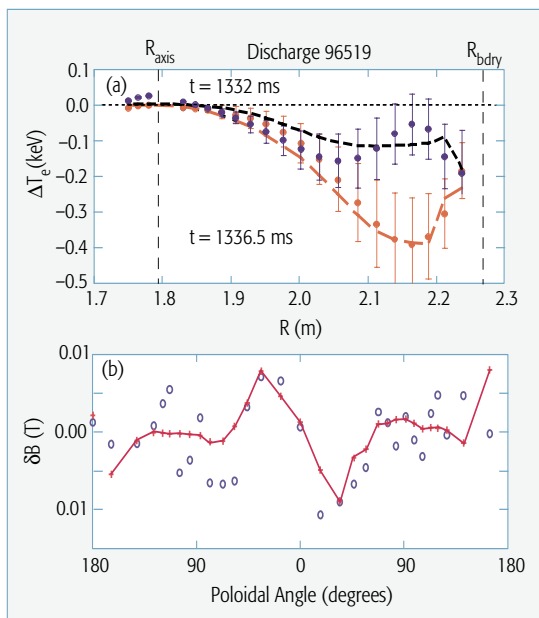
observed stability limits and thresholds can now be obtained to within several percent, and the predicted fluctuations and growth rates to within the estimated experimental errors. Edge instabilities can be explained by a new model for edge localized modes as predominantly ideal low to intermediate  $n$  modes. Accurate ideal calculations are critical to demonstrating RWM stabilization by plasma rotation, and the ideal eigenfunctions provide a good representation of the RWM structure when the rotation slows (Figure 2). Ideal eigenfunctions can then be used to predict stabilization using active feedback.

For non-ideal modes, the agreement is approaching levels similar to those for the ideal comparisons;  $\Delta'$  calculations, for example, indicate that some discharges are linearly unstable to classical tearing modes, consistent with the observed growth of islands in those discharges.

**INVESTIGATORS** A. D. Turnbull, M. S. Chu, L. L. Lao, J. R. Ferron, P. B. Snyder, D. A. Humphreys, R. J. La Haye, T. C. Luce, E. J. Strait, and T. S. Taylor, General Atomics; D. Brennan, Oak Ridge Institute for Science Education; A. M. Garofalo and J. Bialek, Columbia University; I. N. Bogatu, D. H. Edgell, and J. S. Kim, FARTECH; J. D. Callen and K. Comer, University of Wisconsin, Madison; M. S. Chance and M. Okabayashi, Princeton Plasma Physics Laboratory; S. A. Galkin, University of California, San Diego; B. W. Rice, Lawrence Livermore National Laboratory; H. R. Wilson, Culham Laboratory, UK Atomic Energy Authority.

**PUBLICATION** A. D. Turnbull, D. Brennan, M. S. Chu, L. L. Lao, J. R. Ferron, A. M. Garofalo, P. B. Snyder, J. Bialek, I. N. Bogatu, J. D. Callen, M. S. Chance, K. Comer, D. H. Edgell, S. A. Galkin, D. A. Humphreys, J. S. Kim, R. J. La Haye, T. C. Luce, M. Okabayashi, B. W. Rice, E. J. Strait, T. S. Taylor, and H. R. Wilson, "Predictive capability of MHD stability limits in high performance DIII-D discharges," *Nucl. Fusion* (in press).

**URL** <http://web.gat.com/theory/>



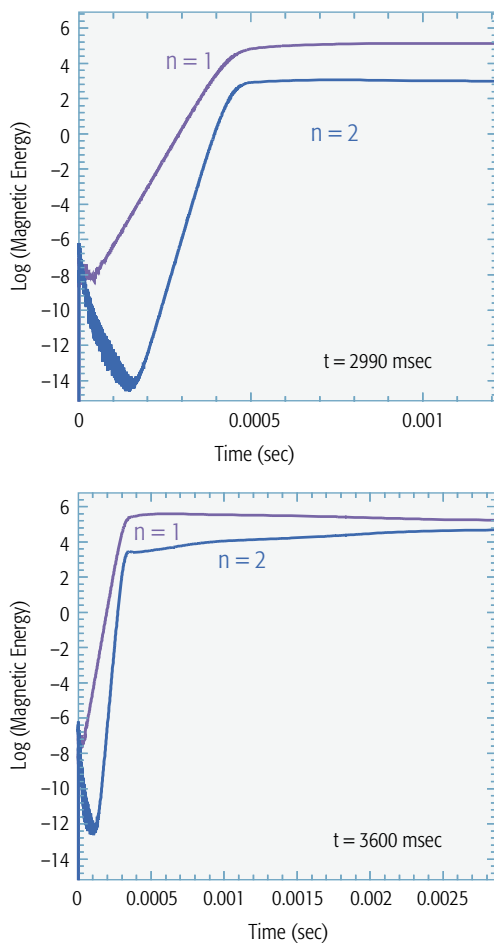
**FIGURE 2** Predicted (a) radial ECE profile and (b) poloidal Mirnov signal for the RWM in DIII-D discharge 96519 compared to measured diagnostic signals. The ECE profile in (a) shows two times with different toroidal phase.

## Nonlinear MHD Dynamics of Tokamak Plasmas on Multiple Time Scales

Long wavelength instabilities in fusion plasmas are often described within the framework of MHD theory. The various types of instabilities have different time scales associated with their growth. In real experiments, an understanding of how the growth rate varies with the free energy source is important for fully understanding the stability limits and the subsequent growth of the mode.

Kruger et al. have used the NIMROD code to explore the onset mechanisms of instabilities in the DIII-D tokamak experiment. In their first simulations, they modeled the disruption occurring in DIII-D discharge 87009 as an ideal MHD instability driven by neutral-beam heating. The mode grows faster than exponential, but on a time scale that is a hybrid of the heating rate and the ideal MHD growth rate as predicted by analytic theory.

The second series of simulations, which occur on a much longer time scale, focus on the seeding of tearing modes by sawteeth, where pressure effects play a role both in the exterior region solutions and in the neoclassical drive terms (Figure 3). The ability to routinely run simulations of tokamak discharges at realistic values of diffusivities (kinetic, electrical, and thermal) has greatly increased the power of these calculations to make quantitative comparisons with experimental results.



**FIGURE 3** Plot of tearing mode energies in DIII-D discharge 86166, where a series of nearly identical sawteeth led to the emergence of a confinement-degrading  $3/2$  mode. Despite similar equilibria, the  $m/n = 3/2$  island grows in the later discharge after the sawtooth.

**INVESTIGATORS** D. D. Schnack and S. E. Kruger, Science Applications International Corporation; D. P. Brennan, General Atomics; T. A. Gianakon, Los Alamos National Laboratory; C. R. Sovinec, University of Wisconsin, Madison.

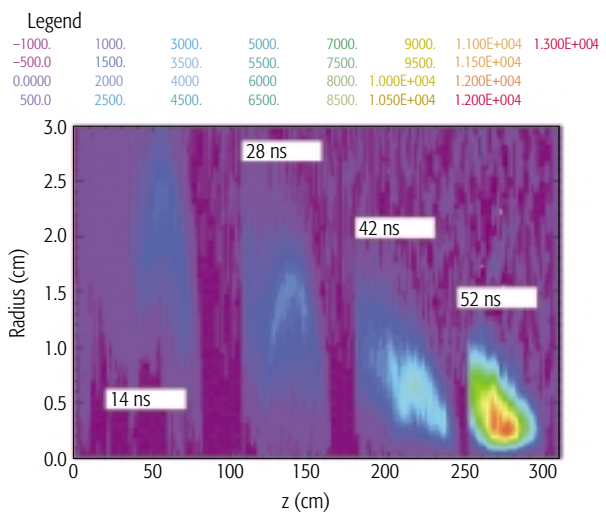
**PUBLICATION** S. E. Kruger, D. D. Schnack, D. P. Brennan, T. A. Gianakon, and C. R. Sovinec, "Nonlinear MHD dynamics of tokamak plasmas on multiple time scales," Nucl. Fusion (in press).

**URL** <http://www.nimrodteam.org/>

## Simulations of Heavy Ion Beams in a Gaseous Fusion Target Chamber

For heavy-ion inertial confinement fusion, ion beams must be transported and focused over several meters through the chamber to the target. A sizable transport distance prevents damage to the final focus section of the accelerator from the target explosion. The selection of transport schemes impacts the design not only of the accelerator but also of the fusion target driven by the beams. Ballistic transport uses a final focusing lens just outside the chamber to focus each beam onto the target and a supply of electrons to provide neutralization. Pinched transport uses a final focusing lens to focus each beam to a small radius at the entrance to the chamber, and then the beam propagates in the chamber at small radius to the target.

Welch et al. have conducted state-of-the-art simulations of three transport scenarios—neutralized-ballistic transport



**FIGURE 4** For the initial NBT plasma simulation, the net current contained within the radius is plotted with time moving clockwise:  $t = 14, 28, 42, 52$  ns. The legend unit is amps.

(NBT, Figure 4), assisted-pinch transport (APT), and self-pinch transport (SPT)—as they pertain to a thick-liquid wall chamber (radius of 3 m). Their intent was to assess strengths, weaknesses, and areas for future work.

No obvious showstoppers were uncovered for any of the transport schemes. Given a judicious placement of plasmas, the simulations suggest a nearly ballistic final spot can be achieved for NBT. Outstanding physics issues for NBT include the 3D effects of beam-beam interactions, target charging, and the interaction with the flibe jets. The APT simulations are encouraging in that nearly 90% energy transport is achieved; the discharge channel naturally guides the beam from the chamber wall to the target, unlike the two other schemes. Future work on APT must include more realistic modeling of beam-plasma interactions and gas chemistry. The meter-long SPT simulation is encouraging in that a stable 2D equilibrium is found with tolerable late-time erosion rate. A key issue may be the transport efficiency, which appears to be degraded by transient beam evaporation.

**INVESTIGATORS** R. Davidson, W. W. Lee, H. Qin, and E. Startsev, Princeton Plasma Physics Laboratory; D. R. Welch, D. V. Rose, B. V. Oliver, T. C. Genoni, and R. E. Clark, Mission Research Corporation; C. L. Olson, Sandia National Laboratories; S. S. Yu, Lawrence Berkeley National Laboratory.

**PUBLICATION** D. R. Welch, D. V. Rose, B. V. Oliver, T. C. Genoni, R. E. Clark, C. L. Olson, and S. S. Yu, "Simulations of intense heavy ion beams propagating through a gaseous fusion target chamber," *Phys. Plasmas* **9**, 2344 (2002).

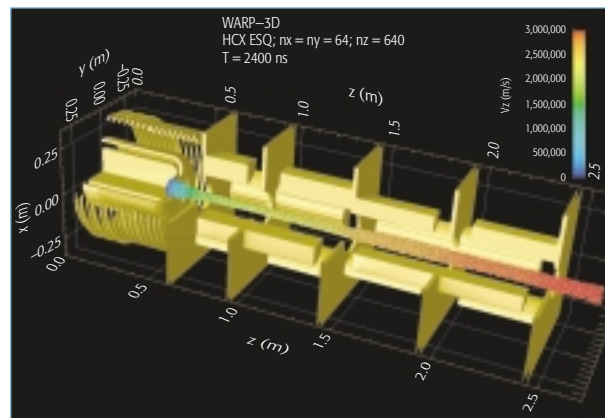
**URL** <http://nonneutral.pppl.gov/best.htm>

## Synthesizing a 4D Beam Particle Distribution from Multiple 2D Views

Discrete-particle simulations are commonly employed to understand the behavior of particle beams in heavy ion fusion. Integrated simulations, beginning at the source and carried out in full time-dependent 3D, or a reduced description when appropriate, offer the promise of the greatest fidelity in describing the long-term beam behavior. However, the source, injector, and beamline upstream of a section of interest in an experiment are usually not completely characterized. Thus,

the beam distribution function in a simulation beginning at the source generally drifts away from the experimentally measured beam distribution, and it can be challenging to adjust the beamline description and other parameters in the simulation to bring them back into agreement.

As a complement to integrated simulations and as a tool for routine experimental analysis, Friedman et al. are developing the ability to launch particle simulations of "real" experiments, using an initial beam particle distribution derived from experimental measurements at a station partway along the machine (Figure 5). Specifically, they have begun developing algorithms to synthesize the 4D phase space distribution of the beams from the reduced 2D experimental data. Their initial simulations verify the importance of such a synthetic procedure, since simulations launched using simpler model distributions with low-order moments matching those of the observed beam fail to reproduce the correct dynamics.



**FIGURE 5** WARP-3D simulation of the electrostatic quadrupole injector at the front end of the High Current Experiment (HCX); the simulated beam at the exit plane was used as a test problem for the new 4D synthesis algorithms.

**INVESTIGATORS** A. Friedman and D. P. Grote, Lawrence Livermore National Laboratory; C. M. Celata and J. W. Staples, Lawrence Berkeley National Laboratory.

**PUBLICATION** A. Friedman, D. P. Grote, C. M. Celata, and J. W. Staples, "Synthesizing a four-dimensional beam particle distribution from multiple two-dimensional views," *Phys. Rev. ST Accel. Beams* (submitted); Lawrence Berkeley National Laboratory report LBNL-49647.

**URL** <http://hif.lbl.gov/>



# High Energy and Nuclear Physics

The DOE Office of High Energy and Nuclear Physics sponsors major experimental facilities and theoretical studies, as well as computational simulations and analyses of experimental data.

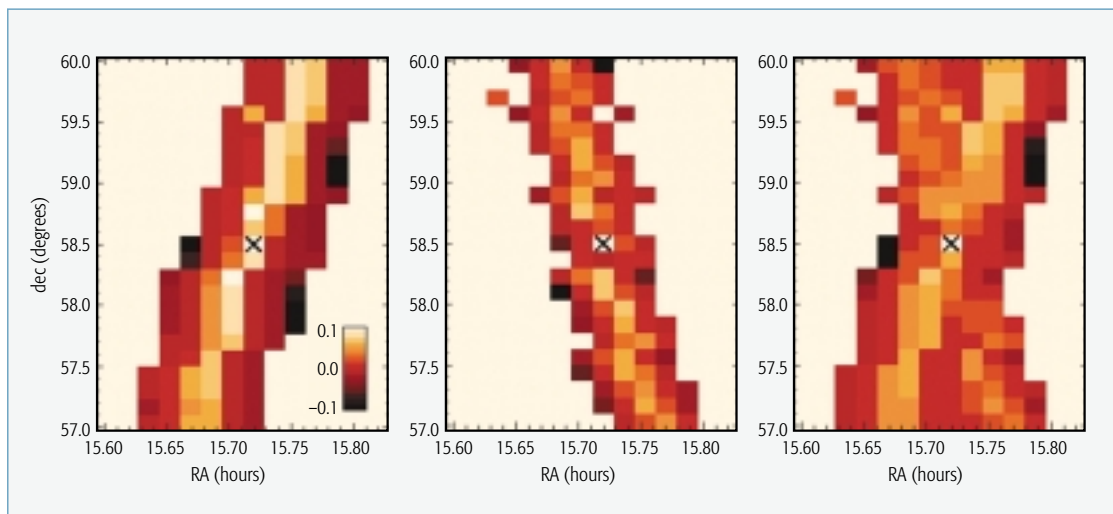
In 2002 the MAXIMA data analysis team documented their successful approach to recovering a map of the cosmic microwave background (CMB); their methods will be applicable to other CMB experiments. Accomplishments in nuclear physics included the only quantum Monte Carlo calculations of 6- through 10-nucleon systems that use realistic interactions and are accurate to 1–2% for the binding energies.

Research in lattice quantum chromodynamics (QCD) included the first simulations to explore the finite temperature phase diagram with an improved staggered fermion action; a study of chiral properties of pseudoscalar mesons with overlap fermions; and simulations of lattice QCD at finite isospin density.

## Making Maps of the Cosmic Microwave Background

The cosmic microwave background (CMB), a “snapshot” of the Universe as it was only 300,000 years after the Big Bang, provides the most powerful discriminant between different cosmological models. To date, CMB datasets have ruled out an entire class of models (based on topological defects) for the generation of primordial density perturbations in the Universe; have demonstrated the spatial flatness of the Universe as a whole; and, coupled with supernova data, have given a first measurement of the overall mass-energy budget for the Universe.

There is much more information still to be mined from CMB data, especially from current and future satellite missions (MAP and Planck), but the size of the datasets presents new challenges for timely and precise data analysis. Stompor et al. have documented how those challenges were met successfully in the analysis of data from the MAXIMA-I balloon-borne experiment, which required improvement of existing methods and tools as well as development and testing of new ones.



**FIGURE 1** Pixel domain correlations of the noise projected on the sky. All three panels show a level of the correlations relative to the rms value of the noise for the same pixel, which is marked with an  $\times$ . This pixel was observed twice during the MAXIMA-I flight. The noise correlations for the first observation are shown in the left panel, and these for the second one in the middle panel. The right panel shows the final co-added noise correlations. Due to the MAXIMA-I scanning strategy and the presence of the noise correlations in the time domain, the noise correlation pattern in pixel domain is highly anisotropic and strongly correlated as a result of any single observation of a pixel. However, the combined noise for all pixels that were observed twice is significantly less correlated and more isotropic.



The MAXIMA collaborators present a comprehensive, consistent approach to recovering a map of the sky and estimating its error matrix in realistic circumstances. Their approach includes data preprocessing and noise estimation; a suite of different map-making methods that simultaneously produce both a map and a corresponding pixel-pixel noise correlation matrix (Figure 1); ways of handling systematic effects within the general framework of maximum likelihood map making; iterative algorithms for time-domain noise estimation; and numerical tests for checking the consistency of the analysis. Their methods are expected to be applicable to other current and future CMB experiments.

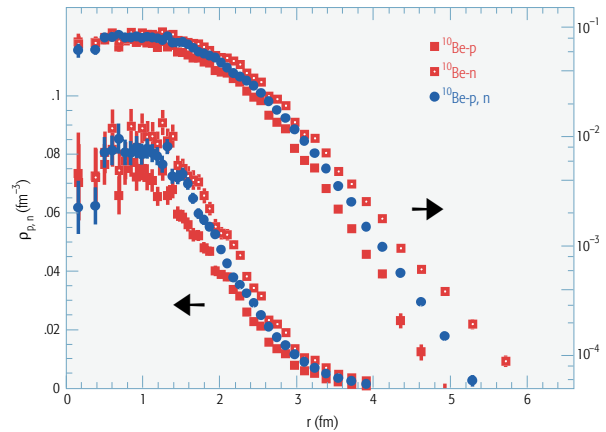
**INVESTIGATORS** J. D. Borrill and G. F. Smoot, Lawrence Berkeley National Laboratory and University of California, Berkeley; R. Stompor, University of California, Berkeley and Copernicus Astronomical Center, Warsaw; A. H. Jaffe, A. T. Lee, S. Oh, B. Rabii, P. L. Richards, C. D. Winant, and J. H. P. Wu, University of California, Berkeley; A. Balbi, Università Tor Vergata, Rome; P. G. Ferreira, University of Oxford; S. Hanany, University of Minnesota.

**PUBLICATION** R. Stompor, A. Balbi, J. D. Borrill, P. G. Ferreira, S. Hanany, A. H. Jaffe, A. T. Lee, S. Oh, B. Rabii, P. L. Richards, G. F. Smoot, C. D. Winant, and J. H. P. Wu, "Making maps of the cosmic microwave background: The MAXIMA example," *Phys. Rev. D* **65**, 022003 (2001).

**URL** <http://www.nersc.gov/~borrill/>

## Exact Calculations of Light Nuclei Using Realistic Interactions

One of the principal goals of nuclear physics is to explain the properties and reactions of nuclei in terms of interacting nucleons (protons and neutrons). There are two fundamental aspects to this problem: (1) determining the interactions between nucleons, and (2) given the interactions (i.e., the Hamiltonian) making accurate calculations of many-nucleon systems. S. C. Pieper and collaborators work in both areas and have made the only calculations of 6- through 10-nucleon systems that use realistic interactions and that are accurate to 1–2% for the binding energies. The resulting wave functions can be used to compute properties measured at electron and hadron scattering facilities (in particular Jefferson Lab), and to compute astrophysical reaction rates, many of which cannot be measured in the laboratory.



**FIGURE 2** Proton and neutron densities for  $A = 10$  nuclei on both linear (left) and logarithmic (right) scales.

Pieper et al. performed quantum Monte Carlo calculations of the ground and low-lying excited states of  $A = 9, 10$  nuclei using realistic Hamiltonians containing a two-nucleon potential alone or with one of several three-nucleon potentials (Figure 2). They concluded that a fairly consistent picture of nuclear binding can be constructed for  $A \leq 10$  nuclei using a single Hamiltonian and a single computational framework. This applies also to the energy differences among isobaric multiplets, which are well reproduced. Electromagnetic moments, within the limitation of the impulse approximation, are in fairly good agreement with experimental data.

**INVESTIGATORS** S. C. Pieper, K. Varga, and R. B. Wiringa, Argonne National Laboratory.

**PUBLICATION** S. C. Pieper, K. Varga, and R. B. Wiringa, "Quantum Monte Carlo calculations of  $A = 9, 10$  nuclei," *Phys. Rev. C* (submitted); preprint nucl-th/0206061 (2002).

**URL** <http://www.phy.anl.gov/theory/research/forces.html>

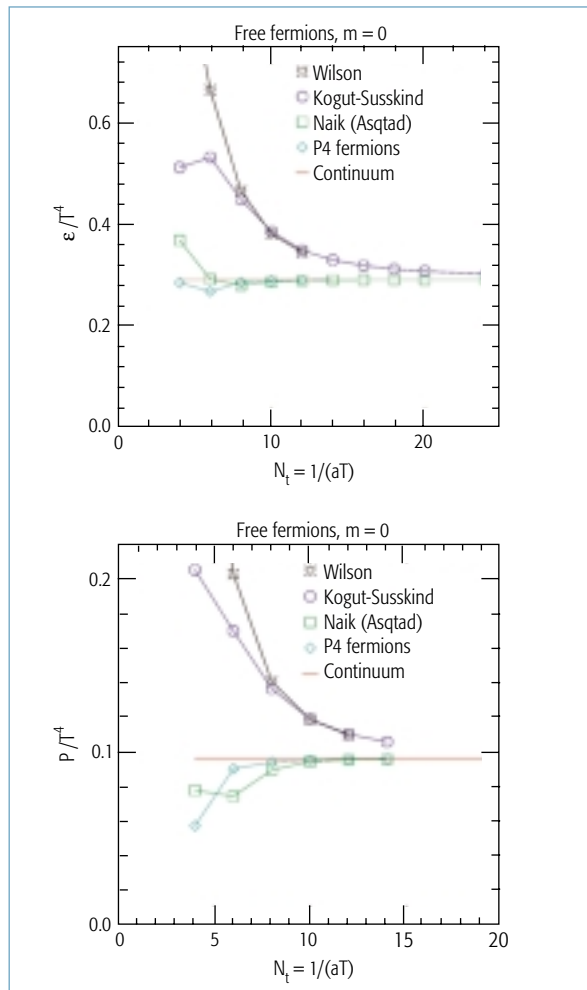
## Thermodynamics with Improved Staggered Quarks

With the Relativistic Heavy Ion Collider now producing data, it has become even more important to understand the phase diagram of QCD at finite temperature, and to determine properties of the high temperature quark-gluon plasma phase with confidence, i.e., with controlled lattice spacing errors.

The MILC Collaboration has published preliminary results from exploring the phase diagram of finite temperature QCD

with three degenerate flavors and with two light flavors and the mass of the third held approximately at the strange quark mass. The simulations used an improved staggered fermion action, the "Asqtad" action, which reduces flavor symmetry breaking so that all pions are lighter than the kaon already at larger lattice spacing. This action also improves rotational symmetry and the dispersion relation, leading to diminished lattice artifacts in energy density and pressure (Figure 3).

**INVESTIGATORS** D. Toussaint and T. Burch, University of Arizona; C. Bernard, Washington University; S. Datta and S. Gottlieb, Indiana University; T. A. DeGrand, University of Colorado; C. E. DeTar, University of Utah; U. M. Heller, Florida State University; K. Orginos, Brookhaven National Laboratory; R. L. Sugar, University of California, Santa Barbara.



**FIGURE 3** The energy density (top) and pressure (bottom) of free massless fermions as function of temporal lattice size  $N_t$ . For free fermions the "Asqtad" action reduces to the Naik action.

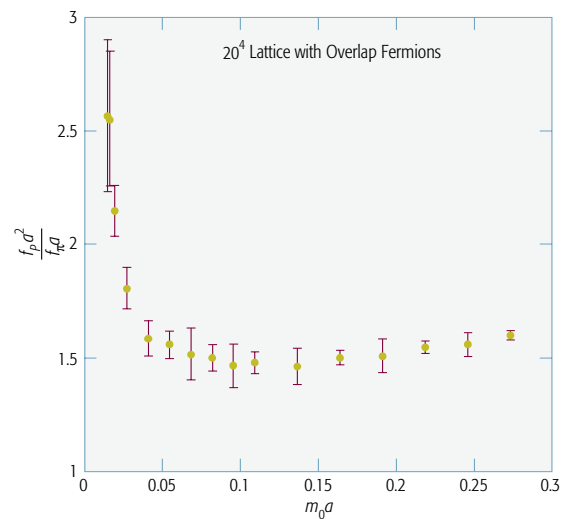
**PUBLICATION** C. Bernard, T. Burch, S. Datta, T. A. DeGrand, C. E. DeTar, S. Gottlieb, U. M. Heller, K. Orginos, R. L. Sugar, and D. Toussaint, "Thermodynamics with 2+1 and 3 flavors of improved staggered quarks," Nucl. Phys. A **702**, 140 (2002).

**URL** <http://www.physics.ucsb.edu/~sugar/poster.ps>

## Chiral Properties of Pseudoscalar Mesons

One of the main goals of lattice QCD is to understand from first principles low-energy phenomenology as a consequence of chiral symmetry. Recent advances in the formulation of chiral fermions on the lattice hold great promise for studying chiral symmetry of QCD at finite lattice spacing.

Dong et al. used the overlap fermion on a quenched  $20^4$  lattice to numerically study the chiral properties of pseudoscalar mesons. They elucidated the role of the zero modes in the meson propagators, particularly that of the pseudoscalar meson. The non-perturbative renormalization constant  $Z_A$  was determined from the axial Ward identity and was found to be almost independent of the quark mass for the range of quark masses studied; this implies that the  $O(a^2)$  error is small. The pion decay constant  $f_\pi$  was calculated, from which the lattice spacing of 0.148 fm was determined. The authors looked for the quenched chiral log in the pseudoscalar decay constants and the pseudoscalar masses and found clear evidence



**FIGURE 4** Renormalized  $f_\rho a^2 / f_\pi a^2$  vs.  $m_\rho^2 a^2$ , which confirms that the chiral log singularity is indeed present in  $f_\rho$ . The solid line is a fit over the lowest 14 points.

for its presence (Figure 4). The chiral log parameter  $\delta$  was determined to be in the range 0.15–0.4, which is consistent with that predicted from quenched chiral perturbation theory.

The overlap fermion was shown to be a reliable tool for studying the chiral symmetry properties of hadrons at low energies, including the quenched chiral logs. Future work will study the continuum limit with different lattice spacings.

**INVESTIGATORS** K. F. Liu, S. J. Dong, T. Draper, and I. Horváth, University of Kentucky; F. X. Lee, George Washington University and Jefferson Laboratory; J. B. Zhang, University of Adelaide, Australia.

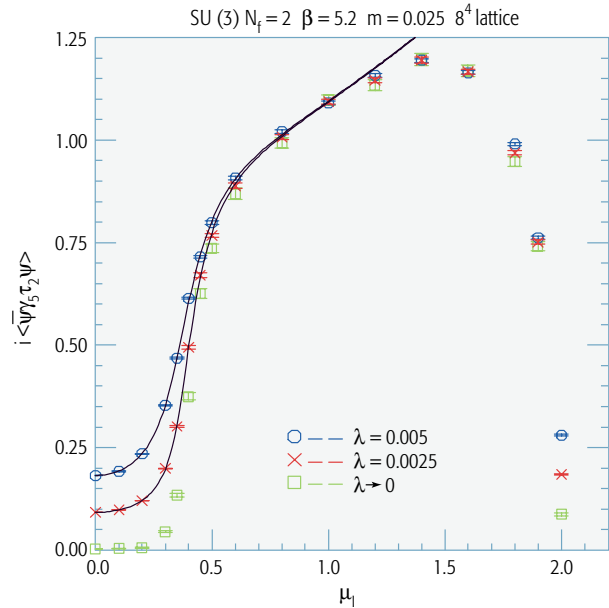
**PUBLICATION** S. J. Dong, T. Draper, I. Horváth, F. X. Lee, K. F. Liu, and J. B. Zhang, "Chiral properties of pseudoscalar mesons on a quenched  $20^4$  lattice with overlap fermions," *Phys. Rev. D* **65**, 054507 (2002).

**URL** <http://www.pa.uky.edu/~liu/>

## Lattice QCD at Finite Isospin Density

QCD at finite temperature and density describes the physics of the early Universe, neutron stars, heavy nuclei, and relativistic heavy ion collisions. Nuclear matter exists not only at finite baryon number, but also at finite negative isospin ( $I_3$ ) density. QCD at finite chemical potential  $\mu_1$  for  $I_3$  has a positive fermion determinant and thus can be simulated using hybrid molecular dynamics methods.

Kogut and Sinclair have simulated QCD at zero temperature,  $\beta = 5.2$ , and finite  $\mu_1$  on  $8^4$  lattices at quark mass  $m = 0.025$  and  $m = 0.05$  with a small symmetry breaking parameter,  $\lambda$ . Preliminary results suggest that for  $\mu_1 > \mu_c$ , this theory forms a charged pion condensate (Figure 5) which spontaneously



**FIGURE 5** The pion condensate as a function of  $\mu_1$ .

breaks  $I_3$ , and the isospin density is non zero. Simulations planned for FY2003 will extend this to a  $12^3 \times 24$  lattice, allowing measurement of the mass of the Goldstone pion that this symmetry breaking implies, measurement of the spectrum of pseudo-Goldstone bosons, and confirmation of the nature of the transition.

**INVESTIGATORS** D. K. Sinclair, Argonne National Laboratory; J. B. Kogut, University of Illinois.

**PUBLICATION** J. B. Kogut and D. K. Sinclair, "Lattice QCD at finite isospin density," *Nucl. Phys. B Proc. Suppl.* **106**, 444 (2002).

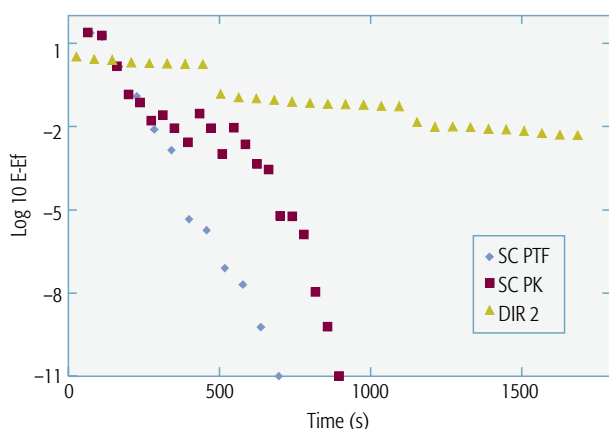
**URL** <http://www.hep.anl.gov/dks/NERSC2002/>

# Advanced Scientific Computing Research

The DOE Office of Advanced Scientific Computing Research, in addition to funding the NERSC Center, supports a variety of research in computer science and applied mathematics. Highlights of this year's accomplishments include development of a faster electronic structure calculation method for metals; a comparison of models for large eddy simulation of turbulent channel flows; modeling of streamwise vorticity formation in a transverse jet; a comparison of experimental, theoretical, and numerical simulation of Rayleigh-Taylor mixing rates; and benchmark testing of the Generalized Portable SHMEM data passing library.

## A Faster Electronic Structure Calculation Method for Metals

Density functional based electronic structure calculations of the properties of specific materials have become essential tools for materials science research. Improved electronic structure algorithms and codes can significantly enhance



**FIGURE 1** Comparison of three methods for calculating the electronic structure of a 20-layer(100) surface of aluminum with 10 layers of vacuum, using 50 bands and a  $2 \times 8 \times 8$  k-point mesh. SC PTF = self-consistent Pulay-Thomas-Fermi; SC PK = self-consistent Pulay-Kerker; DIR 2 = direct method.

researchers' productivity and, in some cases, enable new discoveries. Raczkowski et al. have developed and implemented in code a new method for electronic structure calculations for metals which they call Grassmann-metal conjugate gradient (GMCG). This method is faster than previously used methods for metals and has been tested with large-scale simulations of metal systems that are relevant to experiments. The code can also perform first-principles molecular dynamics calculations.

GMCG is the first all-bands conjugate gradient method for the iterative diagonalization part of the self-consistent method for solving the Kohn-Sham equations that is specifically designed for metallic systems, and as such uses electronic occupations to facilitate convergence. All-bands methods are computationally more efficient than band-by-band methods on modern RISC processors due to the more optimal reuse of the data. GMCG, using two different charge mixing methods (Pulay-Thomas-Fermi and Pulay-Kerker), was compared with a direct method for finding the electronic eigenstates. The two self-consistent methods were typically found to be 300% to 500% faster than other methods (Figure 1).

**INVESTIGATORS** A. Canning, D. Raczkowski, and L. W. Wang, Lawrence Berkeley National Laboratory.

**PUBLICATION** D. Raczkowski, A. Canning, and L. W. Wang, "An iterative diagonalization method for metals using a plane-wave basis set" (in preparation).

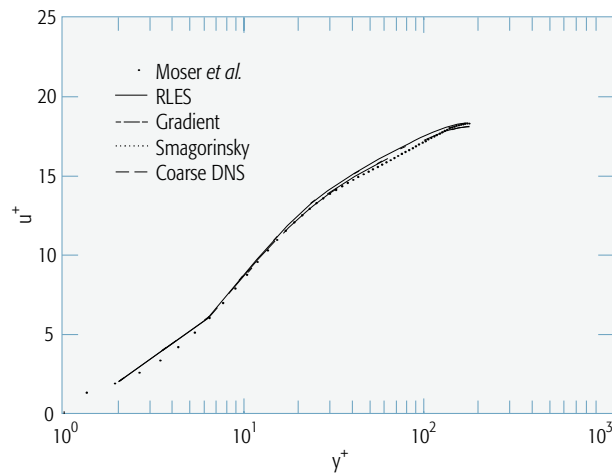
**URL** <http://www.nersc.gov/projects/paratec/>

## Large Eddy Simulation of Turbulent Channel Flows

Large eddy simulation (LES) is one of the most successful techniques in the numerical simulation of turbulent flows. Unlike direct numerical simulation (DNS), which tries to capture all the scales in the flow, LES aims at resolving only the large-scale flow features as defined by a filtering operation. One of the challenges in LES is modeling the subgrid-scale stresses, and a wide variety of models have been developed for this purpose.

Iliescu and Fischer applied the rational LES model (RLES) to numerical simulations of incompressible channel flows at Reynolds numbers based on the friction velocity and the channel half-width  $Re_\tau = 180$  and  $Re_\tau = 395$ . RLES is an approximate deconvolution model based on a rational (Padé) approximation to the Fourier transform of the Gaussian filter and is proposed as an alternative to the gradient model. The authors compared the RLES results with those from the gradient model, the Smagorinsky model, and a coarse DNS with no LES model; all of these were benchmarked against the fine DNS calculations of Moser et al.

The RLES model yielded the best results for the  $Re_\tau = 180$  case and showed much better numerical stability than the gradient model (Figure 2). For the  $Re_\tau = 395$  case, the RLES model and the gradient model yielded comparable results, and the Smagorinsky model performed the best. The next step will be to develop a mixed model, consisting of RLES supplemented by a Smagorinsky model.



**FIGURE 2** Normalized mean streamwise velocity,  $Re_\tau = 180$ . The almost perfect overlapping of the results is interpreted as a measure of success in enforcing a constant mass flux through the channel.

**INVESTIGATORS** P. Fischer, T. Iliescu, G. Leaf, and M. Minkoff, Argonne National Laboratory; J. S. Mullen, Worcester Polytechnic Institute.

**PUBLICATION** T. Iliescu and P. Fischer, "Large eddy simulation of turbulent channel flows by the rational LES model," *Phys. Fluids* (submitted), preprint math.SC/0205264 (2002).

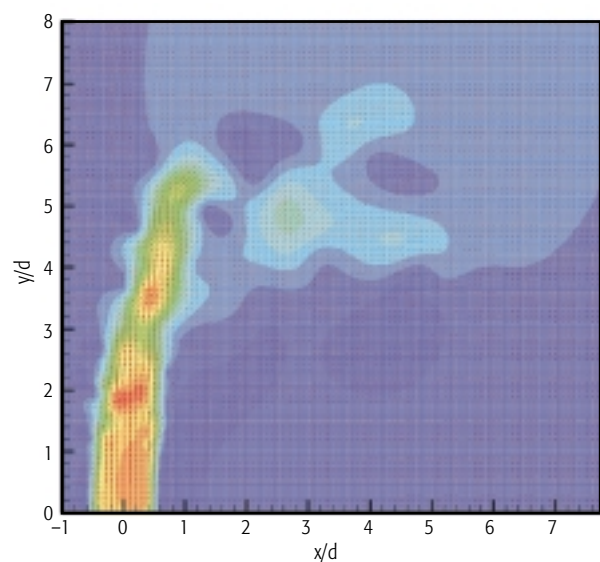
**URL** <http://www-unix.mcs.anl.gov/appliedmath/Flow/cfd.html>

## Streamwise Vorticity Formation in a Transverse Jet

Transverse jets have a wide range of applications in engineering, from propulsion and power generation to exhaust dispersion. The mixing properties of the transverse jet significantly impact the performance of these systems. Experimental studies have identified a small number of coherent flow structures which appear to control the evolution of the jet boundary, suggesting that the mixing characteristics of the transverse jet can be altered by manipulating these structures.

The complexity of the flow renders detailed numerical simulation nearly intractable, but Marzouk and Ghoniem have attempted a careful reduction of the physics in order to reproduce the essential dynamics of the underlying flow structures. They used a vortex filament method to model a transverse jet at high jet-to-crossflow velocity ratio, capturing the mechanisms leading to the formation of streamwise entraining structures—namely, the counter-rotating vortex pair (CVP).

Results show that the formation of the CVP is initiated very close to the nozzle, fed by jet boundary layer vorticity. Large-scale vortex rings form in the early stages of the jet shear layer due to rollup. As each ring convects into the flow, its lee side is lifted upwards and folded backwards, eventually



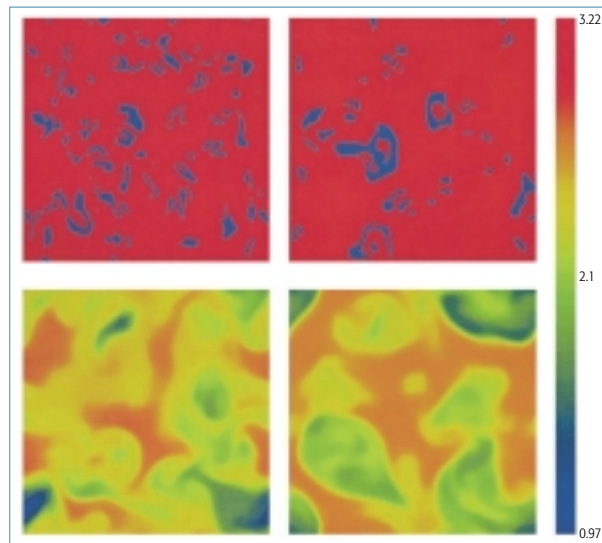
**FIGURE 3** Total velocity magnitude in the centerplane  $z = 0$ ,  $\tilde{t} = 4.50$ .

transforming each ring into two crescent-shaped sections connected by counter-rotating vortices aligned along the jet trajectory. Lee and windward sides of neighboring vortex rings merge, canceling vorticity in a plane normal to the jet trajectory and leaving only the counter-rotating vortex pair. The instantaneous vorticity field supports the assertion that the counter-rotating vortices are driven by the instantaneous dynamics of the flow (Figure 3).

**INVESTIGATORS** A. F. Ghoniem and Y. M. Marzouk, Massachusetts Institute of Technology.

**PUBLICATION** Y. M. Marzouk and A. F. Ghoniem, "Mechanism of streamwise vorticity formation in a transverse jet," American Institute of Aeronautics and Astronautics paper AIAA 2002-1063 (2002).

**URL** <http://centaur.mit.edu/rgd/>



**FIGURE 4** Cross-sectional plots showing density on a common rainbow color scale. The pure light fluid is colored blue and the pure heavy fluid is red. Yellow and green represent various levels of microscopic mixing. The ratio of extreme density values is 3.3:1. (Right) Shown is a higher slice in the  $z$  direction. (Upper) FRONTIER. (Lower) TVD. The simulations are shown at comparable penetration distances, but at different times. The density contrast for the TVD simulation has been reduced by about 50% because of mass diffusion.

## Comparison of Experimental and Simulated Mixing Rates

Rayleigh-Taylor instabilities result when a heavy fluid is supported by a less dense fluid. Gravity causes the heavier liquid to form "fluid fingers" that flow down into the lighter liquid, causing mixing and turbulence. Many natural phenomena, from boiling water to weather inversions to supernovae, show this kind of behavior, which is why numerical simulation of Rayleigh-Taylor instabilities is an important field of research.

George et al. conducted a Rayleigh-Taylor mixing rate simulation with an acceleration rate falling within the range of experiments. The simulation used the high-resolution front-tracking code FRONTIER to prevent interfacial mass diffusion. The results support the assertion that the lower acceleration rate found in untracked simulations such as total variation diminishing (TVD) is caused, at least to a large extent, by a reduced buoyancy force due to numerical interfacial mass diffusion (Figure 4). Quantitative evidence includes results from a time-dependent Atwood number analysis of the diffusive simulation, which yields a renormalized mixing rate coefficient for the diffusive simulation in agreement with experiment. The main result is that all values of the acceleration rate  $\alpha$  (theory, experiment, and simulation) are consistent if the diffusive calculation of  $\alpha$  is renormalized to account for mass diffusion.

**INVESTIGATORS** J. Glimm, E. George, X.-L. Li, A. Marchese, and Z.-L. Xu, State University of New York, Stony Brook.

**PUBLICATION** E. George, J. Glimm, X.-L. Li, A. Marchese, and Z.-L. Xu, "A comparison of experimental, theoretical, and numerical simulation Rayleigh-Taylor mixing rates," PNAS 99, 2587 (2002).

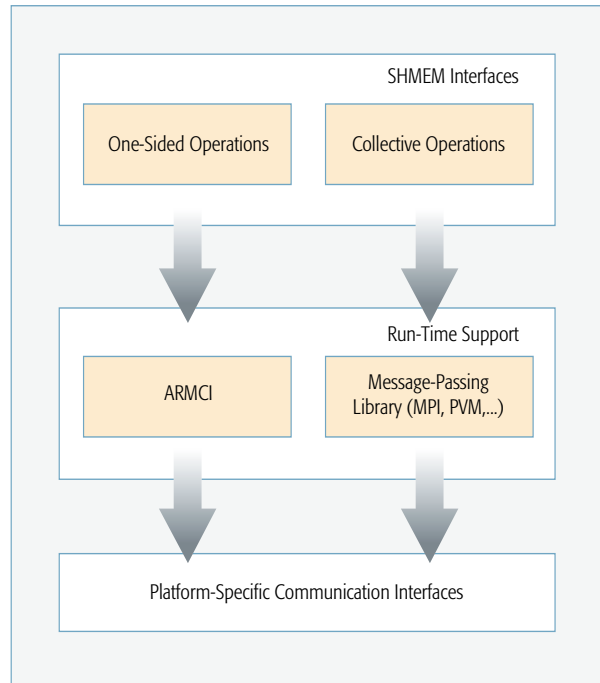
**URL** <http://www.ams.sunysb.edu/~shock/FTdoc/FTmain.html>



## GPSHMEM: Application to Kernel Benchmarks

SHMEM has become a de facto standard for the data passing, distributed shared memory programming model. SHMEM routines minimize the overhead associated with data passing requests, maximize bandwidth, and minimize data latency. Many vendors have packaged their implementation of SHMEM with their systems, but those implementations are still tightly coupled to vendor-specific hardware. The Generalized Portable SHMEM (GPSHMEM) library is poised to achieve for the data passing model what the portable implementations of MPI have done for the message passing model. GPSHMEM aims to provide SHMEM's functionality and at the same time achieve portability across as many platforms as possible, including IBM SP systems and clusters running Linux, FreeBSD, and other UNIX-like systems (Figure 5).

To test the performance of GPSHMEM and its viability as a programming model, Parzyszek and Kendall ported three kernels from the Stanford Parallel Applications for Shared Memory (SPLASH-2) benchmark suite—FFT, radix sort, and LU factorization—and tested the GPSHMEM implementation of these codes on the IBM SP and on a Linux cluster. The measured performance of the GPSHMEM codes mapped directly to the performance of the underlying hardware and software available, and scalability was as expected. Ongoing development of GPSHMEM is being done in cooperation with the Center for Programming Models for Scalable Parallel Computing.



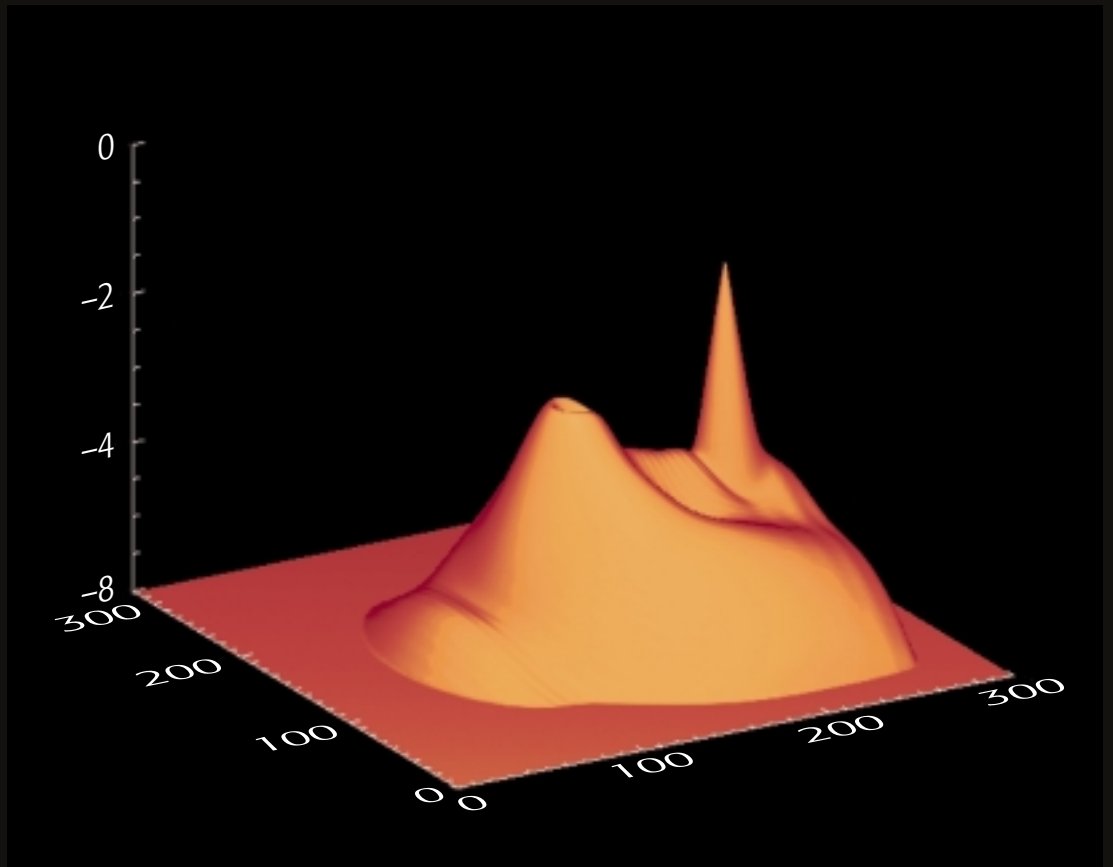
**FIGURE 5** Implementation of the GPSHMEM library. GPSHMEM's portability is achieved by the use of the Aggregate Remote Memory Copy Interface (ARMCI) and its ability to use several message-passing libraries.

**INVESTIGATORS** R. A. Kendall and K. Parzyszek, Ames Laboratory.

**PUBLICATION** K. Parzyszek and R. A. Kendall, "GPSHMEM: Application to kernel benchmarks," *Proc. 14th IASTED Internatl. Conf. on Parallel and Distributed Computing and Systems (PDCS 2002)*, Cambridge, MA, November 2002.

**URL** <http://www.pmodels.org/>





## THE NERSC CENTER

*As a national facility for scientific research, NERSC does much more than operate and provide access to supercomputers. The current model for the NERSC Center involves four areas of activity:*

- **HIGH-END SYSTEMS** – *Balanced introduction of the best new technologies for complete computational and storage systems, coupled with the advanced development activities necessary to wisely incorporate these new technologies.*
- **COMPREHENSIVE SCIENTIFIC SUPPORT** – *Providing the entire range of support activities, from high-quality operations and client services to direct collaborative scientific support, to enable a broad range of scientists to effectively use the NERSC systems in their research.*
- **SUPPORT FOR SCIENTIFIC CHALLENGE TEAMS** – *Supporting SciDAC and other computational science teams, with the goal of bridging the software gap between currently achievable and peak performance on the new terascale platforms.*
- **UNIFIED SCIENCE ENVIRONMENT (USE)** – *Using Grid technology to work toward an integrated science environment, combining experiment, simulation, and theory by facilitating access to computing and data resources, as well as to large DOE experimental instruments.*

*This section provides an overview of these activities during the past year—a behind-the-scenes glimpse into what it takes to make possible the scientific achievements described in the previous section. The section begins with a look at NERSC's clients, sponsors, and advisors.*



# Clients, Sponsors and Advisors

NERSC served 2,594 scientists throughout the United States in FY 2002. These researchers work in DOE laboratories, universities, industry, and other Federal agencies. Figure 1 shows the proportion of NERSC usage by each type of institution, while Figures 2 and 3 show laboratory, university, and other organizations that used large allocations of computer time. Computational science conducted at NERSC covers the entire range of scientific disciplines, but is focused on research that supports the DOE's mission and scientific goals, as shown in Figure 4.

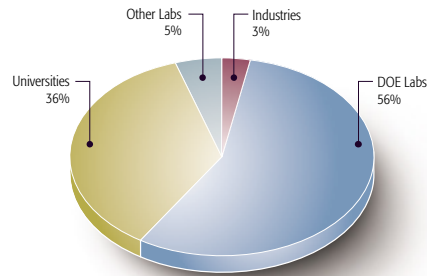


FIGURE 1 NERSC usage by institution type, FY02.

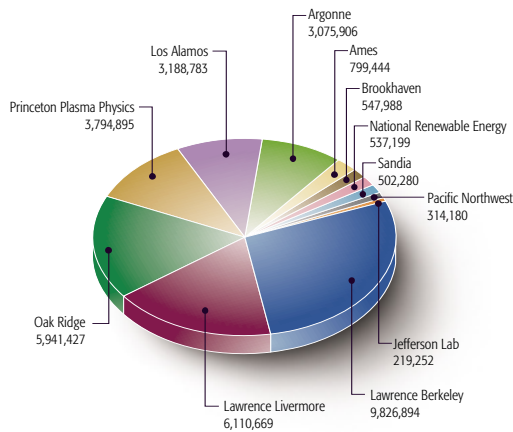


FIGURE 2 Leading DOE laboratory usage at NERSC, FY02 (>200,000 processor hours)

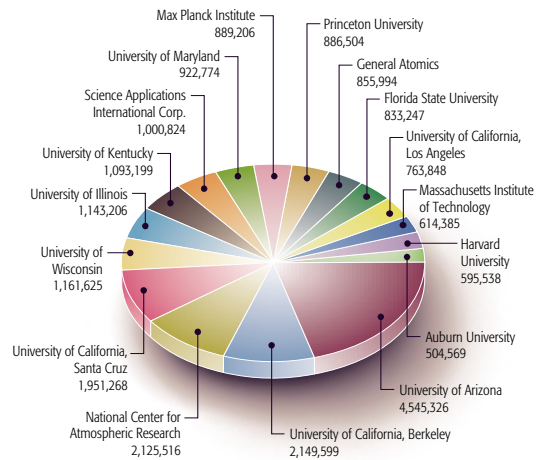


FIGURE 3 Leading academic and related usage at NERSC, FY02 (>500,000 processor hours)

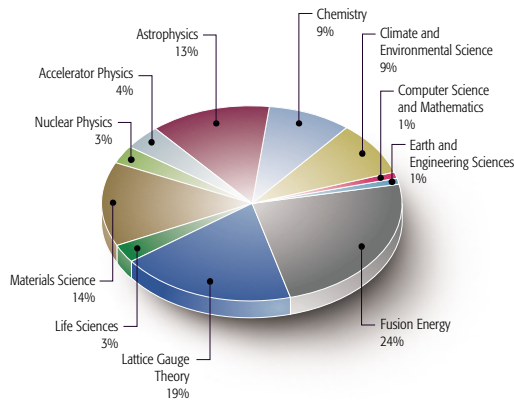


FIGURE 4 NERSC usage by scientific discipline, FY02



## Allocations and Policies

Allocations of computer time and archival storage at NERSC are awarded to research groups, regardless of their source of funding, based on an annual review of proposals. As proposals are submitted, they are subjected to peer review to evaluate the quality of science, how well the proposed research is aligned with the mission of DOE SC, the need for computing resources, and the readiness of the specific application and applicant to fully utilize the computing resources being requested.

The DOE initiated a new allocations process for FY 2003 in which DOE's Supercomputing Allocations Committee (SAC, see Appendix D) reviews and makes award decisions for all production requests, reflecting their mission priorities. In addition, most proposals are reviewed by the Computational Review Panel (CORP, Appendix B) to assess the computational approach, optimization, scalability, and communications characteristics of the applicant's code. Allocations for small startup projects are determined by NERSC.

Two other groups provide general oversight for the NERSC Center: the NERSC Policy Board (Appendix A) advises the Berkeley Lab Director on the policies that determine the impact and performance of the NERSC Center, and the NERSC Users Group (Appendix C) advises the NERSC management and provides feedback from the user community. DOE program management is provided by the Office of Advanced Scientific Computing Research (Appendix E), with advice from the Advanced Scientific Computing Advisory Committee (Appendix F).

## User Survey Results

Three hundred users responded to this year's NERSC User Survey, the highest response level in the survey's five-year history. The survey responses provide feedback about every aspect of NERSC's operation, help us judge the quality of our services, give DOE information on how well NERSC is doing, and point us to areas we can improve.

The average score for overall satisfaction with NERSC in 2002 was 6.32 on a scale of 1 to 7. Areas with the highest user satisfaction were IBM SP uptime (6.56), timely consulting response (6.51), HPSS reliability (6.51), and PDSF uptime (6.51). Areas with the lowest user satisfaction were training (4.99), visualization services (4.83), and PVP batch wait time (4.77). Complete survey results can be found at <http://hpcf.nersc.gov/about/survey/2002/>.

Every year NERSC institutes changes based on the survey. This past year's efforts include:

- With the NERSC User Group we established a queue committee whose task was to investigate queue issues and recommend improvements. (See page xx below for details.)
- NERSC provided more performance analysis tools on the IBM SP along with documentation and training on how to use them.
- NERSC installed new visualization tools on the IBM SP and the visualization server, and streamlined visualization documentation.
- NERSC wrote a number of scripts to improve IBM SP management procedures.
- NERSC started to conduct monthly training sessions on the Internet using Access Grid Node technology. This technology is still not completely mature, and there have been a few rough spots along the way. We will continue working to improve our training program.

# High-End Systems

*If one picture could tell the story of NERSC's high-end systems for FY 2002, perhaps it would be Figure 1, which shows the dramatic increase in usage of NERSC's massively parallel (MPP) systems over the past few years. The demand for time on high performance computers always exceeds the supply, and users immediately take advantage of any increase in capability. The NERSC Users Group documented their future needs in The DOE Greenbook—Needs and Directions in High-Performance Computing for the Office of Science, published in April 2002 (see sidebar on page 54).*

*Because of this high demand, NERSC Center staff are always looking to the future. Even as we upgraded and enhanced existing systems during the past year, we took the next step toward doubling NERSC's capability, and we collaborated on a new strategy for developing future computer architectures that are more useful for computational science.*

## System Upgrades and Expansion

Additional memory was added to NERSC's IBM SP system, called *Seaborg*, which originally had 12 GB of memory in all nodes. After the upgrade, 116 nodes had 16 GB of memory, 64 nodes had 32 GB, and 4 nodes had 64 GB. Fifty nodes were

also added to the compute pool. Seaborg's connection to the High Performance Storage System (HPSS) was upgraded to Jumbo Gigabit Ethernet.

The hardware upgrades were matched by improvements in performance and utilization. In March–April 2002, Seaborg's utilization (30 day moving average) exceeded 96% for the first time. Similarly, CPU utilization exceeded 92%. Given Seaborg's improved stability, NERSC was able to augment MPP allocations by about 6 million hours. All of the NERSC Center's systems achieved more than 98% availability in 2002.

After requesting proposals for a system to replace the Cray T3E and SV1 systems, which were decommissioned in October 2002, NERSC's procurement team, led by Deputy Director Bill Kramer, reviewed proposals from a number of leading super-computer vendors. At the end of a careful deliberation and negotiation process, the team decided to increase the capability of Seaborg. In November, NERSC announced an agreement with IBM to double the size of Seaborg, creating a machine with 6,656 processors and a peak speed of 10 teraflop/s.

The expanded system will have 6,080 processors (380 nodes) for computation. The total system will have 416 16-way Power 3+ nodes with each CPU at 1.5 Gflop/s. The system will include 7.8 terabytes (TB) of aggregate memory (the second-largest memory on any open production system) and a Global Parallel File System with 44 TB of storage. There will be an additional 15 TB of local system disk. Installation of the new equipment began in November, with the full system expected to become available to NERSC users by April 2003.

NERSC's decision to double the size of our existing IBM SP, a system with proven performance, was made in order to have the most immediate and cost-effective impact on the DOE research community, whose computing needs are rising rapidly. The expanded computational capability will be available in only a few months, offering users not only a huge increase in processor hours but also an unprecedented opportunity to explore the scalability of their applications. While some codes are ready to scale immediately beyond 2048 processors, NERSC will start a scalability program to help other users take advantage of the large number of processors. NERSC will also change the queue structure to provide additional

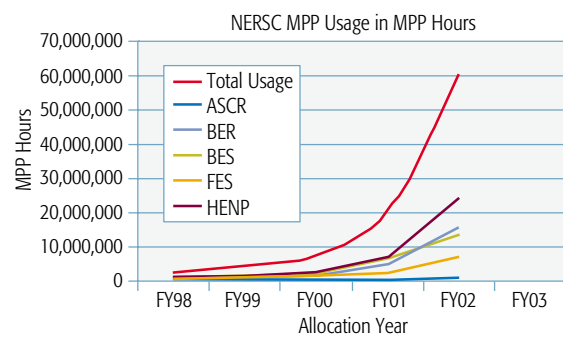
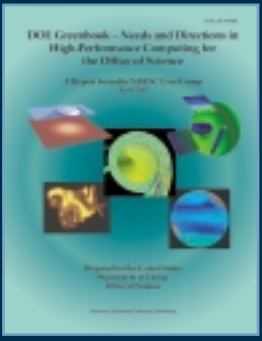


FIGURE 1 Increasing NERSC MPP usage in processor hours.

## DOE GREENBOOK DOCUMENTS

# COMPUTATIONAL CHALLENGES, RECOMMENDATIONS



*The DOE Greenbook—Needs and Directions in High-Performance Computing for the Office of Science* was compiled by Douglas A. Rotman and Paul Harding for the NERSC Users Group and published in April 2002. This report documents the computational science being done at NERSC and other DOE computing centers and provides examples of computational challenges and

opportunities that will guide the evolution of these centers over the next few years. Examples are provided from every research program supported by the DOE Office of Science.

The Greenbook states that a large shared computing center continues to be essential to the scientific mission of the Office of Science, as it provides researchers with resources that could not be supplied locally. The authors believe that parallel computing is now the primary production computing paradigm, although some performance issues remain. The report discusses the need for software and algorithms that enable better utilization of parallel systems, as well as platform configurations that are better aligned with the requirements of computational science. The Greenbook also addresses the use of distributed computational systems and the need for enhanced mass storage, visualization facilities, and networks.

The Greenbook's recommendations include:

- Expand the high-performance computing resources available at NERSC.
- Encourage the continued improvement of algorithms, software (including middleware), and database technology for improved performance on parallel platforms.
- Strengthen the networks to provide reliable, robust, and fast access to Grid resources.
- Coordinate NERSC activities with SciDAC, ISIC, and other Office of Science compute centers.
- Identify mechanisms to provide larger-scale production facilities. A growing number of future simulations will need to run continuously for hundreds of hours, but current computer centers can only handle a few simulations of this type.

The full text of the Greenbook is available at [http://hpcf.nersc.gov/about/NUG/DOE\\_Greenbook.pdf](http://hpcf.nersc.gov/about/NUG/DOE_Greenbook.pdf)

encouragement for large jobs. The size of the expanded system will enable innovative new science-of-scale applications as well as help other projects meet their computational objectives more quickly.

On the storage front, we upgraded our HPSS system to all Fibre Channel disk with 15 TB of disk cache, increasing the bandwidth by 80 to 100%, and we boosted the capacity of the archive to 3.6 petabytes (PB). We enhanced security by turning off all clear-text password access to storage systems. Data transfer rates have accelerated from 40 MB/s to 80 MB/s, thanks to the replacement of HIPPI with Jumbo Gigabit Ethernet and the upgrade of HPSS and HSI software. NERSC currently transfers 2–3 TB of data to and from storage every day, and we expect to have 1 PB in storage within the next year. Near-term plans for HPSS include increasing archive capacity to 7 PB, speeding up transfers to 2 GB/s, adding access to storage using Grid credentials, and providing a Web interface to storage. NERSC continues to contribute to HPSS development, and helped the ASCI (Advanced Simulation and Computing Initiative) program at Los Alamos National Laboratory to convert from CFS to HPSS storage.

The Escher visualization server, which enables NERSC users to perform visualizations from remote locations, has undergone major improvements to enable faster visualization of large-scale datasets. The server itself was upgraded to a Silicon Graphics Onyx 3400 with twelve 600 MHz processors, 24 GB of memory, two Infinite Reality 4 graphics pipes with 1 GB of texture memory each, and a 4 TB RAID-5 disk array with ten 2 GB controllers. Escher now has three Gigabit Ethernet interfaces: one connected to the production network, and two working together connected to the Jumbo Gig-E network to share data between machines, including Seaborg and HPSS. New software on Escher includes Globus, which enables Grid-based remote distributed visualization; VMD for molecular dynamics visualizations; and ParaView, a parallel visualization application for large datasets.

## A New Computer Architecture Strategy: The "Blue Planet" Proposal

In recent years scientific computing in America has been handicapped by its dependence on hardware that is designed and optimized for commercial applications. The performance

of the recently completed Earth Simulator in Japan, which is five times faster than the fastest American supercomputer, dramatically exposed the seriousness of this problem. Typical scientific applications are now able to extract only 5 to 10 percent of the power of American supercomputers built from commercial Web and data servers. By contrast, the design of the Earth Simulator makes 30 to 50 percent of its power accessible to the majority of types of scientific calculations.

It is becoming increasingly clear that the requirements of high performance computing (HPC) for science and engineering, and the requirements of the commercial market are diverging. This divergence can be seen in some computer vendors' reduced interest in the HPC market as well as in the performance limitations of clusters of symmetric multiprocessors (SMPs) used for scientific applications. Communications and memory bandwidth in SMPs are not scaling with processor power, which constrains the performance of scientific codes. The cost of scientific supercomputing, with nearly football-field size computers that consume megawatts of electricity, is also an issue of national strategic importance.

Lawrence Berkeley and Argonne national laboratories, in close collaboration with IBM, have responded to this challenge with a proposal for a new program to bring into existence a new class of computational capability in the United States that is optimal for science. Our strategic white paper, "Creating Science-Driven Computer Architecture: A New Path to Scientific Leadership" (<http://www.nersc.gov/news/blueplanet.html>), envisions a new type of development partnership with computer vendors that goes beyond the mere evaluation of the offerings that those vendors are currently planning for the next decade.



**FIGURE 2** Blue Planet was born here: At a two-day workshop in September 2002, a team of Argonne, Berkeley Lab, and IBM scientists developed the fundamental concepts of Virtual Vector Architecture (ViVA), potentially redefining supercomputing in America.

This strategy includes development partnerships with multiple vendors, in which teams of scientific applications specialists and computer scientists will work with computer architects from major U.S. vendors to create hardware and software environments that will allow scientists to extract the maximum performance and capability from the hardware.

One of the key partnerships, involving IBM, Lawrence Berkeley National Laboratory, and the NERSC Center, will deploy a new architecture called *ViVA* or *Virtual Vector Architecture*. This architecture will use commercial microprocessors but will run programs optimized for vector processors, providing both high sustained levels of performance and cost-effectiveness. *Blue Planet*, a 160 teraflop/s mature implementation of ViVA, has been proposed for installation at NERSC in the second half of 2005. *Blue Planet* is expected to provide twice the sustained capability of the Earth Simulator at half the cost. Computer scientists from Berkeley Lab/NERSC, Argonne, and IBM held two workshops in September and November 2002 (Figure 2), the first to define the *Blue Planet* architecture, and the second for IBM to receive scientists' suggestions on the design of the Power 6 processor.

## Computer Room Expansion

Berkeley Lab began the planned expansion of NERSC's computer room at the Oakland Scientific Facility (OSF) to provide space for the expanded Seaborg system. The expansion includes removing a non-load-bearing wall and extending the seismically enhanced raised floor, HVAC systems, chilled water system, network cable tray systems, and laser-based smoke detection and fire sprinkler systems. The main chilled water system is being completed, and the rooftop cooling towers are being upgraded with variable frequency drives for energy efficiency. The option for additional build-out of the computer room was extended until 2004 with no increase in rent. The OSF was honored by *Buildings Magazine* with an honorable mention in the magazine's 2002 Modernization Awards.

## Advanced Development

Currently NERSC's major development activity for high-end systems is the Global Unified Parallel File System (GUPFS) project. The goal of this project is to provide a scalable, high-

## CRAY DECOMMISSIONING

October 2002 marked the end of an era when NERSC decommissioned its Cray T3E and SV1 supercomputers. This is the first time since 1978 that the NERSC Center does not have a Cray system on the machine room floor.



performance, high-bandwidth, shared file system for all the NERSC production computing and support systems. The GUPFS project is divided into three phases: (1) deployment and integration in the NERSC production environment, (2) integration with HPSS, and (3) integration into a WAN/Grid operating environment.

In December 2001 NERSC completed the installation of the initial Global File System (GFS) testbed, which is configured as a parallel computational cluster to test file systems in a realistic scientific environment. NERSC also developed relationships with file and storage system vendors and with possible collaborators, and began tracking existing and emerging file systems, storage area network (SAN) fabrics, and storage technologies and trends. Testing methodologies and benchmarks were developed for shared/cluster file systems in a parallel environment, and initial testing of two versions of the Sestina GFS file system was completed. Further product evaluation and testing will continue, with the goal of deploying GUPFS in the NERSC production environment by 2006.

In software development, NERSC successfully demonstrated checkpoint/restart on an IBM SP development system using the AIX 5.1 operating system and the PSSP 3.4 cluster management tools. Checkpoint/restart will be implemented on Seaborg in 2003. Other test programs involved the Globus 2.0 Grid software, the MPI 64-bit compiler, and HPSS statistical programs that analyze transfers and cache.

To increase the use of visualization resources by a greater number of users, and to make visualization more available and efficient by bringing the application to the data, NERSC has introduced license servers that enable visualization applications to run on additional machines via floating licenses. Initially deployed to Escher and Seaborg, remote license serving will allow many users to deploy visualization applications at their desktop in the near future. NERSC has also begun testing a utilization logging server (ULOG) that would help monitor and optimize the usage of visualization resources.



# Comprehensive Scientific Support

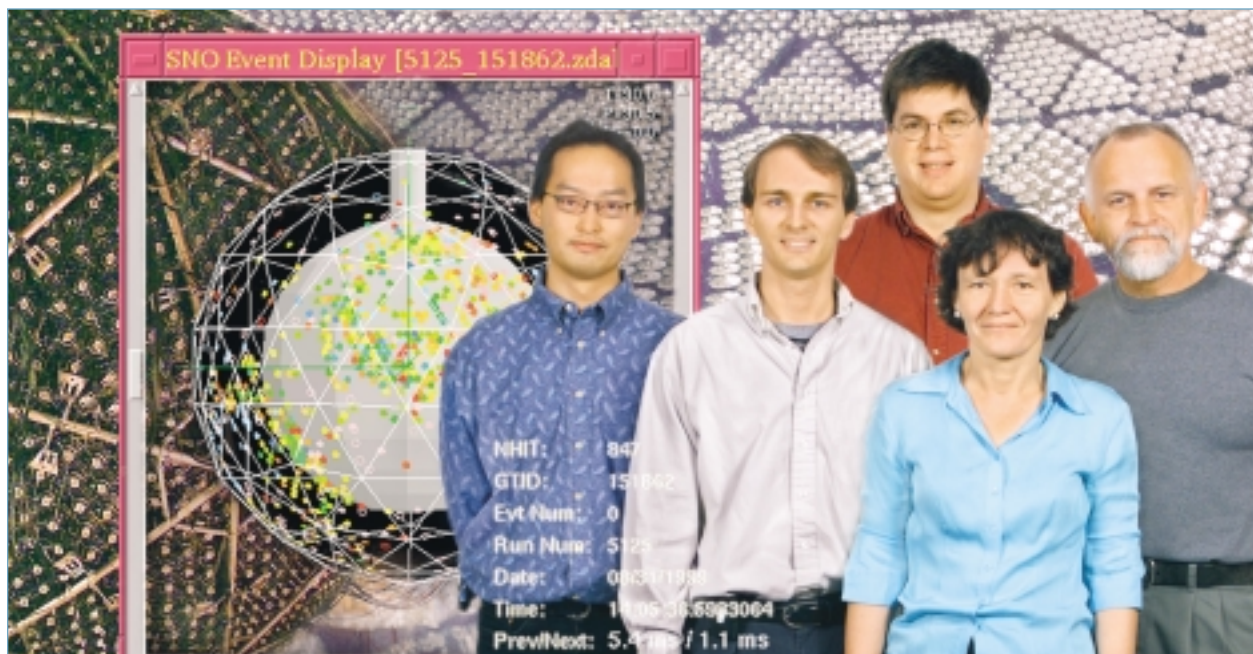
*NERSC's comprehensive scientific support ranges from everyday high-quality operations and client services to direct collaboration with scientists to solve unique computational and data management problems. Whether the challenge involves system software, networks, algorithms, application codes, or visualization tools, NERSC's goal is always the same—to help make the DOE scientific community more productive.*

## Making Systems Productive for Science

NERSC users in 2002 saw significant improvements in job turnaround time thanks to the work of the Queue Committee, made up of NERSC Users Group volunteers and NERSC staff. Based on the committee's recommendations, NERSC improved turnaround time for interactive and debug jobs during prime

time by setting aside 5% of the Seaborg compute nodes for these jobs from 5:00 a.m. to 6:00 p.m. Pacific time, Monday through Friday. To improve fairness, we also implemented priority aging for *regular* class jobs—*regular* jobs in the queue for more than 36 hours will not be preempted by new *premium* jobs. In addition, we provided a new *regular\_long* class with a connection time of up to 24 hours for jobs using 32 nodes or less. A special mechanism was implemented to allow science-of-scale projects to run continuously to use their large allocations.

The NERSC networking team continues working with users at remote sites to improve end-to-end network performance. During the past year, the data transfer rate to and from Princeton Plasma Physics Laboratory was increased from 700 KB/s to 2 MB/s. We achieved a 7× network performance improvement with Fermilab, a 5× improvement with the State University of New York at Stonybrook, and a 2.5× improvement with Brookhaven National Laboratory. Other networking achievements included implementation of an Access Grid node for multicast videoconferencing, and installation of a



**FIGURE 1** The PDSF Team—Steve Chan, Shane Canon, Cary Whitney, Iwona Sakrejda, and Tom Langley—helped the SNO collaboration analyze data that answered longstanding questions about solar neutrinos. (Steve now works in NERSC's Networking and Security Group.)



spam filter on NERSC mail servers. An ESnet link upgrade to OC-48 (2.4 GB/s) is expected to be in production early in 2003.

NERSC's PDSF cluster system is used by several large high energy and nuclear physics collaborations for data analysis and simulations, and NERSC staff work closely with these groups to support their efforts and to improve the PDSF system (Figure 1). When data from the Sudbury Neutrino Observatory (SNO) were analyzed on the PDSF, the results revealed that solar neutrinos do have mass and transform from one "flavor" to another in transit from the core of the sun to the earth. Data from the KamLAND experiment, also analyzed on the PDSF (see page 61), confirmed these results for anti-neutrinos generated by nuclear reactors.

One of the largest users of the PDSF and NERSC's HPSS archive is the Solenoidal Tracker at RHIC (STAR) collaboration, which transfers approximately 1 TB of data per week from Brookhaven National Laboratory to NERSC, with more than 65 TB stored in our HPSS archive to date. Results of the STAR experiment have been analyzed on the PDSF and published in a dozen journal articles, with more to come.

Harsh Anand Passi, a member of NERSC's consulting staff, provides key support for climate modeling researchers (Figure 2). She spearheaded one of the first parallel implementations of the netCDF library, provides initial visualization support

for climate models, and has been the technical leader for installing several climate codes on NERSC systems, most recently the Community Climate System Model (CCSM2). She created methods that allow researchers to modify CCSM manageably, and developed documentation on the code for the NERSC Web site. As a result of her work, NERSC is the only site besides the National Center for Atmospheric Research that runs a fully supported CCSM2.

## Scientific Algorithms and Applications

On leading-edge computational science projects, NERSC staff scientists and mathematicians often collaborate directly with clients to develop methods, algorithms, and codes that address specific research problems. Recent collaborations have included research in nanoscience and materials science, cosmology, and climate modeling.

With the increasing interest in nanoscience, there is an urgent need for electronic structure calculations of ever-larger systems. NERSC staff scientist Lin-Wang Wang collaborates with Alex Zunger's researcher group at the National Renewable Energy Laboratory (NREL) to address this issue. Recently Lin-Wang developed a charge patching method that



FIGURE 2 Harsh Anand Passi installs the latest climate modeling codes on NERSC systems and helps researchers use them effectively.

allows the construction of the *ab initio* charge density of a nanosystem without doing a full self-consistent calculation (Phys. Rev. Lett. **88**, 256402 [2002]). Based on the charge density, the single-particle Schrödinger equation can then be constructed. This procedure enables researchers to do *ab initio* quality electronic structure calculations for tens of thousands of atoms—a big advance over conventional methods, which can only calculate a few hundred atoms with the same accuracy. NREL researchers have used this method to calculate isoelectronic impurity levels for a series of semiconductors, and to calculate  $N$  pairs in gallium arsenide.

Andrew Canning continues to work with Malcolm Stocks and collaborators at Oak Ridge National Laboratory and elsewhere on computational methods for determining the magnetic structure of materials. Recently he collaborated on a study of the magnetic structure of  $\gamma$ -ferromanganese ( $\gamma$ -FeMn) alloy, a rare example of an fcc antiferromagnet, which has become a prototype for pinning layer studies in magnetoelectronic devices (J. Appl. Phys. **91**, 7355 [2002]). The calculations were based on the constrained local moment model and used first-principles spin dynamics to obtain the ground state orientational configuration. Andrew collaborated on testing and optimizing the code for NERSC computers as well as running the code.

NERSC staff scientist Peter Nugent works with Greg Aldering and collaborators on the Nearby Supernova Factory (SNfactory), an international experiment designed to lay the foundation for the next generation of cosmology experiments that will measure the expansion history of the Universe using Type Ia supernovae. Peter is helping this group develop methods to quickly analyze about 50 GB of photometric and spectroscopic data each day in order to identify and calibrate discoveries and then plan and coordinate follow-up observations. These methods involve making statistical comparisons of the newly discovered events with large libraries of astrophysical objects, including stars, galaxies, novae, and supernovae. This work is currently being benchmarked and refined, with an expected implementation date of July 2003 to coincide with first-light for SNIFS, the integral-field-unit spectrograph on the University of Hawaii 2.2-meter telescope.

Two other examples of collaborative support by NERSC staff are described in detail elsewhere in this report: Chris Ding's development of the MPH library for integrating multiple model components (page 17), and Julian Borrill's work on a new generation of cosmic microwave background data analysis tools (page 39).

## Visualization Support

NERSC's visualization support is currently focused on bringing high performance visualization to the remote user. In addition to installing new visualization tools on both Escher and Seaborg this year, NERSC expanded and streamlined its visualization documentation on the Web. This documentation now includes both online and downloadable manuals, links to vendors' Web sites, tutorials, examples, application loading instructions for NERSC machines, and other useful resources. Visualization consulting has been integrated into NERSC's help desk functions (<http://help.nersc.gov>) to make it more easily accessible.

On June 5, 2002, NERSC sponsored a workshop on "Visualization Requirements for DOE-Sponsored Computational Science and Engineering Applications." The goal of the workshop was to identify crucial scientific data visualization needs from all of the DOE Office of Science programs. Eighteen researchers from laboratories and universities contributed to the workshop presentations, and another 49 scientists participated.

Issues discussed at the workshop included ease of use, visualization of large datasets, support for parallel and distributed implementations, multivariate visualization (multiple grids, many species, and many dimensions), drill-down capabilities, visualization support, common data formats and frameworks, and better communication between the visualization and computational science communities. The workshop report and recommendations are available at <http://wwwvis.lbl.gov/Events/VisGreenbookWorkshop-June02/index.html> and will also be published in the Spring 2003 issue of the International Journal of High Performance Computing Applications.

NERSC staff contributed to several major visualization projects this year, including modeling a spectrum synthesis calculation of a supernova atmosphere surrounded by a toroid (Figure 4 on page 8), modeling gravitational waves generated during the collision of black holes (Figure 5 on page 9), and a simulation showing halo particles being tracked backward in an accelerator to their starting points (Figure 17 on page 22).



# Support for Scientific Challenge Teams

*Many of the most important breakthroughs in computational science are expected to come from large, multidisciplinary, multi-institutional collaborations working with advanced codes and large datasets. These teams are in the best position to take advantage of terascale computers and petascale storage, and NERSC provides its highest level of support to these researchers—even when the opportunity to contribute to scientific discovery arrives on short notice, as it did with the KamLAND project described below.*

## Science-of-Scale and SciDAC Projects

The science-of-scale and SciDAC projects described above in the Science Highlights section (beginning on pages 5 and 11, respectively) are the primary recipients of NERSC's high-level support. Many of the special requirements of the science-of-scale projects and the special services NERSC provided are described in that section. Special services that were provided to SciDAC projects, particularly the Integrated Software Infrastructure Centers, included:

- specialized consulting support
- special service coordination for queues, throughput, increased limits, etc.
- specialized algorithmic support
- special software support
- visualization support
- conference and workshop support
- Web sever support for some projects
- consulting support to help projects organize and manage Web content
- CVS servers and support for community code management.

SciDAC will be the catalyst for a fundamental shift in computational science from the principal-investigator model to the collaborative team model. Facilitating this transition is an important part of NERSC's mission.

## Getting the Physics out of KamLAND Data

The Standard Model of Particle Physics, which has successfully explained fundamental physics since the 1970s, predicts that neutrinos have no mass and come in three types or “flavors,” electron, muon, and tau. But for the past four years, solar neutrino experiments at the Super-Kamiokande Observatory (Super-K) in Japan and the Sudbury Neutrino Observatory (SNO) in Canada have offered compelling evidence that neutrinos do have nonzero mass and oscillate between the three flavors while traveling from the sun to the earth, indicating that the three flavors are actually different states of the same particle. While the evidence was strong, a few physicists had nagging doubts about unexpected interactions between neutrinos and the sun's magnetic field. If the same oscillations could be shown for neutrinos from terrestrial sources—or anti-neutrinos, since anti-matter is the mirror image of matter—the doubts would be dispelled.

For this reason, physicists eagerly awaited the results from KamLAND, the Kamioka Liquid scintillator Anti-Neutrino Detector. Located adjacent to Super-K in a mine on the west coast of Japan's main island of Honshu and supported by an



**FIGURE 1** Looking up at KamLAND's photomultipliers. When a neutrino collides with a proton in the liquid scintillator, a flash of light is emitted that is detected by the photomultipliers and converted into an electronic signal for computer analysis.

international collaboration (including DOE), KamLAND is the largest low-energy anti-neutrino detector ever built. KamLAND consists of a weather balloon 13 meters (43 feet) in diameter, filled with about a kiloton of liquid scintillator, a chemical soup that emits flashes of light when an incoming anti-neutrino (generated by nuclear reactors in Japan and Korea) collides with a proton. These light flashes are detected by a surrounding array of 1,879 photomultiplier light sensors which convert the flashes into electronic signals that are collected for analysis on computers (Figure 1).

KamLAND experiments began generating about 200 gigabytes of data per day in January 2002. That amount of data would swamp the slow network connection between the detector and its research host, Tohoku University, so the data are stored on tapes, then driven by car in a seven-hour trip to the university, where the data are transferred from the tapes and stored for analysis.

After gathering data for six months, U.S. scientists running experiments at KamLAND had 800 tapes containing a vast amount of data, and they wanted to present initial results at conferences in September. But they had not determined how to get the data to the U.S.—Internet bandwidth is inadequate—or where in the U.S. they could store and analyze the data. A further complication was that the data were stored on LTO tapes (Linear Tape Open), a new and not yet widely used format.

Fortunately, the NERSC Center had an LTO system on loan from IBM for the Probe storage research project. NERSC's Mass Storage Group had just finished their evaluation of the system and were preparing to return it to IBM in July 2002 when they learned of the physicists' problem. NERSC reached an agreement with IBM to keep the system a few months longer, and the KamLAND tapes were shipped from Japan to Oakland.

NERSC staff had already developed software for the LTO library to interface with our HPSS archive, so the KamLAND group began transferring their data to HPSS.

To avoid interfering with normal NERSC operations, the neutrino group did their data transfers at night and on weekends, increasing the HPSS data traffic by up to 80 percent per day. One weekend they managed to transfer 1.3 terabytes of data in one day. NERSC even reconfigured HPSS to write two data streams for the file size they were using. In all, more than 48 terabytes of data were transferred from the tapes to HPSS.

A second fortunate coincidence was that when the KamLAND data began to pour in, one of the largest PDSF users was idle. With some quick negotiations, the KamLAND group was able to use PDSF to analyze their data (as SNO had done before them), sometimes using the full 400-processor cluster. The KamLAND team was impressed by and grateful for the PDSF staff's efforts to make everything run as smoothly as possible for them.

The NERSC Center's client-oriented services and operational flexibility, together with its large-scale data storage and analysis resources, made possible the timely analysis and announcement of the KamLAND findings, which confirmed the earlier conclusions of the Super-K and SNO researchers. The results were presented at the International Workshop on Neutrinos and Subterranean Science in Washington, DC, September 19–21, 2002, and the 16th International Conference on Particles and Nuclei in Osaka, Japan, September 30–October 4, 2002. The results were also submitted for publication in *Physical Review Letters*.

NERSC remains poised to play its part in the revision of the Standard Model.

# Unified Science Environment (USE)

*This year NERSC took some major steps toward the goal of a Unified Science Environment with the installation and testing of prototype Grid services, the establishment of several Grid testbeds, and another award-winning demonstration of distributed computing and visualization in the SC2002 Bandwidth Challenge competition. All of NERSC's major computing and storage systems are expected to become accessible via the DOE Science Grid in 2003 when all of the initial components of this infrastructure are placed in production.*

## Establishing a Grid Infrastructure

NERSC had originally planned to make its high performance computing systems accessible via the DOE Science Grid by 2004, but the target date was moved up a year when NERSC established a collaboration with IBM to deploy Grid capabilities on the SP and HPSS systems. The goal of this collaboration is to seamlessly integrate IBM's system software with the Globus Grid software. The Globus Toolkit 2 underwent tests on NERSC's development SP cluster during the past year, and some minor problems were identified for correction. DOE Science Grid access to Seaborg is expected by mid-2003. The Globus Security Infrastructure has been integrated with most HPSS tools, and single-stream file transfers to and from HPSS via the Grid should be available on a production basis in early 2003, with parallel file transfers coming a year later. NERSC is working with Argonne National Laboratory to develop a full-featured, Grid-enabled HPSS.

NERSC has been collaborating with other DOE Science Grid sites (Lawrence Berkeley, Argonne, Oak Ridge, and Pacific Northwest national laboratories) to test and implement security procedures and other services in the prototype Grid environment. Pre-production prototypes of various Grid services (e.g., sign-on, certification, portal, firewall, and service monitoring) have been installed and are being tested on NERSC's computing, storage, networking, and security systems.

Working with the Particle Physics Data Grid collaboration, NERSC set up a server to test virtual organization membership schemas; feedback to Globus developers based on these tests resulted in changes in the design of the Globus Community Authorization Service. NERSC's BRO network security monitoring system has been reconfigured to work with Globus, and the NERSC Information Management (NIM) account management system is also being made Grid-aware so that it will be able to use clients' Public Key Infrastructure (PKI) authorization certificates.

NERSC is one of eight laboratory and university sites participating in the U.S. ATLAS Grid testbed, a prototype system to support physicists who collaborate on the ATLAS experiment at CERN's Large Hadron Collider. The goal of the ATLAS Grid is to enable collaborators to access data and perform analysis from their home institutions. In a "data challenge" exercise of this testbed, NERSC's PDSF successfully ran 2,500 jobs submitted over a two-week period.

Tests of distributed computation are expected to begin in the upcoming year, including a subsurface flow simulation involving computers at NERSC and Pacific Northwest National Laboratory.



## Berkeley Lab Team Wins Third Bandwidth Challenge

The Bandwidth Challenge competition at the annual SC conference on high performance computing and networking has been a showcase for emerging Grid technologies and applications. At SC2002, the Berkeley Lab team achieved their third consecutive victory with a data transfer rate five times faster than the previous year's top speed. The team won top honors for the Highest Performing Application, moving data at a peak speed of 16.8 GB/s.

The team used clusters of computers at seven sites in the United States, the Netherlands, and the Czech Republic. Entitled "Wide Area Distributed Simulations Using Cactus, Globus, and Visapult," the winning application modeled gravitational waves generated during the collision of black holes. Participating sites were the PDSF at NERSC and clusters at the SC2002 conference in Baltimore, Argonne National Laboratory, the National Center for Supercomputing Applications, the Pittsburgh Supercomputing Center, the University of Amsterdam, and the Masaryk University in the Czech Republic. Support was provided by the Albert Einstein Institute in Germany, the Poznan Supercomputing and Networking Center in Poland, DOE's Energy Sciences

Network (ESnet), Sandia National Laboratories, SysKonnect, Hewlett-Packard, and Force10 Networks Inc.

The team ran the Visapult volume rendering application (<http://www-vis.lbl.gov/RDProjects/visapult2/>) at SC2002 to create visualizations from the simulations being run on the participating clusters. The OC-192 and OC-48 lines that fed the Baltimore convention center were aggregated into three 10 Gigabit Ethernet links to a Force10 Networks switch that fed the HP/Compaq Linux cluster in the Berkeley Lab booth on the show floor. The team used a cluster of Alpha-based computers loaned by Hewlett-Packard and SysKonnect network interface cards to put together the winning effort.

Wes Bethel, the head of Berkeley Lab's Visualization Group and developer of Visapult, said that improvements in Visapult, along with the evolving networking and Grid infrastructure of hardware, software, and middleware, helped push the team's data transfer to such a high rate.

The High-Performance Bandwidth Challenge encourages teams of researchers from around the world to use, if not swamp, the SC conference network to demonstrate applications using huge amounts of data. The Berkeley Lab team won the first ever Bandwidth Challenge at SC2000, moving data at an average of 596 MB/s over 60 minutes and hitting a peak of 1.48 GB/s over a five-second period. At the SC2001 conference, the team (Figure 1) took the top prize by achieving a sustained network performance level of 3.3 GB/s.



**FIGURE 1** The SC2001 Bandwidth Challenge Team included staff from Berkeley Lab's Computational Research (CRD), Information Technologies and Services (ITSD), and NERSC Center divisions. Shown here are Wes Bethel (CRD), George Smith (NERSC), Alfred Early (ITSD), John Christman (ITSD), Eli Dart (NERSC), Brent Draney (NERSC), Mike Bennett (ITSD), David Paul (NERSC), and John Shalf (CRD). The SC2002 team also included NERSC's Cary Whitney and Shane Canon (see photo on page 87).







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The Supercomputing Allocations Committee (SAC) is responsible for setting the policies associated with the utilization of computing, data storage, and other auxiliary services available to DOE Office of Science (SC) researchers and otherwise coordinating SC's computational projects. The Committee sets the distribution of NERSC and other available Office of Advanced Scientific Computing Research resources for scientific computing applications every year.

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# OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

## MATHEMATICAL, INFORMATION, AND COMPUTATIONAL SCIENCES DIVISION

The primary mission of the Advanced Scientific Computing Research (ASCR) program, which is carried out by the Mathematical, Information, and Computational Sciences (MICS) subprogram, is to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. To accomplish this mission, the program fosters and supports fundamental research in advanced scientific computing—applied mathematics, computer science, and networking—and operates supercomputer, networking, and related facilities. In fulfilling this primary mission, the ASCR program supports the Office of Science Strategic Plan's goal of providing extraordinary tools for extraordinary science as well as building the foundation for the research in support of the other goals of the strategic plan. In the course of accomplishing this mission, the research programs of ASCR have played a critical role in the evolution of high performance computing and networks. Berkeley Lab thanks the program managers with direct responsibility for the NERSC program and the MICS research projects described in this report:

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The Advanced Scientific Computing Advisory Committee (ASCAC) provides valuable, independent advice to the Department of Energy on a variety of complex scientific and technical issues related to its Advanced Scientific Computing Research program. ASCAC's recommendations include advice on long-range plans, priorities, and strategies to address more effectively the scientific aspects of advanced scientific computing including the relationship of advanced scientific computing to other scientific disciplines, and maintaining appropriate balance among elements of the program. The Committee formally reports to the Director, Office of Science. The Committee primarily includes representatives of universities, national laboratories, and industries involved in advanced computing research. Particular attention is paid to obtaining a diverse membership with a balance among scientific disciplines, institutions, and geographic regions.

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