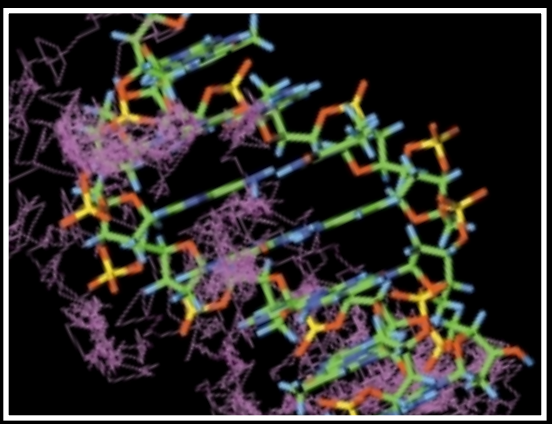
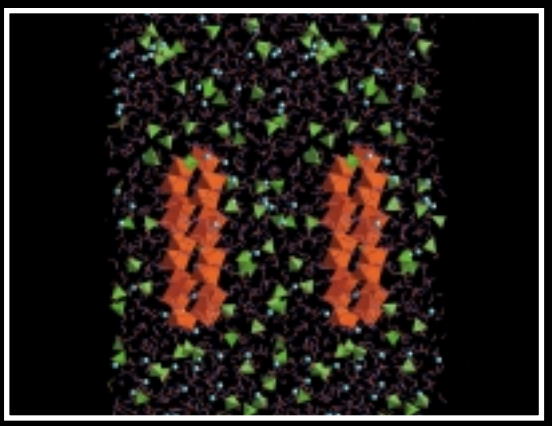
NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

BERKELEY LAB
ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

# *2001 Annual Report*







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BERKELEY NATIONAL LABORATORY

*National Energy Research Scientific Computing Center*

# *2001 Annual Report*

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LBNL-49186, December 2001

NERSC aspires to be a world leader in accelerating scientific discovery through computation. Our vision is to provide 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 technology. The result will be a rate of scientific progress previously unknown.

NERSC's mission is to accelerate the pace of scientific discovery in the Department of Energy Office of Science (SC) community by providing high-performance computing, information, and communications services. NERSC has a threefold strategy for increasing researchers' productivity:

- Providing leading-edge platforms and services that make NERSC the foremost resource for large-scale computation within DOE.
- Introducing the best new computer science tools to SC researchers.
- Providing intellectual services (for example, development of innovative algorithms, simulations, and visualization techniques) that make these complicated technologies useful for computational science.

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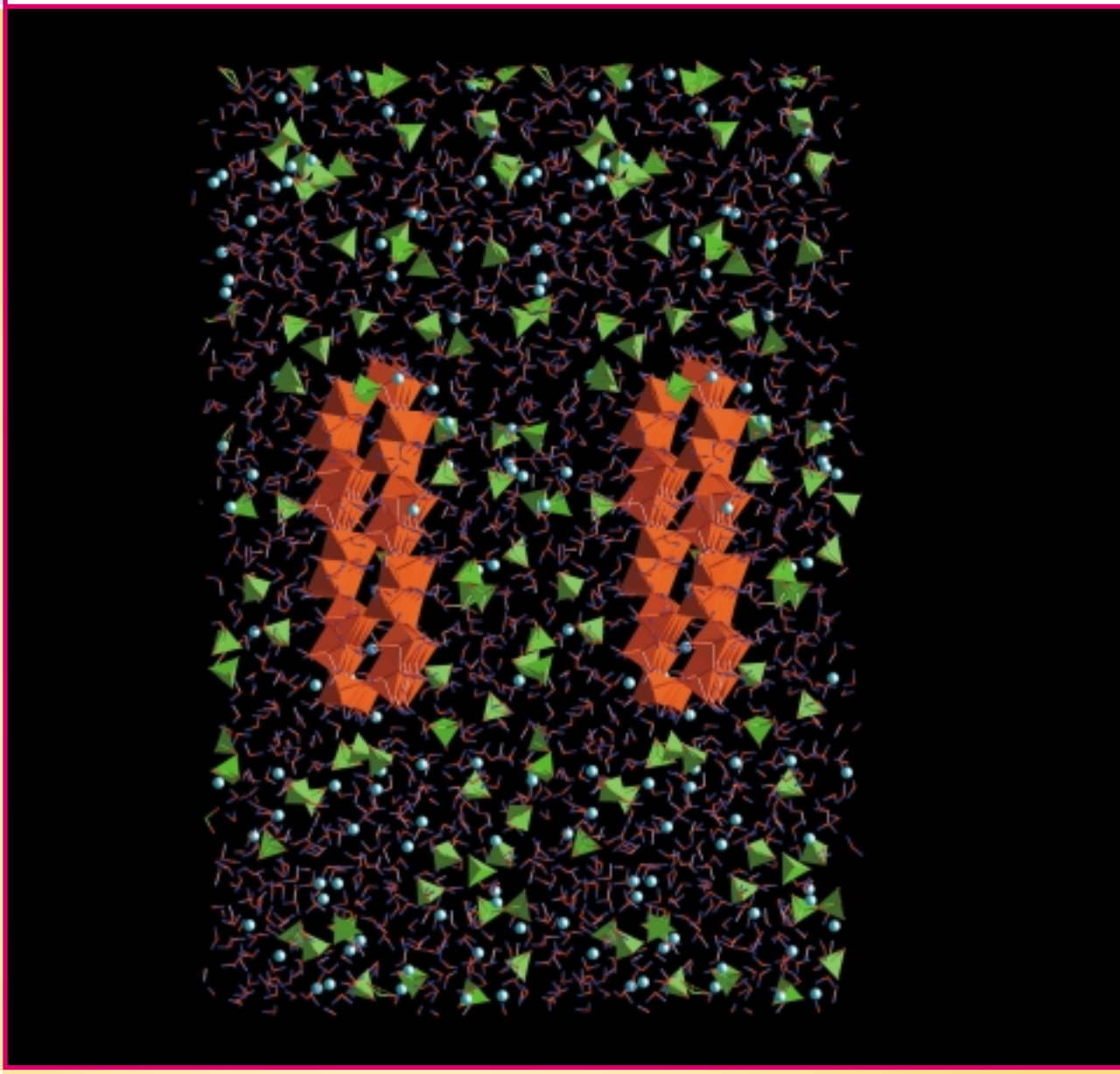
## *Director's Perspective*



*Molecular dynamics simulation of the initial stages of attachment of two goethite nanoparticles in a sodium perchlorate solution.* *See page 39 for details.*

Just before I left for SC2001, a long-expected letter arrived in Berkeley. It was the official DOE response to the NERSC Strategic Plan for 2002–2006, which we had developed earlier this year and submitted to DOE in May. In this letter to Berkeley Lab Director Charles V. Shank, dated November 8, 2001, Dr. C. Edward Oliver, Associate Director of Science for ASCR, accepted the broad outline of the strategic plan and committed to supporting NERSC at Berkeley Lab for the next five years. In these uncertain times, this is a strong commitment to NERSC by DOE. Even more satisfying was the fact that the letter concurred with many of the reviewers' observations that NERSC has provided "world-class hardware, timely technology upgrades and services virtually unsurpassed by any other computer center in the world." Dr. Oliver described the NERSC staff's commitment to excellence as a "vital attribute" of the center, and wrote, "Your proposal presents a sound strategy for providing high-performance scientific computing hardware and services in a manner commensurate with the near-term expectations of the Office of Science."

*Horst Simon, Director of NERSC*

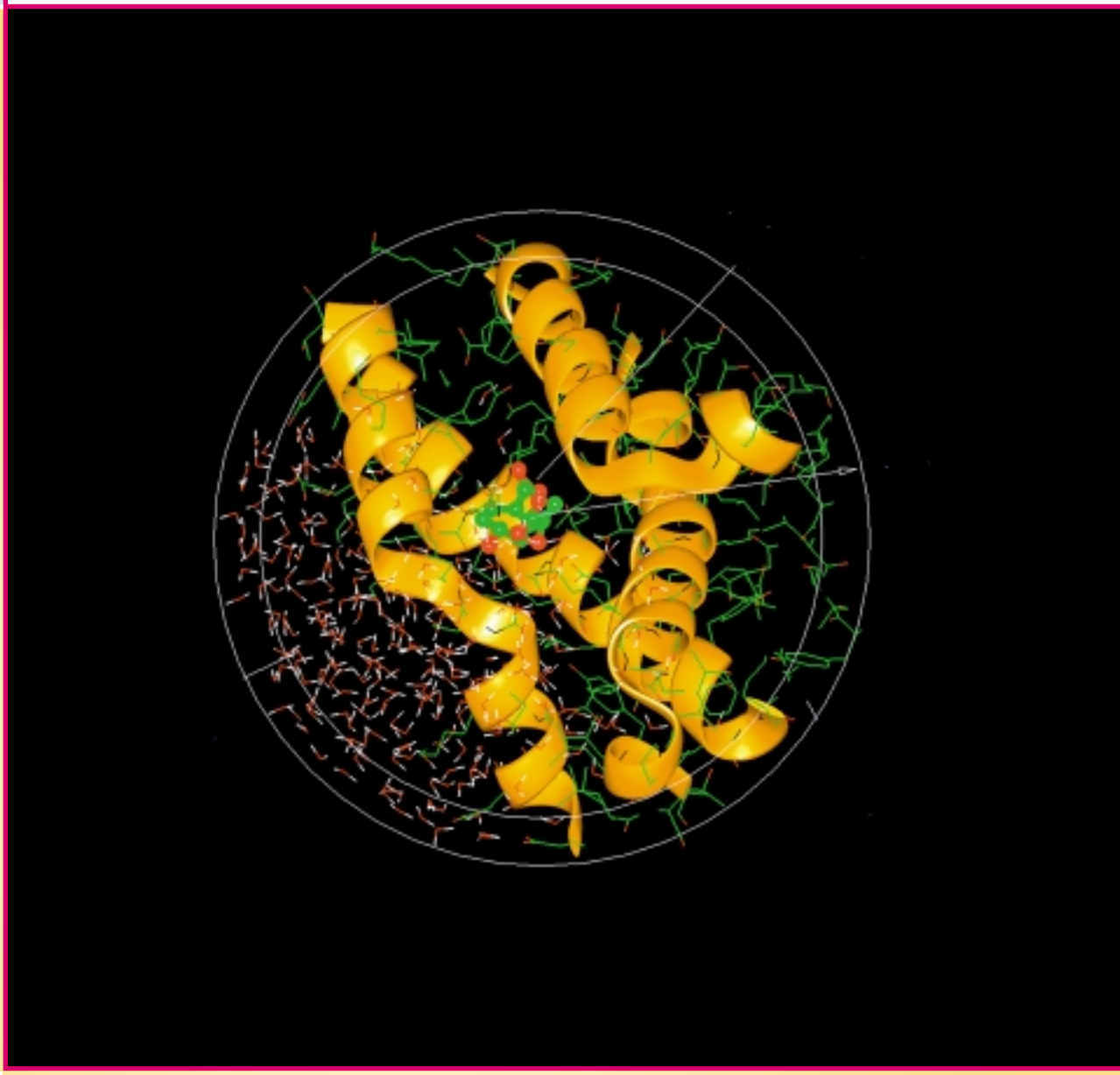
We can be proud of this recognition, which arrived at the end of another very successful year. The high point was NERSC's acceptance of the IBM SP platform, which by October 2001 had been upgraded to deliver almost 5 teraflop/s peak performance. With this new capability, NERSC will deliver 50 million processor hours of compute cycles annually to the DOE Office of Science research community. While many of our colleagues at other sites brag about terascale computing, I believe that in 2002, NERSC will be the first site where users routinely see their applications performing at teraflop/s level. Some are already achieving this, and their remarkable scientific accomplishments are described in this report.

After several years of planning, computational science in the DOE Office of Science finally received a big boost in 2001 through the funding of the Scientific Discovery through Advanced Computing (SciDAC) program. SciDAC opens up the opportunity to further develop and then deploy the results of recent computer science research. Computational science and computer science researchers in Berkeley excelled in the competition and obtained funding for many bold new projects. The leadership for three of the seven new "Integrated Software Infrastructure Centers" (ISICs) as well as for the DOE Science Grid is in the hands of researchers at Berkeley Lab. In addition, we participate in seven other SciDAC projects.

With DOE's recognition of Berkeley Lab and NERSC's leadership in computational science comes a big challenge: we are on the spot to make SciDAC a success. For NERSC as a facility, the challenge is to be ready for these new projects and to enable a whole new generation of computational science. I see it as my personal responsibility to make Berkeley Lab the place where the integration of the SciDAC projects will happen, and NERSC the facility where DOE scientists will first be able to reap the benefits of the newly developed technologies.

With SciDAC projects and the NERSC strategy firmly established, 2001 was the year when we set the agenda and directions for the next five years. With a time of intense new developments ahead of us, I am grateful to our DOE Office of Science sponsors for their continued endorsement of our ambitious plans. It continues to be a pleasure to collaborate with the NERSC Users Group and its executive board members. I would like to thank them for their continued support, especially for their effort to produce the next "Greenbook" documenting the computational requirements of the Office of Science community. 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.

# Computational Science at NERSC



*Model protein-substrate system used in a molecular dynamics simulation of yeast chorismate mutase.*
*See page 55 for details.*

As a national facility for scientific research funded by the Department of Energy, Office of Science (DOE SC), NERSC served 2,130 scientists throughout the United States in FY 2001. 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 utilized around 100,000 MPP processor hours or more during the year. 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.

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.

DOE's Supercomputing Allocations Committee (SAC, see Appendix D) reviews and makes award decisions for all requests, reflecting their mission priorities. In addition, NERSC's Program Advisory Committee (PAC, see Appendix B) peer reviews certain requests and also makes award decisions. The SAC allocates 60 percent of NERSC resources, while the PAC allocates 40 percent.

Two other groups provide general oversight: 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

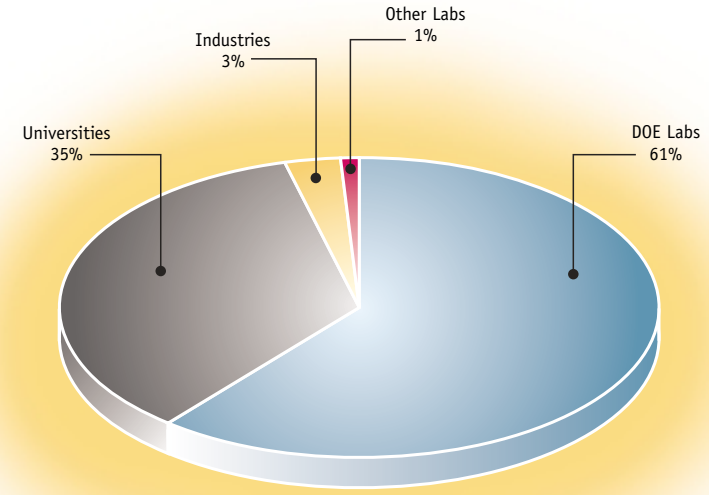



***Figure 1. NERSC MPP usage by institution type, FY01.***

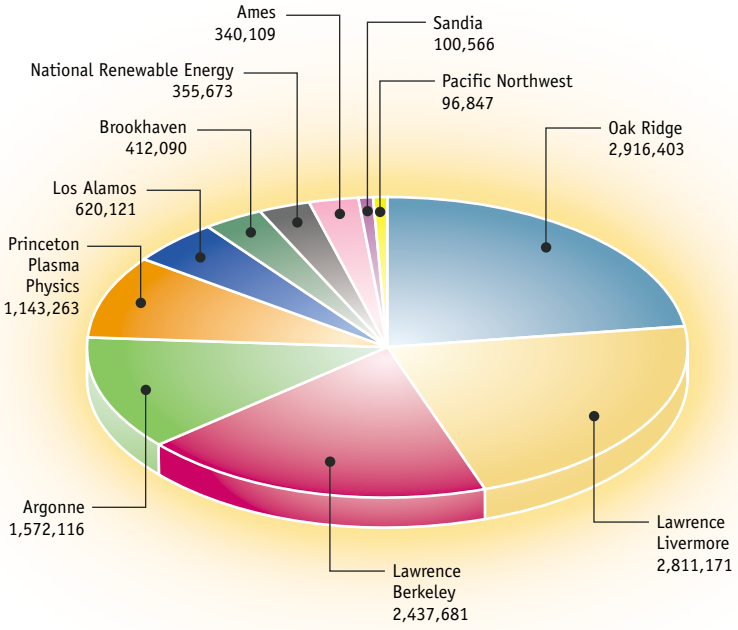



***Figure 2. Leading DOE laboratory usage at NERSC, FY01 (>90,000 MPP processor hours).***

Scientific Computing Avisory Committee (Appendix F).

This section of the Annual Report gives an overview of the research supported by NERSC and points out some of the year's achievements, which are described further in the Science Highlights section.

## Advanced Scientific Computing Research

Research sponsored by DOE's Office of Advanced Scientific Computing Research (ASCR) is having an impact in a number of scientific fields. For example, predicting the formation of pollutants in flames requires detailed modeling of both the carbon chemistry in the flame and nitrogen chemistry that leads to pollutants. Recent flame simulations, performed using a parallel adaptive mesh refinement algorithm, modeled the behavior of 65 chemical species and 447 reactions; the computed results showed excellent agreement with experimental data and provided new insights into the mechanisms of pollutant formation.

Computational studies are also contributing to our understanding of transverse jets, which have been studied extensively for their relevance to aerodynamics and to environmental problems such as pollutant dispersion from chimneys or the discharge of effluents into the ocean. The mixing and combustion dynamics of transverse jets are important to a variety of engineering applications, including industrial furnaces, gas turbines, and oil wells.

ASCR supports a variety of research in computer science and applied mathematics. Some of the more general research involves developing and implementing highly efficient and scalable algorithms for solving sparse matrix problems on various classes of high-performance computer architectures. Sparse matrix problems are at the heart

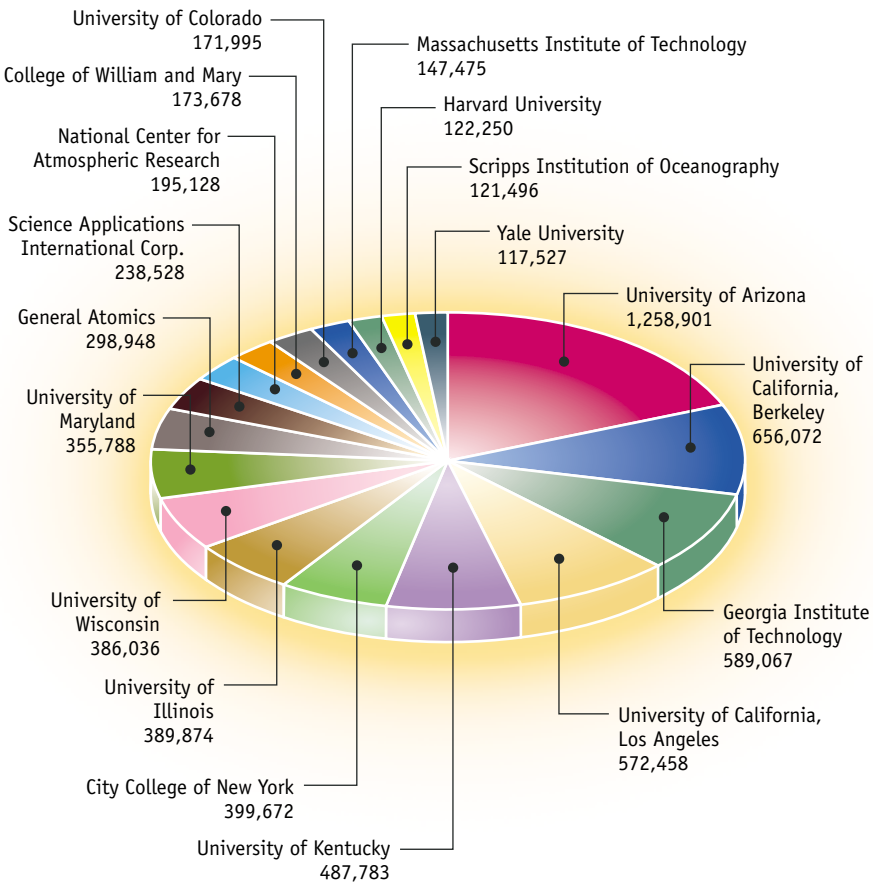



***Figure 3. Leading academic and related usage at NERSC, FY01 (>100,000 MPP processor hours). Includes industry and non-DOE government labs.***

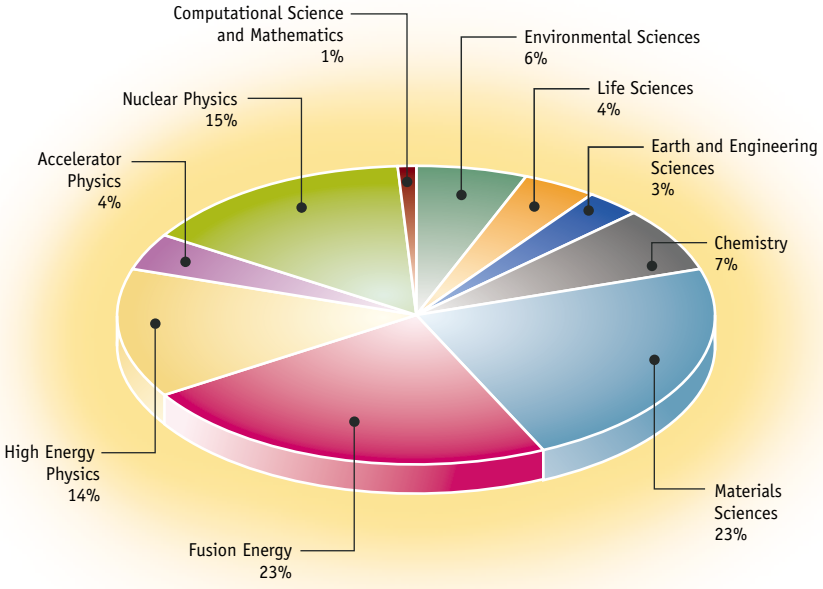



***Figure 4. NERSC MPP usage by scientific discipline, FY01.***

of many scientific and engineering applications, including fusion energy, accelerator physics, structural dynamics, computational chemistry, groundwater simulations, etc. Improved algorithms are expected to have significant impact on the performance of these applications.

Research jointly funded by ASCR and the Office of Biological and Environmental Research has resulted in a global optimization algorithm that performed very well in an international competition to test the performance of various methods of protein structure prediction. The global optimization method produced the best prediction for one of the most difficult targets of the competition, a new fold protein of 240 amino acids. This method relies less on information from databases and more on energy and solvation functions, enabling it to do a reasonable job of discriminating misfolds from correct folds even in relatively novel proteins.

### Basic Energy Sciences

NERSC provides computational support for a large number of materials sciences, chemical sciences, geosciences, and engineering projects sponsored by DOE's Office of Basic Energy Sciences.

Computational materials scientists continue to make important discoveries about a wide range of technologically significant materials, including silicon carbide semiconductors, cadmium selenide nanocrystals, colossal magnetoresistance oxides, and iron-manganese/cobalt interfaces. One research group is developing a first-principles approach to the atomic-scale design of novel catalytic materials, tailored to perform specific reactions with the desired activity and selectivity. Custom-designed catalysts could have widespread applications in pollution prevention technologies, fuel cells, and industrial processes.

Alex Zunger, one of the pioneers of first-principles methods for predicting properties of solids, was named the 2001 recipient of the Rahman Award by the American Physical Society. The award is presented annually to an individual for "outstanding achievement in computational physics research." Zunger, head of the Solid State Theory Group at DOE's National Renewable Energy Laboratory in Colorado, was cited for his "pioneering work on the computational basis for first-principles electronic theory of solids." Zunger developed theoretical methods for quantum-mechanical computations and predictions of the properties of solids through the use of atomic numbers and the laws of quantum physics. Over the 15-plus years since this work was first published, his techniques have become the standard tools for predicting properties of solids from first principles. Zunger's current research has achieved detailed predictions

## *Two Teams of Finalists for 2001 Gordon Bell Prize Used Results Run at NERSC*

The Gordon Bell Prizes are awarded each year at the SC conference to recognize outstanding achievement in high performance computing. This year two teams of finalists, one supported by the Office of Basic Energy Sciences and one by the Office of Biological and Environmental Research, submitted entries based in part on computations run at NERSC.

Several members of the team that won the Gordon Bell Prize for having the fastest application in 1998 were finalists again at SC2001. Their entry, "Multi-Teraflop/s Spin Dynamics Studies of the Magnetic Structure of FeMn/Co Interfaces," achieved a maximum execution rate of 2.46 teraflop/s using 2,176 processors on NERSC's IBM SP. Their large-scale quantum mechanical simulations, involving 2,016-atom super-cell models, revealed details of the orientational configuration of the magnetic moments at the iron-manganese/cobalt interface that are unobtainable by any other means. This work is of fundamental importance in improving magnetic multi-layer computer storage and read head devices. The team included Andrew Canning from NERSC; B. Ujfalussy from the University of Tennessee, Knoxville; T. C. Schulthess, X.-G. Zhang, W. A. Shelton, D. M. C. Nicholson, and G. M. Stocks from Oak Ridge National Laboratory; Yang Wang from the Pittsburgh Supercomputer Center; and T. Dirks from IBM.

Climate models have been notably absent in previous Gordon Bell competitions due to their inability to scale to large processor counts. This year, however, Richard Loft, Stephen Thomas, and John Dennis of the National Center for Atmospheric Research were finalists with the entry "Terascale Spectral Element Dynamical Core for Atmospheric General Circulation Models (GCMs)." This team is working to speed up the integration rate of climate models by using the spectral elements method for the dynamical core; this method gives better performance on SMP architectures than the more commonly used spectral transform method. Using 2,048 processors on the NERSC IBM SP, and achieving a sustained performance of 369 Gflop/s, the NCAR team demonstrated that their GCM dynamical core can be integrated at a rate of 130 modeling years per computing day.

of the effects of nanoscale atomic structures on the electronic and optical properties of semiconductor systems.

Recent simulations of electron-$CO_2$ scattering represent the first time that all aspects of an electron-polyatomic collision, including not only the determination of the fixed-nuclear electronic cross sections but also a treatment of the nuclear dynamics in multiple dimensions, has been carried out entirely from first principles. This computational approach to collision processes will soon be extended to allow study of systems containing more than two electrons. Electron collision processes are central to the problems of interest to DOE, playing a key role in such diverse areas as fusion plasmas, plasma etching and deposition, and waste remediation.

### Biological and Environmental Research

DOE's Office of Biological and Environmental Research is a major supporter of global climate studies as well as computational biological research using NERSC resources. Because the emission of carbon dioxide into the atmosphere from fossil fuel combustion is potentially a major contributor to global warming, the global carbon cycle and carbon sequestration are important areas of research.

This year the highest-resolution-ever global simulations of direct injection of $CO_2$ into the oceans indicated that this may be an effective carbon sequestration strategy. In the simulation, approximately 80% of the injected carbon remains in the ocean permanently, while the 20% of the carbon that leaks back to the atmosphere does so on a time scale of several hundred years. If these results are confirmed by experiments, direct injection of $CO_2$ into the ocean could play an important role in mitigating global warming.

Climate researchers are also developing the first comprehensive coupled climate/carbon cycle model in the U.S. This model will allow better predictions of future climate, because it will take into account feedback effects of climate change on the absorption of carbon by the ocean and the terrestrial biosphere—effects that are ignored in present U.S. climate models. This model will be more useful to policymakers because it will use $CO_2$ emission rates, rather than atmospheric $CO_2$ concentrations, as the fundamental input, thus allowing direct assessment of the climatic impact of specified rates of fossil fuel burning.

Global climate simulations are typically performed on a latitude-longitude grid, with grid cell sizes of about 300 km. Although coarse-resolution simulations can provide useful information on continental and larger scales, they cannot provide meaningful information on regional scales. Thus, they cannot provide information on many of the most

***Figure 5. The genome of the Japanese pufferfish (Fugu rubripes) was draft sequenced using the efficient but computationally demanding whole genome shotgun sequencing method. The unusually short fugu genome will provide important clues for deciphering the human genome.***

important societal impacts of climate change, such as impacts on water resource management, agriculture, human health, etc. A team from Lawrence Livermore National Laboratory, using supercomputers there as well as NERSC's IBM SP, recently ran a global climate change model at 50 km resolution, the highest spatial resolution ever used. Preliminary analysis of the results seems to indicate that the model is very robust to a large increase in spatial resolution, which may improve the realism of the model on both global and regional scales.

On the biological front, a substantial shortcut to the information embedded in the human genome has been taken by an international research consortium with the completion of a draft sequence of the genome of the Japanese pufferfish *Fugu rubripes* (Figure 5). The DOE's Joint Genome Institute (JGI) was one of the leaders of the consortium. Although the fugu genome contains essentially the same genes and regulatory sequences as the human genome, the entire fugu genome is only one-eighth the size of the human. With far less so-called "junk DNA" to sort through, finding genes and controlling sequences in the fugu genome should be a much easier task. The information can then be used to help identify these same elements in the human genome.

The fugu genome is the first vertebrate genome to be draft sequenced after the human genome, and the first public assembly of an animal genome by the whole genome shotgun sequencing method. After the genome was chopped up into pieces that are small enough to sequence, the challenge was to reassemble the genome by putting together nearly four million of these overlapping fragments. Solving this puzzle was made possible by a new computational algo-

rithm, JAZZ, that was developed at JGI to handle large genome assembly projects. JGI used NERSC's IBM SP to develop and test JAZZ, which reconstructs contiguous genome sequences by overlapping the short subsequences.

### Fusion Energy Sciences

Research funded by the Office of Fusion Energy Sciences reached a milestone this year with the first simulation of turbulent transport in a full-sized reactor plasma by researchers at the Princeton Plasma Physics Laboratory. This breakthrough full-torus simulation, which produced important and previously inaccessible new results, used 1 billion particles, 125 million spatial grid points, and 7,000 time steps. It was made feasible by a new generation of software and hardware—better physics models and efficient numerical algorithms, along with NERSC's new 5 teraflop/s IBM SP.

This simulation dealt with a key issue in designing fusion reactors, namely, the realistic assessment of the level of turbulent transport driven by microscopic-scale instabilities (ITG modes). Turbulent transport is a major concern because it can lead to loss of plasma confinement. Up until very recently, the effects of turbulent transport have been assessed by extrapolating to larger reactors the transport properties observed in smaller experimental devices. This approach relied on models of transport scaling that have often stirred debates about reliability. The new simulation of a reactor-sized plasma produced a result that was as welcome as it was surprising—as the size of the plasma increased, the turbulent transport reached a plateau and leveled off. This "rollover" from one scaling mode to another will be an important new topic for future research.

Major progress has also been made in understanding magnetic reconnection, a sudden release of magnetic energy which is the cause of large-scale explosive events in plasma systems. These events include solar flares, storms in the earth's magnetosphere, and sawtooth instability in tokamak experiments. In magnetic reconnection, the magnetic field self-annihilates in locations where it reverses direction, transferring its energy to plasma flows and intense, high-energy beams. The result in fusion experiments is sawtooth instability, which involves sudden changes in magnetic topology and plasma temperature.

The short time scale of this energy release cannot be explained by resistive magnetohydrodynamic models, which break down at the small spatial scales where magnetic reconnection occurs. At these scales, recent simulations show that whistler and kinetic Alfvén waves dominate the dynamics. The dispersive property of these waves causes reconnection to occur quickly in the simulation, consistent with observations, even when the out-of-plane magnetic

## *In Memoriam*

We note with sadness the passing of two pioneers in computational science, John Dawson and Peter Kollman.

*John Dawson*

John M. Dawson, Professor of Physics at UCLA and Director of Special Projects of the Institute for Fusion and Plasma Research, died at his home in Los Angeles on November 17, 2001. He was 71. An international leader in plasma physics, Dawson is considered the father of computer-simulated plasma models and of plasma-based particle accelerators. He created the particle-in-cell modeling technique, which became one of the standard tools of computational plasma research.

Dawson received the James Clerk Maxwell Prize in Plasma Physics in 1977 and the American Physical Society's Aneesur Rahman Prize for Computational Physics in 1994. He holds numerous patents and has published over 300 papers in basic plasma physics, space plasma physics, applications of plasmas to high energy physics, and controlled fusion. More information about his work and a memorial scholarship fund can be found at http://www.physics.ucla.edu/people/faculty_members/dawson.html.

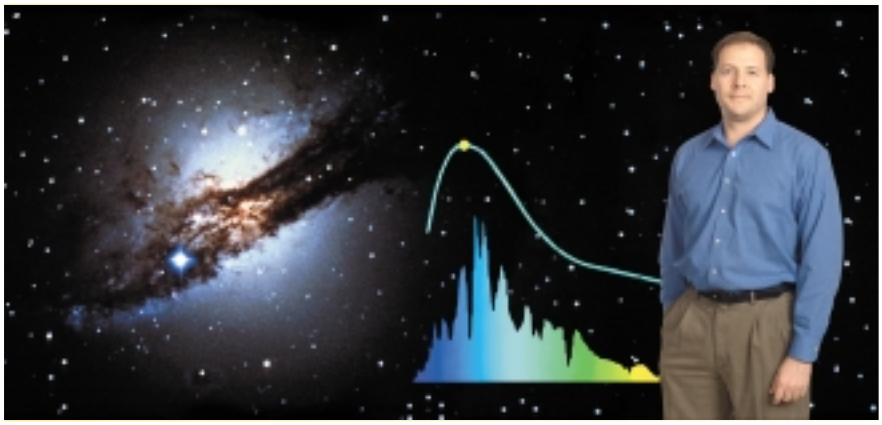
*Peter Kollman*

Peter Kollman died on May 25, 2001 at his home in San Francisco less than a month after being diagnosed with cancer. He was 56. Kollman, Professor of Pharmaceutical Chemistry at the University of California, San Francisco, was an international leader in computational studies of protein folding and molecular interactions. AMBER, the suite of molecular dynamics codes developed under his direction, is one of the most important tools of computational biology.

Kollman received the 1995 American Chemical Society Award for Computers in Chemical and Pharmaceutical Research, and the 1993 Computerworld Smithsonian Award. He was the author of more than 400 scientific journal articles and more than 50 book articles and chapters. His work was the 11th most cited among all chemists in the world during the period 1981–1997. More information about his work and a memorial fund can be found at his home page, http://www.amber.ucsf.edu/amber.

# *Oldest, Most Distant Type Ia Supernova Confirmed by Analysis at NERSC*

An exploding star dubbed SN 1997ff, caught on three different occasions by NASA's Hubble Space Telescope, is the oldest and most distant Type Ia supernova ever seen, according to a recent analysis by Peter Nugent, one of NERSC's two staff astrophysicists. Peter is a member of the team led by Adam Riess at the Space Telescope Science Institute that studied the distant supernova.



*Peter Nugent studies supernovae to answer basic questions about the nature and destiny of the Universe.*

The discovery of the more than 11-billion-year-old supernova is important for several reasons. This supernova is consistent with the cosmological model of an accelerating universe, a universe mostly filled with dark energy. It argues against the notion that observations of distant Type Ia supernovae may be systematically distorted by intervening gray dust or the chemical evolution of the universe. Moreover, the supernova is so ancient that it allows us to glimpse an era when matter in the universe was still relatively dense and expansion was still slowing under the influence of gravity. More recently the dark energy has begun to predominate and expansion has started to speed up.

The Supernova Cosmology Project and the High-Z Supernova Search Team, the two international groups of astronomers and physicists who discovered the accelerating expansion of the universe, use Type Ia supernovae as "standard candles" to measure cosmological parameters. Type Ia spectra and light curves (their rising and falling brightness over time) are all nearly alike, and they are bright enough to be seen at very great distances.

With a redshift (or z) of about 1.7, supernova 1997ff is some 11.3 billion years old, much older—and much fainter—than the previous record of z equals 1.2, which corresponds to an age of about 9.8 billion years old. A supernova at redshift 1.7 is too far away to have been visible from the surface of the Earth. Only a space-based telescope could have found it.

Peter is involved in two related supernova projects, one for accelerating the acquisition of data and one for analyzing the data. The first is the Nearby Supernova Factory, an international collaboration that aims to discover large numbers of Type Ia supernovae as soon as possible after they explode (see page 70 for details). In this project, raw images will be transferred to NERSC nightly from remote observatories; the images will be calibrated and corrected, then compared with baseline sky catalogs; automated search algorithms will then look for indications of supernova activity; and the results will be relayed back to the observatories so that more detailed observations can be made. This close interaction between observation and computation, involving huge datasets, requires high performance computers, storage systems, and Grid technologies. The Supernova Factory is an earth-based observation program that will serve as a development testbed for the next-generation search program, the satellite-based Supernova Acceleration Probe (SNAP).

Peter is also a leader of the Spectrum Synthesis of Supernovae project, which is analyzing data from both nearby and distant supernovae to measure the fundamental parameters of cosmology (see page 75). One of this group's models, which used to take a few months to run, was completed in four days on NERSC's new IBM SP.

field is large and/or the system size is very large. The new model resolves the longstanding discrepancy in the energy release time between models and observations of magnetic reconnection, and recently reported evidence of whistler waves in the magnetosphere bolsters the theory. Computations at NERSC were essential to the discovery and demonstration of the role of dispersive waves.

### 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.

One of this year's most significant physics discoveries provides a solution to a 30-year-old mystery—the puzzle of the missing solar neutrinos. Since the early 1970s, several experiments have detected neutrinos arriving on Earth, but they have found only a fraction of the number expected from detailed theories of energy production in the Sun. This meant there was something wrong with either the theories of the Sun, or our understanding of neutrinos.

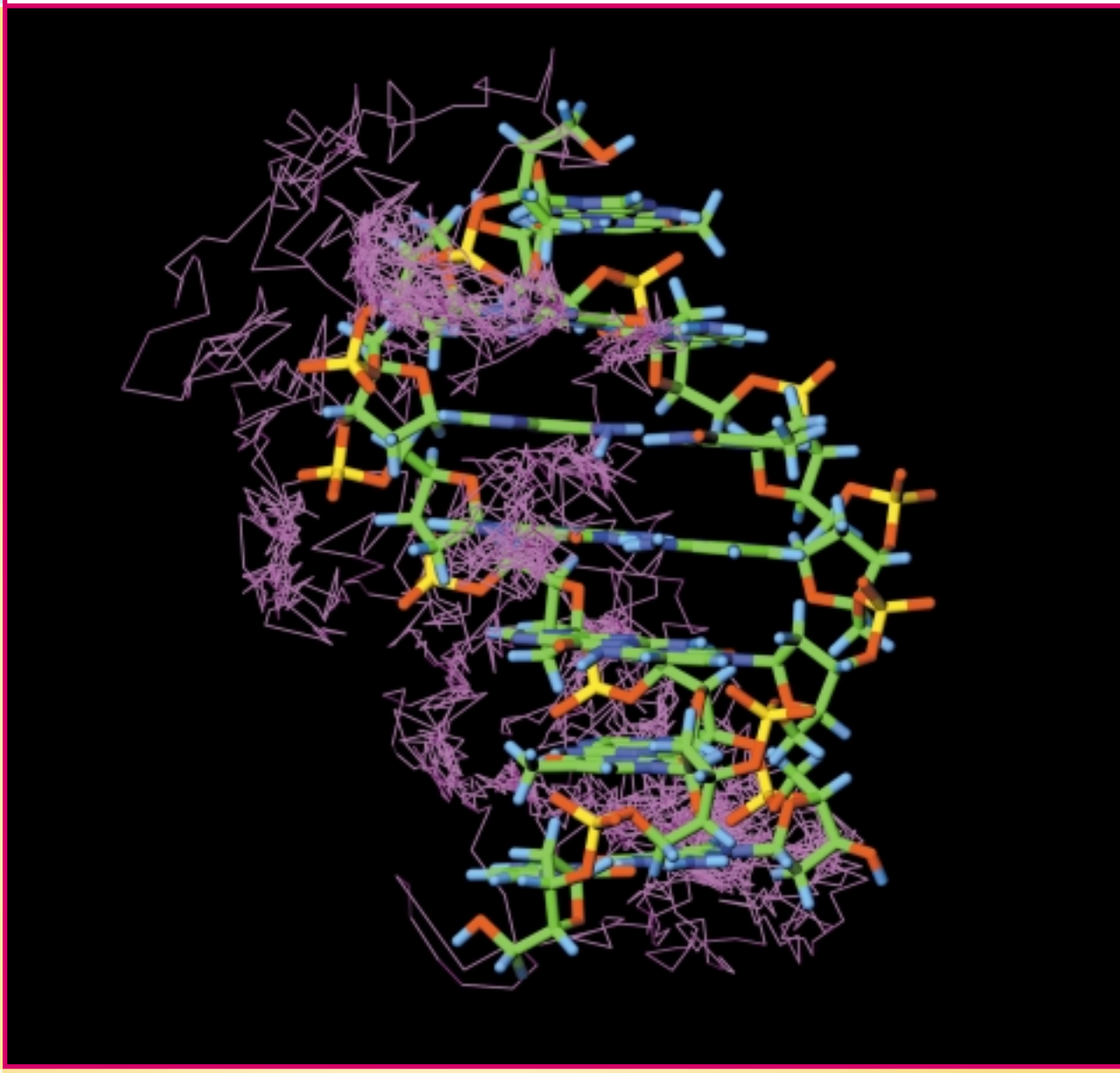
New data from the Sudbury Neutrino Observatory (SNO) shows that the solution lies not with the Sun, but with the neutrinos, which change as they travel from the core of the Sun to the Earth. The new results show that the total number of electron neutrinos produced in the Sun is just as predicted by solar models, but the neutrinos are oscillating in transit, changing in type or "flavor" from electron neutrinos (the flavor produced in the sun) to muon or tau neutrinos. SNO results also show that solar neutrinos do have some small mass, but not enough to account for much of the dark matter in the Universe. These results will require some adjustments to the Standard Model of fundamental particles.

The SNO collaboration has relied on NERSC's HPSS facility for data storage and distribution, and on the Parallel Distributed Systems Facility (PDSF) for algorithm development, detector performance studies, simulations to reduce background data, and analysis of the first year's data.

The STAR detector at Brookhaven National Laboratory also has performed well during its first year's run and has made significant progress in mapping out the soft physics regime at the Relativistic Heavy Ion Collider (RHIC). The measured particle ratios were found to be consistent with quark coalescence. The elliptic flow measured in STAR is larger than observed at lower energies, and is in agreement with calculations using hydrodynamics; this suggests thermalization at an early stage of the collision. Currently, the STAR project yields about 300 gigabytes of data daily which are transferred from Brookhaven to the NERSC HPSS facility. STAR has about 30 terabytes of data in the NERSC HPSS system; extrapolating from current usage, the project is expected to have about 100 terabytes in HPSS by the end of FY 2002.

Among the year's many accomplishments in lattice QCD studies, one research team carried out a production run on a quenched 204 lattice with lattice spacing at 0.15 fm. The size of each direction is thus 3 fm, which is the largest volume that any lattice calculation has attempted. They also pushed the pion mass to as low as ~200 MeV, which is also a record, and found many interesting features of chiral symmetry at such a low mass and large volume. For example, they found that the zero mode contribution to the pion propagator is not negligible at small time region, and its contamination needs to be avoided when extracting pion properties such as the pion mass and decay constant. They also found that after nonperturbative renormalization, the pseudoscalar meson decay constant is very constant in the range between the strange and up/down quark mass.

# NERSC Systems and Services



*Molecular dynamics simulation of DNA with a sodium counter-ion. See page 44 for details.*

The year 2001 was a landmark year for NERSC. It was our first year in Berkeley Lab's new Oakland Scientific Facility, and it was the year we advanced into the terascale computing era by installing what was at that time the most powerful computer in the world for unclassified research. During the year we also made significant upgrades in our mass storage and networking capabilities, and we continued making our services more responsive to client needs.

## Oakland Facility Dedicated

On May 24, Oakland Mayor Jerry Brown and Dr. James Decker, Acting Director of the DOE Office of Science, joined Berkeley Lab Director Charles Shank for the formal dedication of the Oakland Scientific Facility (OSF). (NERSC actually began using the building in November 2000.) Decker noted that the computational research done at NERSC will pay substantial dividends to the city of Oakland, industry partners, the DOE, the Laboratory, and the nation. Mayor Brown praised the "boldness of creativity" evident in the new facility and pledged the city's support.

About 75 guests also heard from Peter Ungaro of IBM; James Payne of Qwest Communications; Peter Wang, Chairman and President of Encinal Broadway, the building's owner; and Jud King, provost and senior vice president for the University of California. Bill McCurdy, associate laboratory director for Computing Sciences, led the machine room tour that followed, pointing to the new IBM SP as "a tool that is our future, the way we will understand our world."

The new 16,000-square-foot OSF computer room was designed for flexibility and expandability. The computer room can be expanded to 20,000 square feet by removing a non-load-bearing wall, resulting in a facility able to accommodate several new generations of computing systems. The facility has a flexible power distribution system with a power supply of 5 MW, and a high-capacity chilled-water air conditioning system to maintain the ideal operating environment.

## 5 Teraflop/s IBM SP Goes Online

In August, after months of rigorous acceptance testing, Phase 2 of the NERSC-3 system was made available to the research community. The 3,328-processor IBM RS/6000 SP system, named "Seaborg" in honor of Berkeley Lab Nobel Laureate Glenn Seaborg, is capable of performing 5 trillion calculations per second (5 teraflop/s). Installed in January,


*With the symbolic connection of cables linking NERSC's supercomputers with its international user community on a high-speed network, the Oakland Scientific Facility was formally dedicated by Oakland Mayor Jerry Brown, Berkeley Lab Director Charles Shank, and Dr. James Decker, Acting Director of the DOE Office of Science.*

the SP underwent extensive configuration and customization for the NERSC production environment and users. NERSC's Sustained System Performance (SSP) benchmark suite was used to test the system with actual scientific applications in a realistic production mode. By the time the system was opened up for general production use, it was running so well that significant scientific results in several fields were produced in just the first few weeks, and users expressed a high level of satisfaction with the system.

Because the NERSC-3 contract was based on specific, firm performance metrics and functional requirements rather than on peak performance or hardware specifications, the Phase 2 IBM SP system has 22% more processing power and 50% more memory than originally planned, and thus will provide 10 million additional processor hours per year to users. Peak performance has grown from the planned 3.8 to 5 teraflop/s, with 3,008 processors available for computation. A unique aspect of NERSC-3 may be its 4.5 terabytes of main memory.

The NERSC-3 contract, defined in 1998–99 and based on IBM's proposal, specified more than 40 performance and 150 functional requirements that stem from the application workload that exists at NERSC. Almost every area of function and performance is covered by overlapping but

independently relevant measures. For example, there are two disk I/O measures, one for large parallel files and another for small parallel and serial files. Both metrics are necessary for an accurate estimate of the true performance for scientists.

The fixed-price contract guaranteed a minimum configuration of hardware—what was projected to meet all the requirements—and IBM also guaranteed to meet the performance requirements. At the end of acceptance testing on the expanded system, IBM had exceeded the performance and functional requirements on the specifications. NERSC also purchased some additional hardware in order to make the system even more suitable for certain applications. As a result, the NERSC-3 system is capable of meeting all the maximum performance requirements, and provides significantly enhanced capability and performance for the typical application requirements.

*The IBM SP acceptance team spent seven months testing, evaluating, and fine-tuning the system's performance. Led by NERSC Deputy Director Bill Kramer, key team members were Lynne Rippe, Gary Mack, Jim Craw, Nick Cardo, Tammy Welcome, Adrian Wong, David Bailey, Jonathon Carter, David Skinner, Dinesh Vakharia, Scott Burrow, and Ronald Mertes. Other contributors included Harsh Anand, Majdi Baddourah, Richard Beard, Del Black, Julian Borrill, Greg Butler, Andrew Canning, Eli Dart, Tom DeBoni, Brent Draney, Aaron Garrett, Richard Gerber, Frank Hale, William Harris, Russell Huie, Wayne Hurlbert, YuLok Lam, Steven Lowe, Nancy Meyer, Robert Neylan, Esmond Ng, David Paul, Jay Srinivasan, David Turner, and Alex Ubungen (not all present for photo).*

## Bigger, Faster, Easier Mass Storage

To stay ahead of the growing needs of our clients and the growing capacity of our computational systems, NERSC works constantly to increase the capacity, bandwidth, and functionality of our HPSS mass storage system. This year NERSC began increasing our disk cache to 20 terabytes by adding more Fibre Channel disks. Internal data transfer rates were improved by the replacement of our HIPPI internal storage network with Jumbo Gigabit Ethernet. Additional high-capacity Fibre tape drives are expanding our archive from 1.3 to 2 petabytes. And we upgraded AFS with a bigger disk cache and faster processors.

Two years ago, NERSC and Oak Ridge National Laboratory established the Probe wide-area distributed-storage testbed to research storage technologies. During the past year NERSC used Probe to test a new, faster version of HSI (the HPSS interface utility) that enables access to multiple HPSS systems, making distributed mass storage simpler and more convenient. A Grid-capable FTP daemon was also tested as another way to bring Grid connectivity to HPSS. NERSC experimented with remote WAN network movers as a way to bypass conventional file transfer methods and stream data quickly between sites. And we conducted a beta test of the new Linear Tape-Open (LTO) Ultrium ultra-high-density tape drives. All of these efforts, together with the GUPFS project described below, will help bring mass storage and Grid technologies together.

## Developing a Global Unified Parallel File System

In a typical high-performance computing (HPC) environment, each large computational system has its own local disk as well as access to additional network-attached storage and archival storage servers. Such an environment prevents the consolidation of storage between systems, thus limiting the amount of working storage available on each system to its local disk capacity. The result is an unnecessary replication of files on multiple systems, an increased workload on users to manage their files, and a burden on the infrastructure to support file transfers between the various systems.

NERSC is using existing and emerging technologies to overcome these inefficiencies. The Global Unified Parallel File System (GUPFS) project aims to provide a scalable, high-performance, high-bandwidth, shared-disk file system for use by all of NERSC's high-performance production computational systems. GUPFS will provide unified file namespace for these systems and will be integrated with the High Performance Storage System (HPSS). Storage servers, accessing the consolidated storage through the GUPFS shared-disk file systems, will provide hierarchical storage management, backup, and archival services. An additional goal is to distribute GUPFS-based file systems to geographically remote facilities as native file systems over the DOE Science Grid.

This environment will eliminate unnecessary data replication, simplify the user environment, provide better distribution of storage resources, and permit the management of storage as a separate entity while minimizing impacts on the computational systems. The major enabling components of this envisioned environment are a high-performance shared-disk file system and a cost-effective, high-performance storage area network (SAN). These emerging technologies, while evolving rapidly, are not targeted towards the needs of high-performance scientific computing. The GUPFS project intends to encourage the development of these technologies to support HPC needs through both collaborations with other institutions and vendors, and active development.

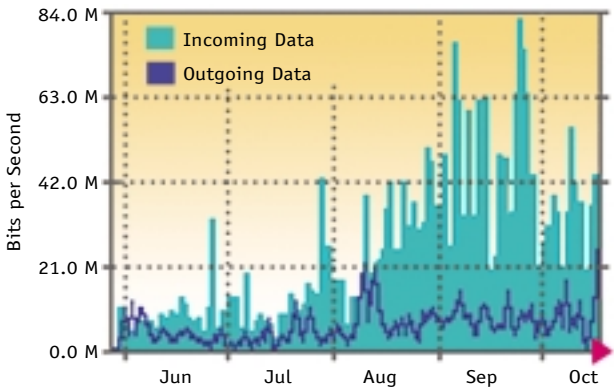



***Figure 6. Network traffic for June through October 2001 shows the impact of the OC-12 ESnet link upgrade and the Phase 2 IBM SP being made available for general production use in August.***

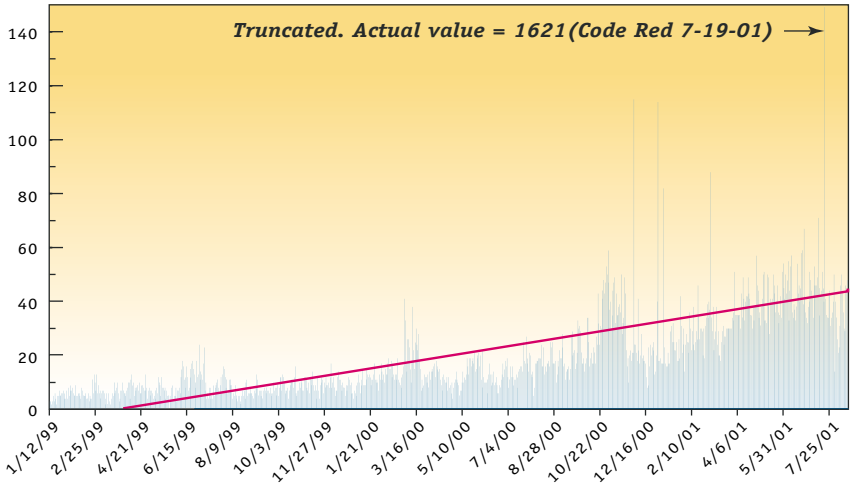



***Figure 7. External daily scans of "lbl.gov" servers from January 1999 to August 2001 show that attempted intrusions are increasing steadily.***

## Providing Fast, Safe Network Connections

To connect our new facilities and systems to the Grid, NERSC has implemented major upgrades to our networking infrastructure. At the end of May, the Oakland Scientific Facility upgraded its ESnet connection to OC-12 (622 Mb/s) to accommodate the growing demands of data-intensive computing (Figure 6). Gigabit Ethernet utilizing Jumbo Frames (9 KB packets) is the new standard for our internal network connecting the IBM SP and HPSS systems; when our current Cray systems are replaced, older HIPPI and FDDI connections will also be phased out. Ongoing network upgrades are being planned for the future to anticipate the ever-increasing bandwidth needs of our users.

As important as the latest networking hardware may be, NERSC's Networking and Security Group is also very concerned with day-to-day performance. They have created a new network statistics Web page (http://hpcf.nersc.gov/network/) which allows NERSC users to monitor network activity in real time. The networking staff themselves monitor traffic for signs of poor performance, and they proactively work with remote users to improve end-to-end rates. For example, they traced slow data transfers from Brookhaven National Laboratory and the Jet Propulsion Laboratory to a bug in the respective labs' firewalls and then worked with Cisco Systems to fix the bug. This kind of creative problem solving has resulted in 4 to 30 times faster data transfer rates from some user sites. (Users desiring to improve their transfer rates should contact NERSC User Services.)

The Networking and Security Group also monitors the network for intrusions and unauthorized use, and responds to security incidents in cooperation with Berkeley Lab's cybersecurity staff. Attempted intrusions have been rising steadily in the last few years (Figure 7), but security research is making progress as well. The NERSC BRO border intrusion detection system can take action to block certain attacks without human intervention. In addition, we have begun working with Juniper Networks, Inc. to test the BRO intrusion detection software at speeds of 2.4 Gb/s (OC-48).

*NERSC's Networking and Security Group—Eli Dart, Brent Draney, group leader Howard Walter, and Steve Lau—are the network detectives, tracking down problems and blocking hackers to ensure high performance and secure connections for NERSC users.*

## Balancing System Utilization and Response Time

Over the years, NERSC has been a pioneer in achieving high utilization on massively parallel systems—in simple terms, keeping as many processors as possible working for as long as possible. High utilization, made possible by customized scheduling and load balancing software, gives researchers more available processor hours and maximizes the value of the computing resource. NERSC's Cray T3E reached 95% utilization (averaged over 30 days) in February 2001; and taking advantage of our experience with the T3E, we were able to get 85% utilization on the IBM SP, better than the T3E's first year.

An occasional side effect of high utilization—and an undesirable one from the user's viewpoint—is a long wait for a job to run, if that particular job is not the right size for the system's current load balance. Because response time is an important factor in researchers' productivity—and scientific productivity is the ultimate measure of NERSC's success—we are now working with a user committee to find the optimum balance of utilization and response time. The committee will research solutions and develop guidelines to be implemented on NERSC systems.

## Expanded PDSF Brings Cosmic Mysteries to Light

Eighty-two new servers and significant improvements in the overall computing and networking infrastructure were added this year to the PDSF (Parallel Distributed Systems Facility), a large Linux-based computer cluster that is currently operated as a partnership between NERSC and the Berkeley Lab Nuclear Science and Physics divisions.

Computing power was expanded to 395 processors, and the number of disk vaults grew from 15 to 40, with a total 24 terabytes of shared storage. Gigabit Ethernet networking for the high-bandwidth compute nodes enables the PDSF to run MPI jobs that require up to 50 nodes (100 processors). In addition, Gigabit Ethernet for the disk vaults makes it possible to take advantage of the server-side performance improvements of the 2.4 Linux kernel.

The PDSF serves the data-intensive computing needs of international high energy and nuclear physics experiments at the world's most powerful accelerator centers—including the AGS/RHIC complex at Brookhaven National Laboratory (STAR, E895), CERN (NA49, ATLAS, ALICE), and Fermilab (CDF, E871)—as well as neutrino detectors in Canada (SNO) and Antarctica (AMANDA), and other experiments that are expanding our knowledge of the universe.

The PDSF is the primary computing facility for analysis of data from the STAR experiment, which is generating 300 terabytes of data each year, and was also used to verify several major discoveries at CERN's NA49 experiment. Access to the PDSF greatly speeded up publication of initial results from STAR, E895, AMANDA, and SNO. Scientific questions the PDSF is helping to answer range from the mass of solar neutrinos to the characteristics of the quark-gluon plasma that existed briefly after the Big Bang.

## Proposals Sought for NERSC-4 System

NERSC acquires a new capability-focused computational system about every three years. The three-year interval is based on the length of time it takes to introduce large systems, the length of time it takes for NERSC clients to become productive on new systems, and the types of funding and financial arrangements NERSC uses. At any given time, NERSC has two generations of computational systems in service, so that each system will have a lifetime of five to six years. This overlap provides time for NERSC clients to move from one generation to the next, and provides NERSC with the ability to fully test, integrate, and evolve the latest generation while maintaining service on the earlier generation.

NERSC uses the "Best Value" process for procuring its major systems. Rather than setting mandatory requirements and using a quantitative rating scheme, the Best Value method requests baseline and value-added characteristics. These characteristics are not meant to design a specific solution but rather to signify a range of parameters that will produce an excellent and cost-effective solution. Thus, Best Value does not limit a site to the lowest common denominator requirements, but rather allows NERSC to push the limits of what is possible in order to get the best solution. Vendors indicate they prefer this method as well, because it provides them more flexibility in crafting their best solution.

A request for proposals for the NERSC-4 system was issued in November 2001, with proposals due in February 2002. Like the NERSC-3 contract described above, the NERSC-4 contract will be based on performance metrics and functional requirements, especially NERSC's Sustained System Performance (SSP) benchmark suite and Effective System Performance (ESP) test. One new feature of this contract is that the SSP value will no longer be based on the NAS Parallel Benchmarks, but will be based on the NERSC Application Performance Suite. Delivery of the initial NERSC-4 system is expected in early 2003.

## User Survey Provides Valuable Feedback

NERSC's annual user survey provides feedback about every aspect of NERSC's operation, and every year we institute changes based on the survey results. Here are some of the changes resulting from the FY 2000 survey:

- In last year's survey, one of the two top IBM SP issues was that the "SP is hard to use." Based on comments we received, we wrote more SP documentation for the Web and made changes to the user environment. This year only 12% of the comments (compared with 25% last year) indicated that the SP is hard to use.
- We made changes that were suggested to the IBM SP disk configuration.
- We added queue resources and created a new queue for the Cray T3E, resulting in improved satisfaction with T3E turnaround time.
- Last year we moved PVP interactive services from the J90 to the SV1 architecture and provided more disk resources. Overall PVP satisfaction was rated higher in this year's survey.

In the FY2001 survey, there were significant increases in user satisfaction in the available computing hardware, the allocations process, and the PVP cluster. Other areas showing increased satisfaction were T3E and SP batch wait times, SP disk configuration, SP Fortran compilers, and HPSS. Areas with continuing high user satisfaction included HPSS reliability, performance, and uptime; consulting responsiveness, quality of technical advice, and follow-up; Cray programming environment; PVP uptime; and account support.

When asked what NERSC does well, some respondents pointed to our stable and well managed production environment, while others focused on NERSC's excellent support services. Other areas singled out include well done documentation, good software and tools, and the mass storage environment. When asked what NERSC should do differently, the most common responses were to provide more hardware resources and to enhance our software offerings. Other areas of concern were visualization services, batch wait times on all platforms, SP interactive services, training services, and SP performance and debugging tools.

Several sample responses give the flavor of the users' comments:

*"NERSC makes it possible for our group to do simulations on a scale that would otherwise be unaffordable."*

*"The availability of the hardware is highly predictable and appears to be managed in an outstanding way."*

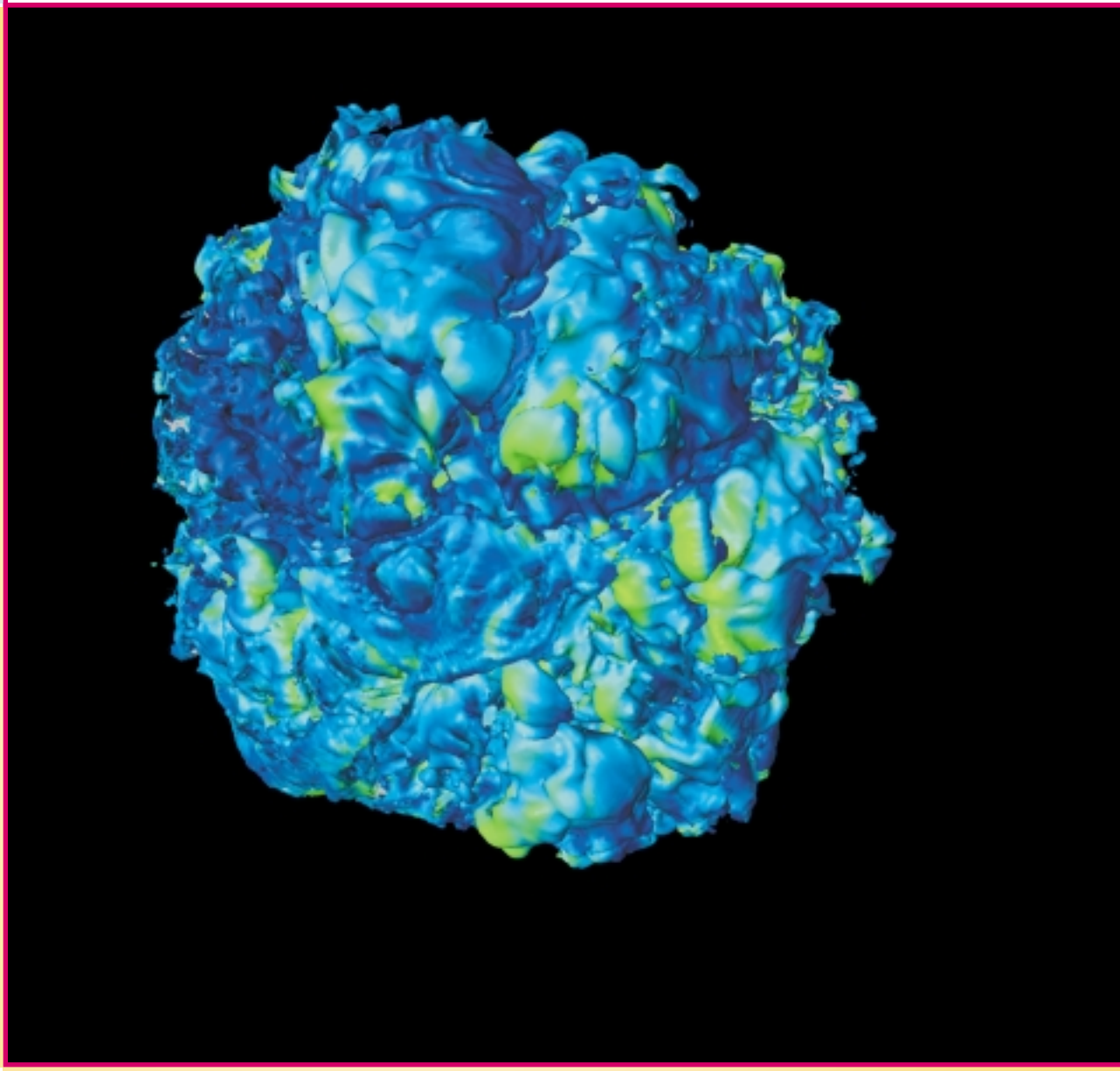
*"Provides computing resources in a manner that makes it easy for the user. NERSC is well run and makes the effort of putting the users first, in stark contrast to many other computer centers."*

*"Consulting by telephone and e-mail. Listens to users, and tries to set up systems to satisfy users and not some managerial idea of how we should compute."*

*"The web page, hpcf.nersc.gov, is well structured and complete. Also, information about scheduled down times is reliable and useful."*

Complete survey results can be found at http://hpcf.nersc.gov/about/survey/2001/.

# High Performance Computing R&D at Berkeley Lab



*This 3D supernova simulation shows the turbulent environment beneath the supernova shock wave.*
*See page 73 for details.*

The NERSC Program is part of the Computing Sciences organization at Berkeley Lab and works closely with two other departments within Computing Sciences: the High Performance Computing Research Department and the Distributed Systems Department. These two departments conduct a large number of independently funded research and development efforts in applied mathematics, computer science, and computational science. Some of their staff members also work on tasks matrixed from the NERSC Program, such as the advanced development of scientific computing infrastructure, and focused high-end support for NERSC clients in areas such as algorithms, software tools, and visualization of data.

This close association of research activities and a leading-edge computing facility is mutually beneficial—it gives NERSC users access to the latest technologies and tools, while encouraging developers to address the critical needs of computational scientists. Some of the highlights of this year's R&D efforts are described in this section, particularly those that are relevant to SciDAC.

## Applied Mathematics

Applied mathematics research at Berkeley Lab ranges from involvement in three SciDAC projects, which are expected to yield major scientific benefits within a few years, to investigating the randomness of certain mathematical constants, which represents a major step toward answering an age-old question.

### *Applied Partial Differential Equations*

Led by Phil Colella, head of the Applied Numerical Algorithms Group (ANAG), the Applied Partial Differential Equations (PDE) Integrated Software Infrastructure Center (ISIC) will develop a high-performance algorithmic and software framework for solving PDEs arising from three important mission areas in the DOE Office of Science: magnetic fusion, accelerator design, and combustion. This framework will provide investigators in these areas with a new set of simulation capabilities based on locally structured grid methods, including adaptive meshes for problems with multiple length scales; embedded boundary and overset grid methods for complex geometries; efficient and accurate methods for particle and hybrid particle/mesh simulations; and high performance implementations on distributed-memory multiprocessors. One of the key results of this effort will be a common mathematical and software framework for multiple applications.

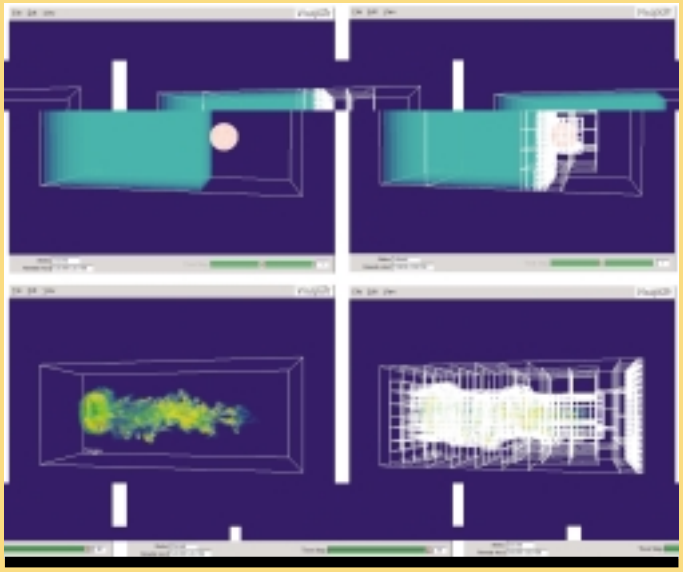


***Figure 8. CCSE and the Berkeley Lab/NERSC Visualization Group collaborated on this simulation of shock-wave physics that shows what happens to a bubble of argon when subjected to a shock wave. This sequence shows images from early and late simulation time steps, with and without the underlying AMR grid. It was produced with Visapult, our research prototype application and framework that performs image-based-rendering-assisted volume rendering of large, 3D and time-varying AMR datasets.***

Members of ANAG and the Center for Computational Sciences and Engineering (CCSE), led by John Bell, have more than 15 years of experience in developing adaptive mesh refinement (AMR) algorithms and software, culminating last year in the release of Berkeley Lab AMR, a comprehensive library of AMR software and documentation. This experience is the foundation of their leadership role in the Applied PDE ISIC, which includes collaborators from Lawrence Livermore National Laboratory, the University of California at Davis, New York University, the University of North Carolina, the University of Washington, and the University of Wisconsin.

The research of CCSE and ANAG to date has focused primarily on turbulent combustion processes, and their methods have matured to the point that several of their recent simulations have accurately reproduced experimental results. Because small-scale turbulent fluctuations modify the physical processes such as kinetics and multiphase behavior, an important goal of their research is to develop techniques that accurately reflect the role of small-scale fluctuations on the overall macroscopic dynamics. They are also working on improved techniques for visualizing AMR data (see Figure 8).

# *Berkeley Lab Provides Both Leadership and Support for SciDAC Projects*

Berkeley Lab will help lead the development of a new generation of tools and technologies for scientific computing under a new $57 million program announced on August 14, 2001 by the DOE. Under the Scientific Discovery through Advanced Computing (SciDAC) program, scientists and mathematicians in Berkeley Lab's Computing Sciences organization are leading four of the projects and are collaborating in another seven projects.

SciDAC is an integrated program that will help create a new generation of scientific simulation codes. The codes will take full advantage of the extraordinary computing capabilities of terascale computers to address ever larger, more complex problems. The program also includes research on improved mathematical and computing systems software that will allow these codes to use modern parallel computers effectively and efficiently. Additionally, the program will develop collaboratory software to enable geographically separated scientists to effectively work together as a team, to control scientific instruments remotely, and to share data more readily. In all, 51 projects were funded nationwide, involving collaborations among 13 DOE national laboratories and more than 50 colleges and universities.

Here are the SciDAC programs that Computing Sciences staff will be leading:

- *DOE Science Grid* — This collaboratory will 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. (PI: Bill Johnston)
- *Performance Evaluation Research Center (PERC)* — As one of several SciDAC Integrated Software Infrastructure Centers (ISICs), this project will focus on how specific scientific applications can best be run on high-performance computers. The results of this research are expected to permit the generation of realistic performance levels, and to determine how applications can be written to perform at the highest levels and how this information can be applied to the design of future applications and computer systems. (PI: David Bailey)
- *Scientific Data Management ISIC* — Terascale computing and large scientific experiments produce enormous quantities of data that require effective and efficient management, a task that can distract scientists from focusing on their core research. The goal of this project is to provide a coordinated framework for the unification, development, deployment, and reuse of scientific data management software. (PI: Ari Shoshani)
- *Applied Partial Differential Equations ISIC* — The goal is to develop a high-performance algorithmic and software framework for solving partial differential equations arising from problems in magnetic fusion, accelerator design, and combustion—key mission areas for the DOE. (PI: Phil Colella)

Berkeley Lab computer scientists and mathematicians will also be collaborating with other national laboratories and universities on the following SciDAC projects:

- *Advanced Computing for 21st Century Accelerator Science and Technology* — This project will work on simulating particle accelerators, some of the largest and most complex scientific instruments. A new generation of accelerator simulation codes will help us to use existing accelerators more efficiently and will strongly impact the design, technology, and cost of future accelerators. (Lead institutions: Lawrence Berkeley National Laboratory and Stanford Linear Accelerator Center)
- *Collaborative Design and Development of the Community Climate System Model for Terascale Computers* — A multi-institutional team will develop, validate, document, and optimize the performance of this coupled climate model using the latest software engineering approaches, computational technology, and scientific knowledge. (Lead institution: Los Alamos National Laboratory)
- *Earth Systems Grid II: Turning Climate Databases into Community Resources* — This project will create a virtual collaborative environment that links distributed centers, users, models, and data, significantly increasing the scientific productivity of U.S. climate researchers by turning climate datasets into community resources. (Lead institution: Argonne National Laboratory)

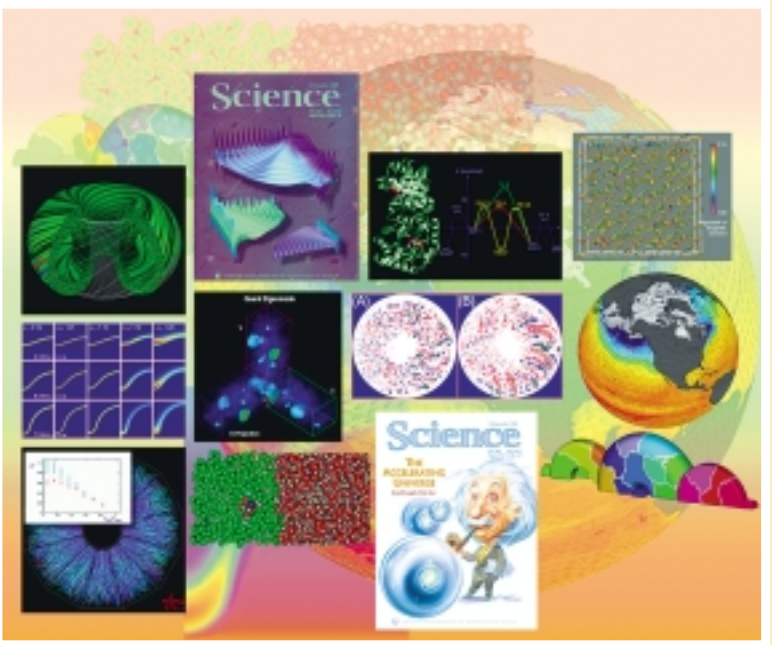



*Figure 9. Building on the DOE Office of Science's past achievements in computational science, SciDAC will help create a new generation of scientific simulation codes that take full advantage of terascale computers and Grid technologies.*

- *National Collaboratory to Advance the Science of High Temperature Plasma Physics for Magnetic Fusion Energy* — The National Fusion Collaboratory will promote more effective integration of experiment, theory, and modeling by enabling networked real-time data analysis and instantaneous communication among geographically dispersed teams of experimentalists and theoreticians. (Lead institution: General Atomics)

- *Particle Physics Data Grid Collaborative Pilot* — This pilot project will develop, acquire, and deliver vitally needed Grid-enabled tools for the data-intensive requirements of particle and nuclear physics. (Lead institutions: University of Wisconsin, California Institute of Technology, and Stanford Linear Accelerator Center)

- *Scalable Systems Software ISIC* — This project will address the lack of software for effective management and utilization of terascale computing resources. This project will develop an integrated suite of machine-independent, scalable systems software needed for the SciDAC program. The goal is to provide open-source solutions that work on systems ranging in size from small to large. (Lead institution: Oak Ridge National Laboratory)

- *Terascale Optimal PDE Solvers (TOPS) ISIC* — Large-scale simulations of importance to the DOE often involve the solution of partial differential equations (PDEs). In such simulations, continuous (infinite-dimensional) mathematical models are approximated with finite-dimensional models. To obtain the required accuracy and resolve the multiple scales of the underlying physics, the finite-dimensional models must often be extremely large, thus requiring terascale computers. This project focuses on developing, implementing, and supporting optimal or near-optimal schemes for PDE simulations and closely related tasks. (Lead institution: Old Dominion University)

In addition to Berkeley Lab's participation in the projects mentioned above, NERSC is providing specialized consulting and algorithmic support for SciDAC projects. A consulting project facilitator has been assigned to each scientific discipline to help define project requirements, get resources, and tune and optimize codes, as well as coordinate special services (queues, throughput, increased limits, etc.). Algorithmic project facilitators have been assigned to develop and improve algorithms, enhance performance, and coordinate software development with the various ISICs.

NERSC's strategic plan for the next five years involves two new elements—Support for Scientific Challenge Teams and the Unified Science Environment—specifically designed to support the kinds of scientific collaborations envisioned by SciDAC. NERSC's strategic plan is described in a special section of this report beginning on page 30.

### *TOPS and Accelerators*

Esmond Ng, leader of the Scientific Computing Group, is a collaborator on two SciDAC projects: the Terascale Optimal PDE Solvers (TOPS) ISIC, led by David Keyes of Old Dominion University, and the Advanced Computing for 21st Century Accelerator Science and Technology project, led by Kwok Ko of Stanford Linear Accelerator Center and Robert Ryne of Berkeley Lab.

The TOPS ISIC will research, develop, and deploy an integrated toolkit of open source, optimal complexity solvers for the nonlinear PDEs that arise in many Office of Science application areas, including fusion energy, accelerator design, global climate change, and reactive chemistry. These algorithms, primarily multilevel methods, aim to reduce computational bottlenecks by one to three orders of magnitude on terascale computers, enabling scientific simulation on a scale heretofore impossible.

The 21st Century Accelerator Project will develop a new generation of accelerator simulation codes, which will help to use existing accelerators more efficiently and will strongly impact the design, technology, and cost of future accelerators. These simulations use a wide variety of mathematical methods; for example, the electromagnetic systems simulation component utilizes sparse linear solvers for eigenmode codes.

Esmond Ng was one of the first researchers to develop and implement efficient algorithms for sparse matrix computation on parallel computer architectures, and some of his algorithms have been incorporated into several scientific computing libraries. Several other Berkeley Lab and NERSC staff members also have eigenanalysis and sparse linear systems expertise which the SciDAC projects will be able to take advantage of. In related research during the past year, the MUMPS general-purpose sparse solver was tuned, analyzed, and compared with the SuperLU code developed by Sherry Li and James Demmel.

### *Are the Digits of Pi Random?*

David Bailey, NERSC's chief technologist, and his colleague Richard Crandall, director of the Center for Advanced Computation at Reed College, Portland, Oregon, have taken a major step toward answering the age-old question of whether the digits of pi and other mathematical constants are truly random. Their results were reported in the Summer 2001 issue of *Experimental Mathematics*.

Numbers like pi have long been thought to be "normal," meaning that in base 10, for example, any single digit occurs one-tenth of the time. While the evidence to date supports this assumption, no naturally occurring math constant—such as pi, the square root of 2, or the natural logarithm of 2—has ever been formally proved to be normal in any number base.

Bailey and Crandall have translated this heretofore unapproachable problem to a more tractable question in the field of chaotic processes. They propose that the normality of certain constants is a consequence of a plausible conjecture in the field of chaotic dynamics, which states that sequences of a particular kind are uniformly distributed between 0 and 1—a conjecture they refer to as "Hypothesis A." If even one particular instance of Hypothesis A could be established, the normality of important mathematical constants would follow.

## Computer Science

Computer science research and development at Berkeley Lab runs the gamut from programming languages and systems software to scientific data management, Grid middleware, and performance evaluation of high-end systems. The expertise of our computer scientists and the relevance of their research can be seen in the projects highlighted below.

### *DOE Science Grid Collaboratory*

Led by Bill Johnston, head of the Distributed Systems Department, the DOE Science Grid SciDAC Collaboratory will 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.

The DOE Science Grid will provide uniform access to a wide range of DOE resources, as well as standard services for security, resource access, system monitoring, and so on. This will enable DOE scientists and their collaborators in projects such as the Particle Physics Data Grid (PPDG), the Extensible Computational Chemistry Environment (ECCE), the Earth Systems Grid (ESG), and the Supernova Factory Collaboratory to much more readily employ computational and information resources at widely distributed institutions. It will also facilitate development and use of collaboration tools that speed up research and allow scientists to tackle more complex problems. All of these services will be available through secure Web/desktop interfaces in order to produce a highly usable environment.

Bill Johnston and the Distributed Systems Department staff have more than a decade of R&D experience in this field, in addition to Bill's experience as project technical manager for NASA's Information Power Grid. NERSC Deputy Director Bill Kramer is co-principal investigator on this SciDAC project; other collaborators are at Argonne National Laboratory, Pacific Northwest National Laboratory, and Oak Ridge National Laboratory. Several other projects of the Distributed Systems Department are described below.


*The Grid Technologies Group—student intern Wesley Lau, group leader Keith Jackson, and staff members Jason Novotny and Joshua Boverhof—are working to make Grid middleware more user friendly so that scientists can more easily create their own Grid connections and working environments.*

### *Developing Grid Technologies*

The Distributed Systems Department this year formed a new Grid Technologies Group, with Keith Jackson as group leader, to research and develop technologies needed for the DOE Science Grid. Their current focus is on developing high-level tools to make the Grid easier to use and program. The group is developing Commodity Grid Kits (CoG Kits), which allow one to utilize basic Grid services through commodity technologies such as frameworks, environments, and languages, to allow easier development of Grid applications. (Some examples of these technologies are CORBA, Java, Perl, and Python.)

The group's preliminary work in this field includes the Grid Portal Development Kit, which provides common components used to construct portals allowing secure access to Grid resources via an easy-to-use Web interface; and pyGlobus, an interface to the Globus toolkit from Python (an interactive, object-oriented scripting language). The group is also developing versions of the industry standard Simple Object Access Protocol (SOAP) that use the Grid Security Infrastructure (GSI) to provide authentication and delegation. Building on this foundation, the group is developing a more comprehensive CoG Kit for designing science application Web portals and problem-solving environments.

### *Navigating Network Traffic*

Today's computer operating systems come configured to transfer network data at only one speed—usually slow—regardless of the underlying network. To take advantage of high-speed networks like ESnet, the Net100 Project is creating software that allows computer operating systems to tune themselves and adjust dynamically to changing network conditions. Net100 is a collaboration of the Pittsburgh Supercomputing Center, the National Center for Atmospheric Research, Berkeley Lab, and Oak Ridge National Laboratory, with Brian Tierney and the Distributed Data Intensive Computing Group leading Berkeley Lab's effort. The network sensing components of Net100 will be based on NetLogger and other tools developed here, and our main contribution will be the Network Tools Analysis Framework.

Dealing with network traffic problems from the perspective of Grid applications is the Self-Configuring Network Monitoring Project, led by Brian Tierney and Deb Agarwal. For a distributed application to fully utilize the network, it must first know the current network properties and what is happening to its data along the entire network path, including local and wide-area networks. Without this information, the end-to-end system is often unable to identify and diagnose problems within the network. This project is designing and implementing a self-configuring monitoring system that uses special request packets to automatically activate monitoring along the network path between communicating endpoints. This passive monitoring system will integrate with active monitoring efforts and provide an essential component in a complete end-to-end network test and monitoring capability.

### *Reliability and Security on the Grid*

The DOE Science Grid and the availability of distributed resources enable applications such as shared remote visualization, shared virtual reality, and collaborative remote control of instruments. These applications require reliable and secure distributed information sharing and coordination capabilities, usually provided by collaboration and security tools that use server-based systems. Unfortunately, the need to run and support servers often prevents small collaborations from installing the tools, while the scaling problems of server-based systems can limit the size of large collaborations. Collaborations are naturally built in an incremental and ad hoc manner, and this dynamic and scalable peer-to-peer model is not supported well by a rigid server-based structure. Two coordinated projects in the Distributed Systems Department are addressing these problems, one focusing on the communication issues, the other on security.

The goal of the Reliable and Secure Group Communication Project, led by Deb Agarwal, is to develop the components necessary for a peer-to-peer group communication infrastructure that provides reliability, security, and fault-tolerance while enabling scalability on the Internet scale. The InterGroup protocols are being used to provide reliable delivery of messages, ordered delivery of messages, and membership services, while the Group Security Layer provides the secure group communication mechanisms. The long-term goal is to integrate these components, being developed by Berkeley Lab's Collaboration Technologies Group, into the DOE Science Grid infrastructure.

The Distributed Security Architectures project, led by Mary Thompson, is working to provide assured, policy-based access control for Grid systems and services. The foundation of this project is the Distributed Security Research Group's Akenti certificate-based authorization system, which provides multiple-stakeholder control over distributed resources accessed by physically and administratively distributed users. The Akenti access policy documents are created and maintained by stakeholders independent of the resource server platform. Current work focuses on integrating the Akenti authorization mechanism with emerging standards such as the IETF's Transport Layer Security (TLS), the Grid Security Interface (GSI), WebDAV protocols, and Generic Authentication and Authorization interface (GAA). Integrating Akenti with GSI is being done as part of the SciDAC National Fusion Collaboratory proposal. A standalone Akenti server will also be available on the DOE Science Grid nodes for Grid applications to use to as an option for authorization.

### *Making Collaborations More Productive*

Many of the tools currently available for remote collaboration focus on rigidly structured applications such as videoconferencing. While these are important when a high level of interaction is needed, our experience building distributed collaboratories has revealed a more basic need for less intrusive and more flexible ways for people to stay in touch and work together on the daily tasks required by large research efforts. These tasks include not only communications and document sharing, but also tracking workflow, such as data archiving and analysis.

The Pervasive Collaborative Computing Environment (PCCE) project, led by Deb Agarwal and Chuck McParland, is researching, developing, and integrating the software tools required to support a flexible, secure, seamless collaboration environment that supports the entire continuum of interactions between collaborators. This environment is envisioned as a persistent space that allows participants to locate each other; use asynchronous and synchronous messaging; share documents, applications, progress, and results; and coordinate daily activities.

The PCCE project is leveraging existing and recently proposed tools such as Grid Web Services, Internet Relay Chat (IRC), Web Distributed Authoring and Versioning (WebDAV), electronic notebooks, Basic Support for Cooperative Work (BSCW), and videoconferencing capabilities. By basing our environment on the DOE Science Grid computing and data services, we hope to maximize its applicability to a wide range of collaborative research efforts and present users with a familiar, consistent, and secure activity management and coordination environment. The collaborative workflow tools will also help DOE researchers take full advantage of the flexible computing and storage resources that will be available on the Science Grid.

### *Managing Scientific Data*

Terascale computing and large scientific experiments produce enormous quantities of data that require effective and efficient management, a task that can distract scientists from focusing on their core research. In some fields, data manipulation—getting files from a tape archive, extracting subsets of data from the files, reformatting data, getting data from heterogeneous distributed systems, and moving data over the network—can take up to 80% of a researcher's time, leaving only 20% for scientific analysis and discovery. The goal of the SciDAC Scientific Data Management ISIC, led by Ari Shoshani, head of the Scientific Data Management Group in the High Performance Computing Research Department, is to reverse that ratio by making effective scientific data management software widely available.

This ISIC will provide a coordinated framework for the unification, development, deployment, and reuse of scientific data management software. It will target four main areas that are essential to scientific data management: storage and retrieval of very large datasets, access optimization of distributed data, data mining and discovery of access patterns, and access to distributed, heterogeneous data. The result will be efficient, well-integrated, robust scientific data management software modules that will provide end-to-end solutions to multiple scientific applications.

*The Future Technologies Group performs research and development on infrastructure for scientific computing; their current projects include checkpoint/restart for Linux, Unified Parallel C, and performance analysis of high-end systems. Members include (front) Mike Welcome, Erich Strohmaier, Sonia Sachs, Eric Roman, Kathy Yelick, (back) Costin Iancu, new group leader Brent Gorda, Paul Hargrove, Jason Duell, (not shown) David Culler, James Demmel, Lenny Oliker, Evan Welbourne, and Richard Wolski.*

The research and development efforts will be driven by the needs of the initially targeted application areas: climate simulation, computational biology, high energy and nuclear physics, and astrophysics. Several of the teams involved in this project have developed procedures, tools, and methods addressing scientific data management and data mining for individual application areas. But this project is the first attempt to unify and coordinate these efforts across all the data management technologies relevant to the DOE mission and across all the SciDAC scientific applications. Collaborators include Argonne National Laboratory, Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, Georgia Institute of Technology, North Carolina State University, Northwestern University, and the University of California, San Diego.

Ari Shoshani and his group have been pioneers in developing a comprehensive approach to scientific data management, and they are also collaborating on two other SciDAC data management projects: the Particle Physics Data Grid Collaborative Pilot, and the Earth Systems Grid II: Turning Climate Datasets into Community Resources.

### *Checkpoint/Restart for Linux*

Members of the Future Technologies Group, drawing on their previous experience with the Linux kernel, are developing a hybrid kernel/user implementation of checkpoint/restart. Their goal is to provide a robust, production-quality implementation that checkpoints a wide range of applications, without requiring changes to be made to application code. This work focuses on checkpointing parallel applications that communicate through Message Passing Interface (MPI), and on compatibility with the software suite produced by the SciDAC Scalable Systems Software ISIC.

The Scalable Systems Software ISIC, led by Al Giest of Oak Ridge National Laboratory, is developing an integrated suite of machine-independent, scalable systems software for effective management and utilization of terascale computational resources. The goal is to provide open-source solutions that work from small to large-scale systems. Berkeley Lab's contribution, spearheaded by Paul Hargrove, includes the checkpoint/restart implementation for Linux as well as standard interfaces between checkpoint/restart and other components in the software suite. Paul is also heading the process management working group within the ISIC.

The Future Technologies Group's effort will be the first completely open checkpoint/restart implementation designed for production supercomputing. Other production implementations have been developed commercially, but no information is available on how they work. Other open-source implementations also exist, but were designed with an emphasis on research, not on production computing. Our work will deliver not only the benefits of checkpoint/restart to our users, but also all of the lessons learned necessary to undertake similar efforts in the future.

# *Sabbatical Gives Insight into European Approach to Grids*

Brian Tierney, leader of the Data Intensive Distributed Computing Group, has spent a productive sabbatical year working as a Scientific Associate in the Information Technology Division at CERN, the European Organization for Nuclear Research in Geneva, Switzerland. Not many non-Europeans are invited to work at CERN, but they wanted to take advantage of Brian's expertise in transferring large datasets across wide-area networks.

Brian has primarily been working on "Work Package 2" of the European DataGrid Project, funded by the European Union. "WP2" is responsible for the data management architecture of the project, including data access and migration, data replication, meta data management, secure and transparent data access, and query optimization. In addition, Brian has been a guest consultant on the Architecture Task Force for the DataGrid, so he's been contributing to all aspects of Grid middleware, including scheduling, security, monitoring, PC farm management, mass storage interfaces, and more.

Technologically, pretty much the same tools, such as Globus, are being used for Grids on both sides of the Atlantic, Brian says. But he does see two major differences in approach.

The biggest difference is the scale of the EU DataGrid Project, which has over 200 people working on it. Coordinating such an effort is quite a challenge, especially given the cultural clashes between disciplines (physics vs. computer science) and nationalities (for example, northern vs. southern European approaches to management and problem solving).

The other big difference is that the EU DataGrid is focused more on production, while many Grid projects in the U.S. are focused more on research. The EU really hopes to have the DataGrid in daily use at over 40 sites by the end of 2003. The ultimate goal of the EU DataGrid is to provide computing on-tap to libraries, schools, and homes, as well as scientific researchers.

*Brian Tierney has been applying his expertise in high-speed distributed data systems to the architecture of the European DataGrid.*

### *Implementing Unified Parallel C*

Shared memory programming models are more attractive to many users than the message passing programming model. The ability to read and write remote memory with simple assignment statements is much easier than writing code using all the conventions of a message-passing library. However, in order to write efficient code for large-scale parallel machines, programmers need a language that allows them to exploit data locality on a variety of memory architectures. Unified Parallel C (UCP) is exactly such a language.

UPC is an extension of the C programming language designed for high-performance computing. UPC uses a Single Program Multiple Data (SPMD) model of computation, in which the amount of parallelism is fixed at program startup time, typically with a single thread of execution per processor. The communication model is based on the idea of a shared, partitioned address space, where variables may be directly read and written by multiple processors, but each variable is physically associated with a single processor. The language provides a uniform programming model for shared memory and distributed memory hardware, with some of the programmability advantages of shared memory and the control over data layout and performance of message passing.

The goal of the Future Technologies Group's UPC effort is to build portable, high-performance implementations of UPC for large-scale multiprocessors, PC clusters, and clusters of shared memory multiprocessors. There are three major components to this effort: (1) developing a runtime layer for UPC that allows for lightweight communication calls using the most efficient mechanism available on the underlying hardware, (2) optimizing the UPC compiler, and (3) developing a suite of benchmarks and applications to demonstrate the features of the UPC language and compilers, especially targeting problems with irregular computation and communication patterns. The project is being led by Kathy Yelick, a joint member of the Future Technologies Group and professor of computer science at the University of California, Berkeley.

### *High-End Computer System Performance*

The SciDAC Performance Evaluation Research Center (PERC), under the leadership of NERSC's Chief Technologist, David Bailey, will focus on how one can best execute a specific application on a given platform. The research results from this effort are expected to permit the generation of realistic bounds on achievable performance, and to answer three fundamental questions: (1) why do these limits exist; (2) how can we accelerate applications toward these limits; and (3) how can this information drive the design of future applications and high-performance computing systems.

PERC will develop a *science* for understanding the performance of scientific applications on high-end computer systems, and *engineering* strategies for improving performance on these systems. The goals of the project are to optimize and simplify the profiling of real applications, measurement of machine capabilities, performance prediction, performance monitoring, and informed tuning. Studying the convoluted interactions of application signatures and machine signatures will provide the knowledge necessary to achieve those goals.

In addition to his own significant contributions to the field of benchmarking and performance analysis, David will have a wealth of experience to draw on from other Berkeley Lab and NERSC staff, including Horst Simon, Bill Kramer, Erich Strohmaier, Adrian Wong, Lenny Oliker, and others. Other SciDAC participants include Argonne National Laboratory, Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, the University of Illinois, the University of Maryland, the University of Tennessee, and the University of California, San Diego.

## Computational Science

Berkeley Lab staff work closely with scientists in a variety of fields to develop and improve software for simulation and data analysis, with the ultimate goal of making computational science more productive. Some recent examples are discussed below.

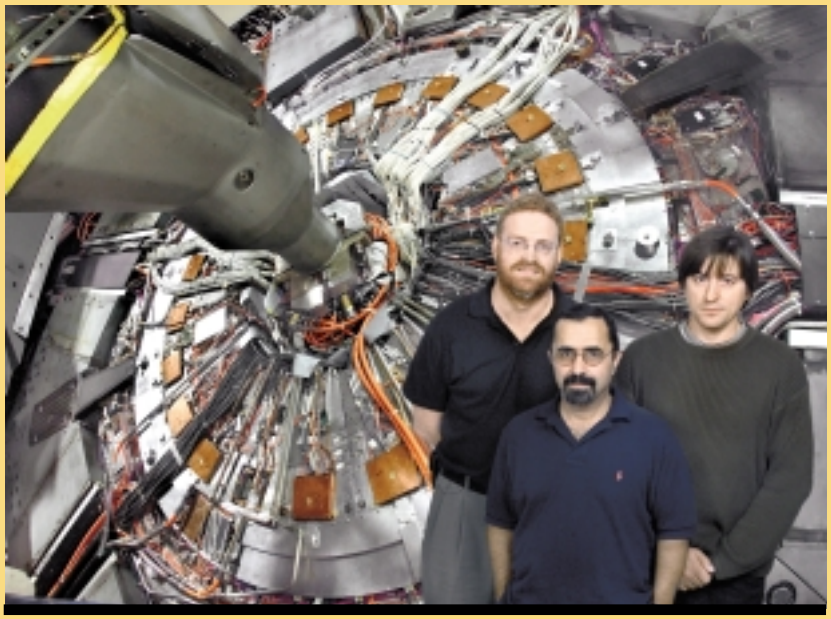
### *BaBar Detects Clear CP Violation*

Why is there more matter than antimatter in the Universe? One plausible explanation is CP violation occurring in the first seconds after the Big Bang. CP violation means violation of the combined conservation laws associated with charge conjugation (C) and parity (P) by the weak nuclear force, which is responsible for reactions such as the decay of atomic nuclei. The existence of CP violation was experimentally demonstrated decades ago, but there are conflicting theories to explain it.

The Asymmetric B Factory and BaBar detector at the Stanford Linear Accelerator Center were built to provide new data to help solve the matter/antimatter puzzle. On July 6, 2001, after analyzing data from 32 million pairs of B mesons, the international BaBar Collaboration announced that BaBar had found 640 pairs that exhibited unmistakable differences in the ways that the matter and antimatter B mesons decayed—clear evidence of CP violation in agreement with the Kobayashi-Maskawa model, one of the two leading theories.

Part of the software infrastructure for BaBar data analysis was recently upgraded by the HENP Computing Group, which

develops software for large, international high energy and nuclear physics experiments. Specifically, Simon Patton, Akbar Mokhtarani, and Igor Gaponenko completed a major upgrade of the BaBar database that allows data processing to scale to multiple petabytes of data, with further improvements feasible in the future. They also discovered ways of storing data more efficiently and improved the parallel accessibility and reliability of the database. These upgrades will help accommodate larger datasets resulting from improved accelerator luminosity and changing physics goals.



*Simon Patton, Akbar Mokhtarani, and Igor Gaponenko upgraded the database for the BaBar detector, helping researchers sort through millions of subatomic events to find clues to the asymmetry of matter and antimatter.*

### *Quantum Rods Emit Polarized Light*

A collaboration between experimental and computational scientists at the University of California and Berkeley Lab has made a significant discovery in nanoscience. In the June 15, 2001 issue of *Science*, the research team reported that colloidal quantum rods of cadmium selenide (CdSe) exhibit linearly polarized emission, which may make them useful as light emitters in a wide range of nanotechnology applications, such as biological labeling, flat panel displays, and lasers.

The article "Linearly Polarized Emission from Colloidal Semiconductor Quantum Rods" (*Science* 292, 2060) was written by Jiangtao Hu, Liang-shi Li, Weidong Yang, Libero Manna, and A. Paul Alivisatos (all of the Berkeley Lab Materials Science Division and the UC Berkeley Chemistry Department), and Lin-wang Wang of the Scientific Computing Group. The computation was done on NERSC's Cray T3E with the Escan code developed by Lin-wang, which can calculate million-atom systems using the folded spectrum method for non-self-consistent nanoscale calculations. The calculation showed that the photoluminescence of the CdSe quantum dot changes direction from non-polarized to linearly polarized after the shape changes from spherical to rod-like, at the aspect ratio of 2. This result was confirmed by experimental measurements.

This discovery showed that optical emission properties of quantum dots can be tailored by adjusting the height, width, and shape of the potential that confines electrons and holes. The technological significance is that colloidal rods can be produced by comparatively simple solution methods and are photochemically robust, making them good candidates for a variety of light emission applications.

### *New Parallel Electronic Structure Code*

Andrew Canning of the Scientific Computing Group gave a presentation on a new parallel electronic structure code, P-FLAPW, at the International Conference for Computational Physics in September 2001. Andrew developed the parallel code in collaboration with Wolfgang Mannstadt of Marburg University and Arthur Freeman's group at Northwestern University.

FLAPW (for full-potential linearized augmented plane-wave) is one of the most accurate and widely used methods for determining structural, electronic, and magnetic properties of crystals and surfaces. Until the work by this group, the method was limited in scope because it did not have a parallelized version, so it could only be applied to small systems. Now with the parallel code P-FLAPW, it is possible to perform calculations on systems of hundreds of atoms, which means technologically important systems such as nanostrutures, impurities, and disorded systems can be studied with this highly accurate first-principles method. Use of the parallel eigensolvers from the ScaLAPACK library allows the P-FLAPW code to scale up efficiently to hundreds of processors, which is a computational requirement for the study of large systems. ScaLAPACK is one of the many

computational tools that form the Department of Energy's ACTS Toolkit (see below).

### *Neutrino Data from the South Pole*

Jodi Lamoureux of the Scientific Computing Group took a business trip to the South Pole this past year as part of her work collaborating on the software infrastructure for the AMANDA project (Antarctic Muon and Neutrino Detector Array). AMANDA is a neutrino observatory that searches for high-energy neutrinos from cosmic sources to verify that active-galactic nuclei and gamma-ray bursters are proton accelerators.

Jodi's usual routine at home includes analyzing AMANDA data with algorithms and visualization tools that she helped develop for data filtering and reconstruction, but she flew to Antarctica during the local summer to work on AMANDA data handling. In addition to taking detector calibration measurements, she also helped with satellite transfers and organized various processes that select data samples for monitoring and quick analysis.

Initial results validating the AMANDA technology, computed at NERSC, were published in the March 22, 2001 issue of *Nature* as "Observation of High-Energy Neutrinos Using Čerenkov Detectors Embedded Deep in Antarctic Ice" by E. Andrés et al. (*Nature* 410, 441).

### *Improving Climate Model Performance*

A multi-institutional team has been collaborating to merge two of the world's most advanced computer climate models, the Climate System Model (CSM) and the Parallel Climate Model (PCM). The merged Community Climate System Model (CCSM) is being designed to include the best features of both models and to perform well on a variety of computer architectures. Chris Ding, Helen Yun He, and Woo-Sun Yang of the Scientific Computing Group have been working to optimize parallel input/output and to optimize performance of the coupler (the top-level model that integrates the component models) on distributed memory architectures.

A major contribution of Chris's team this year was development of the Multi Program-Components Handshaking Utility (MPH). Many large and complex scientific applications are based on semi-independent program components developed by different groups or for different purposes (in this case, CSM and PCM). MPH handles the initial component handshaking and registration process necessary for combining codes on a distributed memory architecture. MPH supports two software integration mechanisms—multi-component multi-executable, and multi-component single-executable, with processor overlapping or non-overlapping—as well as a modular approach in which each component builds its own executable. With this utility, one can change execution modes relatively easily without extensive rewriting of codes. Although developed for CCSM, this flexible component coupling system could be used by a wide range of applications.

The climate team also has optimized the three most time-consuming subroutines in the PCM coupler: the flux conservation, the ocean-to-atmosphere regridding, and the atmosphere-to-ocean regridding. These optimizations improved the total coupler timing by 20% on 64 processors, and they have been adopted in production codes. Other team activities have included assessing various I/O and file systems, studying methods to increase climate simulation reproducibility, and improving the performance of finite difference methods. All of these efforts will contribute to the SciDAC project "Collaborative Design and Development of the Community Climate System Model for Terascale Computers."

### *ACTS Toolkit Explicated*

The ACTS Toolkit is a set of DOE-developed tools that make it easier to write parallel scientific programs. The ACTS Online Information and Support Center (http://acts.nersc.gov/), operated by Osni Marques and Tony Drummond of the Scientific Computing Group, is a centralized source of information about these tools. But not content to sit back and respond to inquiries, Tony and Osni have taken a proactive role in promoting the ACTS tools.

In October 2001 they organized a three-and-a-half-day workshop at Berkeley Lab, "Tools for Advanced Computational Testing and Simulation—Solving Problems in Science and Engineering," aimed at familiarizing researchers in various scientific disciplines with the ACTS tools. The workshop included a range of tutorials on the tools, discussion sessions focused on solving specific computational needs of the participants, and hands-on practice using NERSC's computers. More than 50 presenters and participants took part in the workshop.

As part of the Los Alamos Computer Science Institute's Second Annual Symposium, also held in October, Osni and Tony organized a full-day workshop on "High-Performance Numerical Libraries for Science and Engineering," with Sherry Li also giving a presentation. Topics included introduction to the tools, panel discussion on the tools and applications, tool interoperability, panel discussion on the frameworks and standards for software interoperability, scientific and engineering applications, and panel discussion on usage and applicability of commercial and noncommercial software.

# *Lab Wins 2nd Network Bandwidth Challenge As RAGE Robot Roams SC2001 Conference*

For the second year in a row, a Berkeley Lab-led team took top honors in a contest to move the most data across the network built around SC, the annual conference of high-performance computing and networking. Meanwhile, the Lab's Remote Access Grid Entity (RAGE) robot was rolling around the conference floor, demonstrating the next generation of video conferencing technology.

SC2001, held in Denver, marked the second staging of the Network Bandwidth Challenge, in which researchers with high-bandwidth applications using huge amounts of distributed data were invited to push SCinet, the conference fiber-optic network, to its limits. The SCinet infrastructure featured a 14.5 gigabit wide-area network connection over multiple OC-48 links to the exhibit floor and connections to most high-speed national research networks.

Our Network Bandwidth Challenge entry, "Visapult: WAN-Deployed Distributed and Parallel Remote Visualization," simulated a grazing collision of two black holes using the Cactus simulation code developed by collaborators at the Albert Einstein Institute in Germany. Data from the simulation, running in real time at both NERSC and the National Center for Supercomputing Applications in Champaign, Illinois, was sent to Denver via ESnet and the Abilene network, where it was volume-rendered in parallel by the Visapult application running on a cluster of PCs in the Berkeley Lab booth on the SC2001 show floor. The application provided highly interactive visualization and computational steering of a production-scale simulation code over a wide-area network, and achieved a sustained network performance level of 3.3 gigabits per second.

Collaborators on the winning team were John Shalf, Wes Bethel, Michael Bennett, John Christman, Eli Dart, Brent Draney, and David Paul of Berkeley Lab; Peter Deiner and Gabrielle Allen of the Albert Einstein Institute/Max-Planck-Institute for Gravitation Physics, Germany; Werner Benger of the Albert Einstein Institute/Konrad Zuse Institute, Berlin, Germany; Jim Ferguson of the National Center for Supercomputing Applications/National Laboratory for Applied Network Research; and Tony Rimovsky of NCSA.

The RAGE robot made its debut at the SC2001 conference, capturing both technical presentations and less formal human interactions in the exhibit hall, and feeding the information into the Access Grid, and thence to the world. With its four-wheel drive and four-wheel steering, RAGE was designed to take the Access Grid beyond the walls of its specially built, inherently immobile nodal facilities.


*Built entirely from off-the-shelf components, RAGE takes video conferencing where it has never gone before.*

RAGE is connected to its remote operator by wireless network technology. It is equipped with an on-board PC and video conferencing software, as well as speakers, a microphone, a video camera, and a flat-panel screen. With these capabilities, RAGE can provide Access Grid interaction in many locations not equipped with a node. Once it returns to Berkeley Lab, RAGE is expected to provide remote tours of the Oakland Scientific Facility.

RAGE was designed and built by John Shalf, Zach Radding, Deb Agarwal, Keith Jackson, Marcia Perry, Martin Stoufer, Joshua Boverhof, Dan Gunter, and Clayton Bagwell of the Computing Sciences organization, and Eve Edelson of the Environmental Energy Technologies Division.

### *Visualization Group Tackles AMR Data*

During the past year, Wes Bethel accepted the position of Group Leader for the Berkeley Lab/NERSC Visualization Group, whose mission is to apply scientific visualization principles and practices to scientific data in a multidisciplinary setting, and to anticipate, define, and develop new visualization technologies that are appropriate for contemporary and future applications. To meet the needs of production requirements, the Visualization Group installs and maintains a portfolio of visualization software on NERSC platforms. To meet the evolving needs of remote users, the Visualization Group has defined a roadmap for expanding the breadth and depth of services to the remote user constituency.

*John Shalf, new members Ken Schwartz and Cristina Siegerist, and group leader Wes Bethel make up the core of the Berkeley Lab/NERSC Visualization Group.*

An ongoing focus of the group's research is Visapult, an application and framework for remote and distributed visualization. Visapult uses parallel computers, a desktop workstation, and a remote data source that are coupled together into a distributed application that implements image-based rendering assisted volume rendering. This application has a unique feature of effectively decoupling interactivity on the desktop from the delays inherent in network-based applications.

The Visualization Group has broadened its scope of research activities to include faculty and staff from the University of California at Davis's Center for Image Processing and Integrated Computing (CIPIC). Together, the two groups have focused on methods for direct volume rendering of adaptive mesh refinement (AMR) data (see figure 8 on page 17). AMR data visualization poses special challenges, particularly when the datasets are large and network connections to remote locations are slow. The group plans to begin to deploy these research prototypes, as well as Visapult, into a limited production environment using Web-based portal technology. The portal technology will serve to simplify user access to the remote and distributed visualization software components.

## Components of the Next-Generation NERSC


*The four principal components of the next-generation NERSC are designed to serve the DOE science community.*

Over the five years that NERSC has been located at Ernest Orlando Lawrence Berkeley National Laboratory, it has built an outstanding reputation for providing both high-end computer systems and comprehensive scientific client services. At the same time, NERSC has successfully managed the transition for its users from a vector-parallel to a massively parallel computing environment. In January 2001, DOE's Mathematical, Information, and Computational Sciences (MICS) program asked Berkeley Lab to develop a strategic proposal which, building on a foundation of past successes, presents NERSC's vision for its activities and new directions over the next five years. The proposal was delivered in May 2001, and this section of the Annual Report summarizes its main themes.

NERSC proposed a strategy consisting of four components in order of priority. The two ongoing components, which will be enhanced over the next five years, are:

- *High-End Systems* — NERSC will continue to focus on 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* — NERSC will continue to provide 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.

The two new strategic components are:

- *Support for Scientific Challenge Teams* — NERSC will focus on supporting these teams, with the goal of bridging the software gap between currently achievable and peak performance on the new terascale platforms.

- *Unified Science Environment (USE)* — Over the next five years, NERSC will use Grid technology to deploy a capability designed to meet the needs of 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.

## High-End Systems

*Providing the most effective and most powerful High-End Systems possible.* This is the foundation upon which NERSC builds all other services in order to enable computational science for the DOE/SC community. High-End Systems at NERSC mean more than highly parallel computing platforms—they also include a very large-scale archival storage system, auxiliary and developmental platforms, networking and infrastructure technology, system software, productivity tools for clients, and applications software. Our successful High-End Systems strategy includes advanced development work, evaluating new technologies, developing methodologies for benchmarking and performance evaluation, and acquisition of new systems.

There are three major areas of system design and implementation at NERSC: the computational systems, the storage system, and the network. The balance of the entire Center is determined by the requirements that evolve from the increased computational capability, plus independent requirements for other resources. Enhanced storage systems must be designed to support not just current work, but future workloads as well. Figure 10 shows the evolution of the NERSC system architecture between 2001 (left) and 2006 (right), with the introduction of the Global Unified Parallel File System and the Unified Science Environment integrating the discrete computational and storage systems.

We expect that NERSC-4 and very likely NERSC-5 will be commercial integrated SMP cluster systems. Special architectures will be considered, but it is not likely that these will be ready for high-quality production usage in the next five years. Commodity cluster systems will also be considered, but based on our technology assessments, we do not believe it likely that these systems will be able to support the diverse and communication-intense applications at NERSC in this time frame. Equivalently balanced cluster hardware will at best have a modest performance-per-dollar advantage, but cluster software in particular is significantly less mature than vendor-supplied software. NERSC will use the "best value" process for procuring its major systems, as described above on page 15.

Between now and 2006, NERSC plans to augment both the aggregate capacity and the transfer rate to and from the mass storage system. NERSC will continue collaborating in

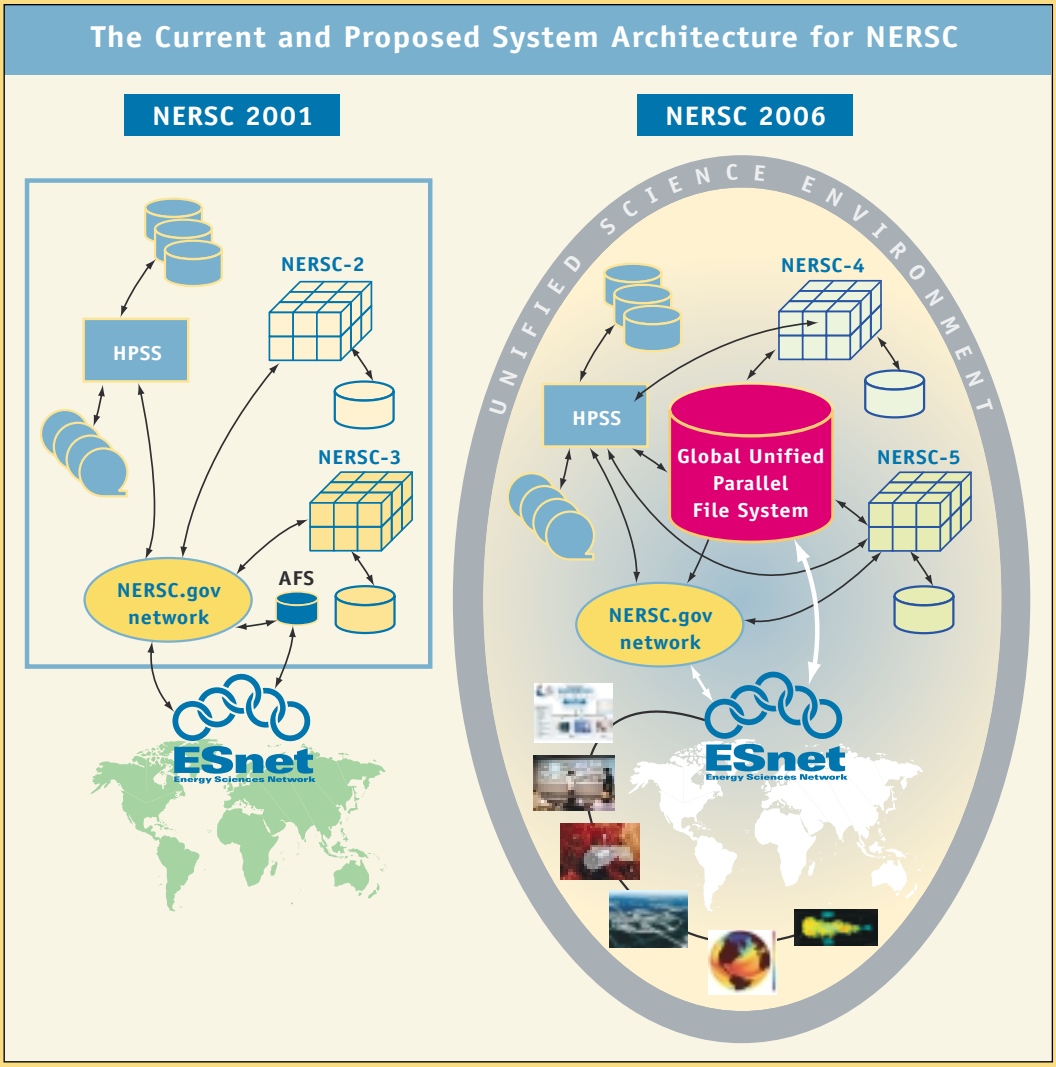



*Figure 10. Evolution of the NERSC system architecture between 2001 (left) and 2006 (right).*

High Performance Storage System (HPSS) development, in order to improve archive technology. In particular, NERSC will help develop schemes to replicate data over long distances and to import and export data efficiently.

As high-performance computing becomes more network-centric (the Grid, HPSS, cluster interconnects, etc.), the network will become the "glue" that holds everything together. NERSC must become a center of excellence in network engineering; this is the only way we will be able to deliver the full capability of our systems to our users. NERSC will expand its networking and data communication capacity regularly as applications become more bandwidth intensive, and we will take advantage of the latest enhancements in networking systems and protocols to enable NERSC clients to access the system and move data.

## Comprehensive Scientific Support

As described above, NERSC continues to provide early, large-scale production computing and storage capability to the DOE/SC computational science community. The NERSC systems will be of such a scale as to be unique or nearly unique in many aspects (e.g., computational abilities, storage capacity, etc.). The goal of NERSC's Comprehensive Scientific Support function is to make it easy for DOE computational scientists to use the NERSC high-end systems effectively by:

- Providing consistent high-quality service to the entire NERSC client community through the support of the early, production-quality, large-scale capability systems.

- Aggressively incorporating new technology into the

production NERSC facility by working with other organizations, vendors, and contractors to develop, test, install, document, and support new hardware and software.

- Ensuring that the production systems and services are the highest quality, stable, secure, and replaceable within the constraints of budget and technology.

- Participating in other work to understand and address the unique issues of using large-scale systems.

Comprehensive Scientific Support is the heart of the strategy that sets NERSC apart from other sites and greatly enhances the impact of NERSC's High-End Systems. Elements of this support include:

- System monitoring and operational support on a 24 x 7 x 365 schedule.

- Advanced consulting support during business hours.

- Direct collaborative support by staff scientists on major projects.

- Up-to-date and convenient training and documentation.

- Account management and allocations support.

- Efficient system management, including cyber security.

- System hardware and software improvements, implemented with little or no service disruption.

### Support for Scientific Challenge Teams

The arrival of large, highly parallel supercomputers in the early 1990s fundamentally changed the mode of operation for successful computational scientists. In order to take full advantage of the new capabilities of these parallel platforms, scientists organized themselves into national teams. Called "Grand Challenge Teams," they were a precursor to the "Scientific Challenge Teams" that NERSC anticipates as its leading clients in the next decade. These multidisciplinary and multi-institutional teams engage in research, development, and deployment of scientific codes, mathematical models, and computational methods to maximize the capabilities of terascale computers. NERSC responded by creating the "Red Carpet" plan, which revolved around building individual relationships with the users as well as providing a NERSC staff member as a point of contact to expedite any problems or concerns.

In March 2000 DOE launched a new initiative called "Scientific Discovery through Advanced Computing" (SciDAC). SciDAC defines and explicitly calls for the establishment of Scientific Challenge Teams. These teams are characterized by large collaborations, the development of community codes, and the involvement of computer scientists and applied mathematicians. In addition to high-end computing, teams will also have to deal increasingly with issues in data management, data analysis, and data visualization. The expected close coupling to scientific experiments supported by the USE environment (described below) will be an essential requirement for success for some teams. Scientific Challenge Teams represent the only approach that will succeed in solving many of the critical scientific problems in SC's research programs. These teams are the culmination of the process of users moving to ever-higher computing capability, and NERSC's new structure enables that entire process (Figure 11).

NERSC's strategy for the next five years is to build a focused-support infrastructure for the Scientific Challenge Teams consisting of four components:

- integrated support and collaboration from the NERSC staff

- deployment of tools developed by the SciDAC Integrated Software Infrastructure Centers (ISICs)

- deployment of grid and collaboration technologies (USE).

### Unified Science Environment (USE)

A second new component of the NERSC strategy addresses another change in the practice of scientific computing. In recent years rapid increases in available networking bandwidth, combined with continuing increases in computer performance, are making possible an unprecedented *simultaneous* integration of computational simulation with theory and experiment. This change will have a fundamental impact on areas of science that have not yet made much use of high-end computing. By deploying critical parts of a *Unified Science Environment (USE)*, NERSC anticipates playing a role in the emergence of a new paradigm in computational science.

Examples of the potential of—and the necessity for—a unified approach to computing and science may be found in many of DOE's large-scale science projects, such as accelerator-based science, climate analysis, collaboration on very large simulation problems, and observational cosmology. These activities occur in widely distributed environments and under circumstances that are constrained by the timing of the experiments or collaborations, and are essential to advancing those areas of science. The USE will help support this integration and facilitate DOE's large-scale science.

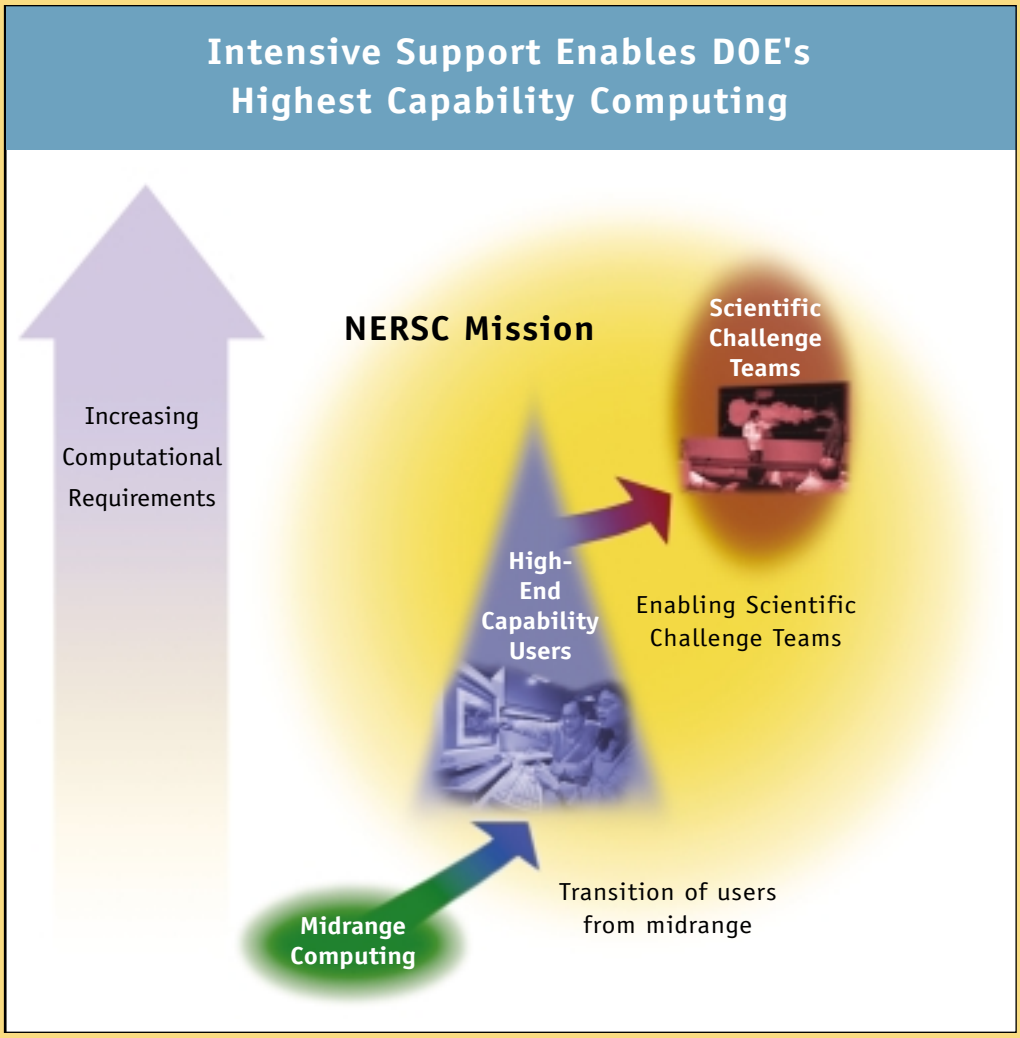



***Figure 11. NERSC facilitates the transition to high-end capability computing, and enables Scientific Challenge Teams through intensive support.***

Grids will play an important role in NERSC, and NERSC will play an important role in Grids. Though Grids provide the middleware for managing and accessing widely distributed resources, NERSC will add the very high-end computing and storage for Grids when it is feasible. Grid middleware provides the user with a uniform view of the job- and data-management environment across heterogeneous systems. This environment has a single, consistent security model and strong security services that are not obstructive. Tools are available in this environment to manage complex sequences of tasks. Inclusion of NERSC in the DOE Science Grid will make high-end services available to NERSC computational scientists through the uniform Grid environment (Figure 12). The resulting combination of Grid access to desktop, midrange, and high-end services creates the USE.

### Collaborations

Finally, NERSC will expand its collaborations with other institutions, especially with the other DOE SC laboratories, to systematically integrate into its offerings the products of their efforts in computational science. With this strategy NERSC will enhance its successful role as a center that bridges the gap between advanced development in computer science and mathematics on one hand, and scientific research in the physical, chemical, biological, and earth sciences on the other. Implementing this strategy will position NERSC to continue to enhance the scientific productivity of the DOE SC community, and to be an indispensable tool for scientific discovery.

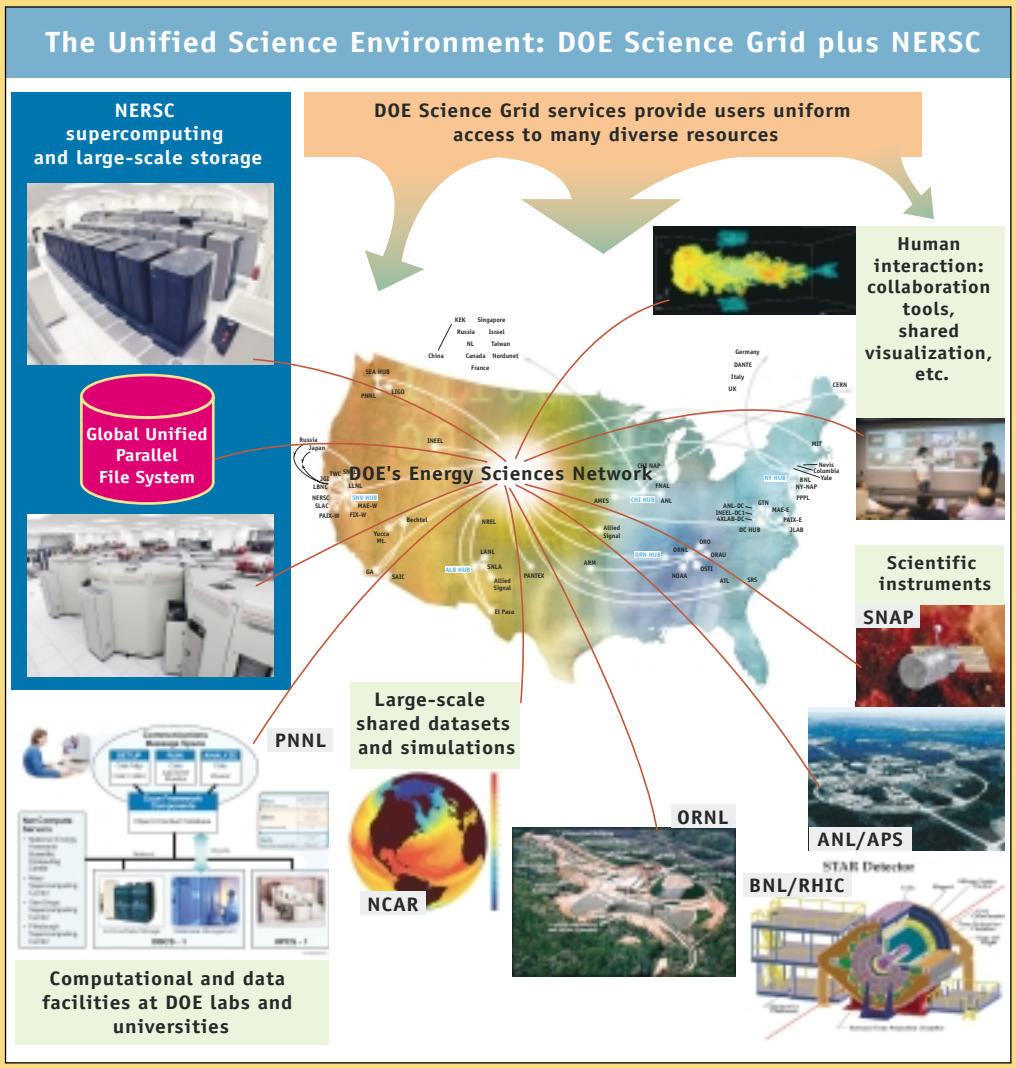
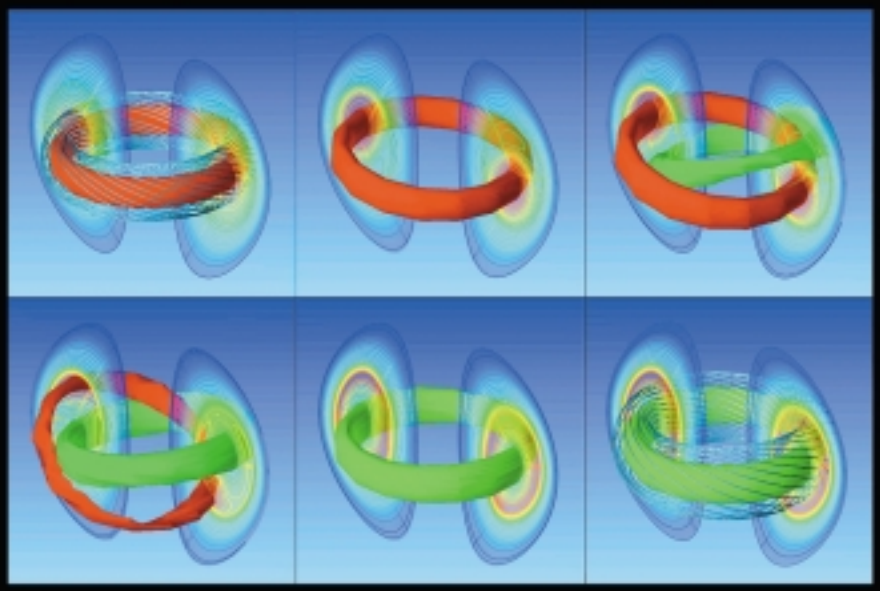



*Figure 12. The role of NERSC as the largest computational resource in the DOE Science Grid.*

## Concurrence

The NERSC Strategic Proposal was anonymously reviewed by 15 independent experts in high performance scientific computing. The proposal and the reviewers' comments were analyzed by the DOE Office of Advanced Scientific Computing Research (ASCR) and discussed with representatives of other Office of Science programs. At the conclusion of this review process, the DOE accepted the broad outline of the strategic plan and committed to supporting NERSC at Berkeley Lab for the next five years. The ASCR program managers agreed with the four components of the plan and their order of priority, emphasizing High End Systems and Comprehensive Scientific Support.

In a letter to Berkeley Lab Director Charles V. Shank, dated November 8, 2001, Dr. C. Edward Oliver, Associate Director of Science for ASCR, wrote, "Your proposal presents a sound strategy for providing high-performance scientific computing hardware and services in a manner commensurate with the near-term expectations of the Office of Science." Dr. Oliver described the NERSC staff's commitment to excellence as a "vital attribute" of the center, and concurred with many of the reviewers' observations that NERSC has provided "world-class hardware, timely technology upgrades and services virtually unsurpassed by any other computer center in the world."



*Time sequence of a simulated "reconnection event" in the National Spherical Torus Experiment (NSTX). See page 64 for details.*

# *Direct Numerical Simulation of Turbulent Combustion: Compression Ignition, Front Propagation, and Burnout of Hydrocarbon Fuels in Engine Environments*

*Jacqueline Chen, Scott Mason, and Tarek Echekki,*
*Sandia National Laboratories*
*Reddy Raghumara, Pittsburgh Supercomputing Center,*
*Carnegie Mellon University*

## RESEARCH OBJECTIVES

This project seeks to further develop and apply direct numerical simulation (DNS) to understand the influence of turbulence on compression ignition, flame propagation, and burnout in compression ignition engine environments. With the insights obtained from these simulations, control strategies for the combustion timing and burn rate will be devised and optimized such that improved efficiencies and lower pollutant generation (especially NOx) will be achieved.

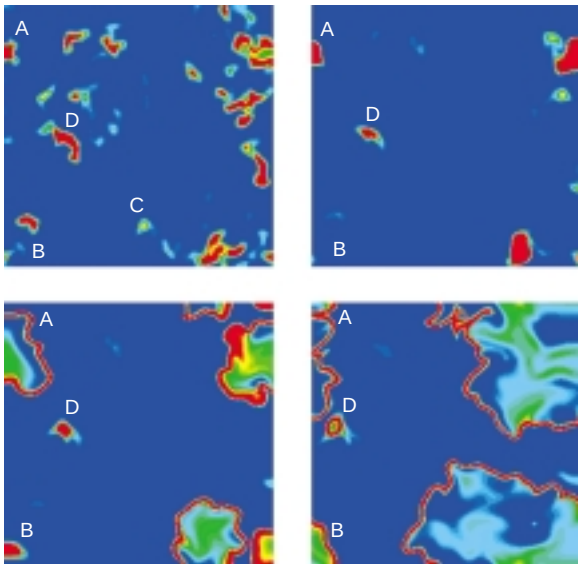
## COMPUTATIONAL APPROACH

DNS is used to solve the compressible turbulent reacting governing equations along with boundary and initial conditions. Higher-order temporal and spatial discretization is used (8th order in space, 5th order in time) along with error monitoring. The method is fully explicit, and the code has been written in MPI for scaleable parallelism. The code scales nearly linearly on Cray T3E, IBM SP3, SGI Origin 2000, and Compaq cluster platforms up to as many as 2048 processors.

## ACCOMPLISHMENTS

*Interaction of premixed turbulent flames:* The global burning rate response of twin premixed hydrogen/air flames embedded in homogeneous turbulence was determined with DNS with detailed chemistry. Superequilibrium radical bursts appear during mutual flame annihilation for fuel-rich mixtures, resulting in enhanced postflame burning rates that contribute to the global response.

*Autoignition of inhomogeneous premixed hydrogen-air flames:* The effect of turbulent mixing on autoignition of hydrogen/air mixtures in the second ignition limit were determined by DNS with detailed chemistry. Unlike in previous studies, it was shown that the scalar dissipation history influences the radical pool history during the induction phase, and also determines the rate of thermal runaway.




*Time sequence showing autoignition of hydrogen/air mixtures in a turbulent field. Isocontours of $HO_2$ mass fractions at 1/2, 1, 3/2, and 2 autoignition induction times (from top left to lower right). The color ranges correspond to mass fractions of 0 for blue to maximum values of 0.001 for red. The color ranges and the corresponding scales are the same for all times, except the induction-phase image, where $HO_2$ mass fractions are multiplied by 100. Ignition kernels A, B, and D show transition of the kernels to propagating fronts, while kernel C undergoes extinction due to high mixing rates.*

## SIGNIFICANCE

A homogeneous charge compression ignition (HCCI) engine operates on the principle of compressing a dilute premixed charge until it autoignites volumetrically. This is a relatively new realm of combustion, wherein the mixture is often sufficiently dilute so as to prevent flame propagation—hence, combustion occurs volumetrically. However, in practice, it is seldom the case that mixtures are truly homogeneous. In fact, mixture inhomogeneities are desirable to spread out the pressure rise in time so as to avoid engine knock. HCCI engines are an attractive alternative to diesel engines, offering the potential for diesel-like efficiencies, while concurrently producing extremely low emissions without expensive aftertreatment. The primary technical challenge of HCCI is to control the in-cylinder fluid motion to obtain the desired heat release time profile across the load-speed map of the engine.

## PUBLICATIONS

J. H. Chen and H. G. Im, "Stretch effects on the burning velocity of turbulent premixed hydrogen-air flames," in *Proceedings of the Twenty-Eighth Symposium (International) on Combustion,* (Edinburgh, Scotland, July 30–August 4, 2000).

T. Echekki and J. H. Chen, "Direct numerical simulation of autoignition in inhomogeneous hydrogen-air mixtures," Paper 184, in *Proceedings of the Second Joint Meeting of the U.S. Sections of the Combustion Institute* (2001).

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*Jacqueline Chen, Scott Mason, and Tarek Echekki,*
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*Reddy Raghumara, Pittsburgh Supercomputing Center,*
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## COMPUTATIONAL APPROACH

DNS is used to solve the compressible turbulent reacting governing equations along with boundary and initial conditions. Higher-order temporal and spatial discretization is used (8th order in space, 5th order in time) along with error monitoring. The method is fully explicit, and the code has been written in MPI for scaleable parallelism. The code scales nearly linearly on Cray T3E, IBM SP3, SGI Origin 2000, and Compaq cluster platforms up to as many as 2048 processors.

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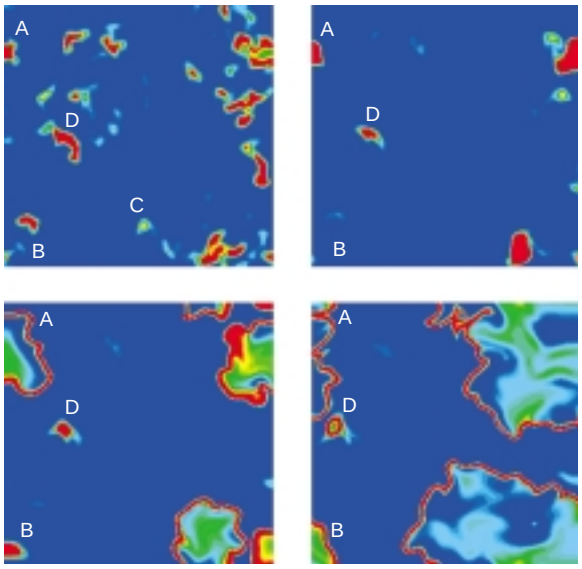
*Interaction of premixed turbulent flames:* The global burning rate response of twin premixed hydrogen/air flames embedded in homogeneous turbulence was determined with DNS with detailed chemistry. Superequilibrium radical bursts appear during mutual flame annihilation for fuel-rich mixtures, resulting in enhanced postflame burning rates that contribute to the global response.

*Autoignition of inhomogeneous premixed hydrogen-air flames:* The effect of turbulent mixing on autoignition of hydrogen/air mixtures in the second ignition limit were determined by DNS with detailed chemistry. Unlike in previous studies, it was shown that the scalar dissipation history influences the radical pool history during the induction phase, and also determines the rate of thermal runaway.




*Time sequence showing autoignition of hydrogen/air mixtures in a turbulent field. Isocontours of $HO_2$ mass fractions at 1/2, 1, 3/2, and 2 autoignition induction times (from top left to lower right). The color ranges correspond to mass fractions of 0 for blue to maximum values of 0.001 for red. The color ranges and the corresponding scales are the same for all times, except the induction-phase image, where $HO_2$ mass fractions are multiplied by 100. Ignition kernels A, B, and D show transition of the kernels to propagating fronts, while kernel C undergoes extinction due to high mixing rates.*

## SIGNIFICANCE

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# Numerical Simulations of Interfaces, Grain Boundaries, and Nanocrystals

*John Cooke, Oak Ridge National Laboratory*

## RESEARCH OBJECTIVES

This research involves the investigation of the atomic-scale structure and the electronic properties of interfaces, grain boundaries, and nanocrystals using *ab initio* density functional calculations. The computation is done in conjunction with Z-contrast scanning transmission electron microscopy measurements, which provide atomic-resolution imaging of the structures of interest, and electron energy loss spectroscopy (EELS) measurements of local electronic structure.

## COMPUTATIONAL APPROACH

We use the density-functional theory in the local-density approximation, either in the plane-wave pseudopotential implementation (VASP code) or in the full-potential linearized augmented plane waves implementation (WIEN code).

## ACCOMPLISHMENTS

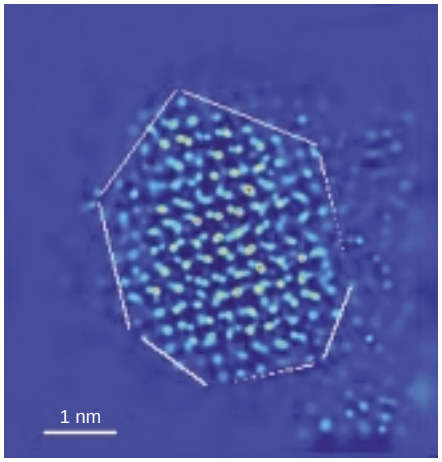
*Localized defects at the SiC-$SiO_2$ interface:* Theoretical studies of the Si-$SiO_2$ interface showed that contrary to expectation, a flat interface was energetically preferred, and therefore the observed defect states were the result of suboxide intrusions through the growth process. We have found that Si-Si suboxide bonds induce gap states near the conduction-band edge, while carbon precipitates at the interface determine an increase in the density of states near the valence-band edge.

*Origin of electrical barriers at grain boundaries in $SrTiO_3$:* We have shown through a combination of Z-contrast imaging, EELS, and theory that non-stoichiometry is an intrinsic effect at grain boundary dislocation cores. Theory then examined model structures consistent with the experimental data and showed that non-stoichiometry leads to lower energy boundaries.

*CdSe nanocrystals:* We have started investigating small CdSe clusters (10–30 atoms) as intermediate steps in the formation of CdSe nanocrystals in the nanometer size regime. We have determined the geometry of these clusters in the presence of organic passivants. We have found that organic ligands favor specific atomic configurations and surface coverages, and may determine the overall shape of the nanocrystals. This we expect will explain why the crystals grow with the asymmetric structure observed in a Z-contrast image.

## SIGNIFICANCE

SiC is becoming the semiconductor of choice for high-voltage, high-power applications, but its technological impact is still limited, mainly because of the poor electronic and transport properties of the SiC-$SiO_2$ interface. A better understanding of extended and localized defects at the interface is necessary to overcome the technological difficulties.




*Reconstructed Z-contrast image of a CdSe nanocrystal embedded in a polymer film revealing the polarity of the lattice and an asymmetric shape. While the Cd terminated end is flat, the Se terminated end is pointed, appearing to end in just a single atomic site. This is not expected on the basis of the Wulff construction for equilibrium shapes, and indicates that the shape can be controlled by choice of passivating ligand (in this case TOPO).*

Perovskite oxides are the basis for a number of new materials systems with unusual and potentially very useful properties, such as high-temperature superconductivity, giant magnetoresistance, and ferroelectricity. In these systems the grain boundaries are electrically active, which sometimes is a serious problem. We have demonstrated the origin of the electrical barriers in $SrTiO_3$ to be non-stoichiometry.

Semiconductor nanocrystals can now be grown by chemical synthesis methods with a relatively high degree of control over the size and shape distribution. However, a microscopic understanding of the growth process and of the equilibrium shape as a function of the chemical environment and the growth conditions is still missing.

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R. Buczko, S. J. Pennycook, and S. T. Pantelides, "Bonding arrangements at the Si-$SiO_2$ and SiC-$SiO_2$ interfaces and a possible origin of their contrasting properties," Phys. Rev. Lett. **84**, 943 (2000).

S. T. Pantelides, G. Duscher, M. di Ventra, R. Buczko, K. McDonald, M. B. Huang, R. A. Weller, I. Baumvol, F. C. Stedile, C. Radtke, et al., "Atomic-scale engineering of the SiC-$SiO_2$ interface," Materials Science Forum **338**, 1133 (2000).

M. Kim, G. Duscher, N. D. Browning, K. Sohlberg, S. T. Pantelides, and S. J. Pennycook, "Nonstoichiometry and the electrical activity of grain boundaries in $SrTiO_3$," Phys. Rev. Lett. **86**, 4056 (2001).

# Computational Studies in Molecular Geochemistry and Biogeochemistry

*Andrew Felmy, E. J. Bylaska, K. M. Rosso, J. R. Rustad, and T. P Straatsma, Pacific Northwest National Laboratory*

## RESEARCH OBJECTIVES

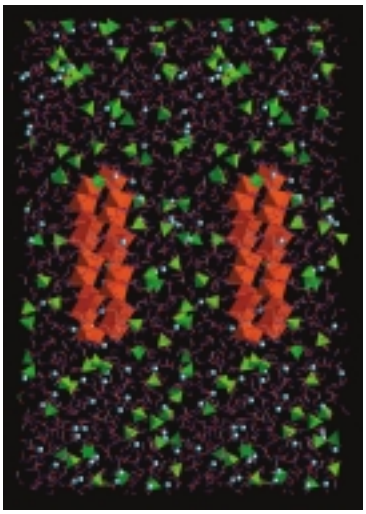
Our effort consists of two types of molecular level simulations in key areas of geochemistry/biogeochemistry: (1) in microbial surface-mediated processes, the effects of lipopolysaccharides present on gram-negative bacteria; (2) in mineral surface interactions, providing a molecular-scale understanding of surface complexation reactions at oxide, oxyhydroxide, and silicate minerals through the use of molecular modeling calculations.

## COMPUTATIONAL APPROACH

We use a variety of computational chemistry methods (density functional theory [DFT], molecular mechanics/dynamics, Car-Parrinello, kinetic theories), and codes that are a part of NWChem. Besides NWChem, we also use parameterized classical potential models to calculate bulk and surface properties for the interaction of water and hydroxide with Fe/Al surfaces. These models are based upon parameterizations from *ab initio* calculations, and they have been particularly successful in predicting structures, surface charging, and water chemistry of iron-oxide surfaces.

## ACCOMPLISHMENTS

A molecular model for the rough lipopolysaccharide (LPS) membrane of *Pseudomonas aeruginosa* was designed based on experimentally determined structural information. An electrostatic model was based on Hartree-Fock self-consistent-field calculations of the complete LPS molecule to obtain partial atomic charges. Molecular dynamics simulations of the rough LPS membrane of *P. aeruginosa* were carried out under periodic boundary conditions, such that the membrane consists of a periodic double layer of LPS/phospholipid molecules externally exposed to aqueous environments.



*Molecular dynamics simulation of the initial stages of attachment of two goethite (a-FeOOH) nanoparticles in a sodium perchlorate solution.*

The Parallel Projector Augmented-Wave Code (PAW) method allows us to simulate many new types of materials at a first-principles level, including iron-oxides. During FY01 we modified the PAW program to add load balancing, and we added a mulipole ewald sum (i.e., not just s-component charges) to the program to calculate solids.

We performed free-space PAW and Gaussian DFT NWChem simulations for a series of first-row transition metal monoxides and dioxides, ScO, TiO, VO, CrO, MnO, FeO, $TiO_2$, $VO_2$, $CrO_2$, and $FeO_2$. These small molecules, which are well characterized experimentally, are an extreme test of the reliability of an *ab initio* method because they have a large number of low-lying states, many with high spin multiplicity. For the monoxides, the agreement in structural parameters was quite good between the two methods and with experiment. The worst-case difference was for the CrO molecule, with absolute differences in distance, frequency, and binding energy. For the dioxides, the agreement between the two methods was also quite good. The worst-case difference was for the $TiO_2$ molecule, with absolute differences in distance, angle, frequency, and atomization energy.

## SIGNIFICANCE

(1) Subsurface microbial processes can control the rates of oxidation/reduction reactions, modify and enhance mineral dissolution and precipitation reactions, and adsorb metals and other ions at the microbial surface, but our theoretical understanding of these processes is very limited. (2) The ubiquitous occurrence, high specific surface area, and strong binding to a large number of cations, anions, metal ions, and organic chelates makes Fe/Al oxides and oxyhydroxides important adsorbing surfaces. Difficulties in characterizing the structure and energetics of these sites obstruct the development of improved thermodynamic models for adsorption.

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James R. Rustad, "Molecular models of surface relaxation, hydroxylation, and surface charging at oxide-water interfaces," Reviews in Mineralogy and Geochemistry **42**, 169 (2001).

R. D. Lins and T. P. Straatsma, "Computer simulation of the rough lipopolysaccharide membrane of *Pseudomonas aeruginosa*," Biophys. J. **81**, 1037 (2001).

Eric J. Bylaska, Marat Valiev, Ryoichi Kawai, and John H. Weare, "Parallel implementation of the projector augmented plane wave method for charged systems," Comp. Phys. Comm. (submitted).

# Energetics, Bonding Mechanism and Electronic Structure of Metal/Ceramic Interfaces

*Arthur Freeman, Northwestern University*

## RESEARCH OBJECTIVES

Our research focuses on the structural, electronic, and magnetic properties of metal/ceramic interfaces. We investigate the total energies, band structures, and Fermi surfaces of double-layered colossal magnetoresistance (CMR) oxides with different doping (doping level and type of dopant), with different Mn-O octahedral distortions corresponding to temperature and doping variation, and with different spin configurations (ferromagnetic [FM] and antiferromagnetic [AFM]).

## COMPUTATIONAL APPROACH

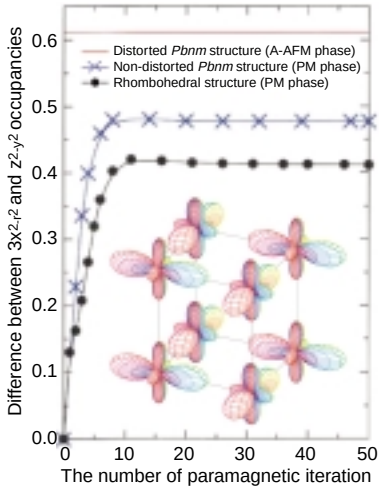
The first-principles calculations within the local density approximation are performed by solving the Kohn-Sham equations self-consistently in a variational approach using the highly precise full-potential linearized augmented plane wave (FLAPW) method, the full-potential linear muffin-tin orbital (FLMTO) method, and the tight-binding linear muffin tin orbital method within the atomic sphere approximation (LMTO-ASA), and with the local spin density approximation with on-site Coulomb interaction taken into account (LSDA+U).

## ACCOMPLISHMENTS

Our major accomplishment with the Cray T3E and the IBM SP was the full and optimized parallelization of the all-electron FLAPW method, done together with Andrew Canning at NERSC. To our knowledge, this is the first all-electron electronic structure method that has been successfully parallelized.

We have investigated the influence of the Coulomb interaction parameter on both the electronic structure and the magnetic ordering of $LaSr_2Mn_2O_7$. The main factors governing band formation in this manganite are (1) the exchange splitting with almost unoccupied minority spin Mn-3*d* states, (2) the ligand field splitting of the $t_{2g}$ and $e_g$ states, and (3) further splitting of the $e_g$ states with increase of *U*, which we consider an essential factor in the layered manganites. We have examined FM and A-type AFM ground states of this compound by comparing their total energy differences for a number of *U* values (from 0 to 10 eV) and found that the experimentally observed magnetic ordering is reproduced within LSDA+U only for $U > 7$ eV — in contrast with the 3D manganites ($LaMnO_3$), where LSDA gives the true magnetic ground state.

Our first-principles FLMTO-GGA electronic structure calculations of the new medium-$T_C$ superconductor (MTSC) $MgB_2$ and related diborides indicate that superconductivity in these compounds is related to the existence of $p_{x,y}$-band holes at the Γ point. Based on these calculations, we explained the absence of medium-$T_C$ superconductivity for $BeB_2$, $AlB_2$, $ScB_2$, and $YB_2$. The simulations




*In this model of orbital order in paramagnetic $LaMnO_3$, the investigations of coupling between spin, orbital, and lattice degrees of freedom have been started by performing model average spin state calculations, which allow one to treat an orbital order in a paramagnetic state.*

of a number of $MgB_2$-based ternary systems using a supercell approach demonstrates that the electron doping of $MgB_2$ and the creation of isoelectronic defects in the boron sublattice are not favorable for superconductivity, and that a possible way of searching for similar MTSC should be via hole doping of $MgB_2$ or $CaB_2$ or via creating layered superstructures of the $MgB_2/CaB_2$ type.

## SIGNIFICANCE

There is a great demand for simple but realistic models describing essential electronic interactions in CMR materials. A detailed investigation of electronic structures is therefore important for a better understanding of the physics of CMR materials and for potential device applications. The investigations on properties and fundamental electronic structure characteristics of the new superconductor $MgB_2$ and related binary and ternary compounds will provide a theoretical basis for experimental efforts of solid-state chemists and physicists in searching for new superconductors with unusual and valuable properties.

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# Electronic and Structural Properties of Surfaces and Interfaces

*Bruce Harmon, Cai-Zhuang Wang, James Morris, Kai-Ming Ho, and Dave Turner, Ames Laboratory*

## RESEARCH OBJECTIVES

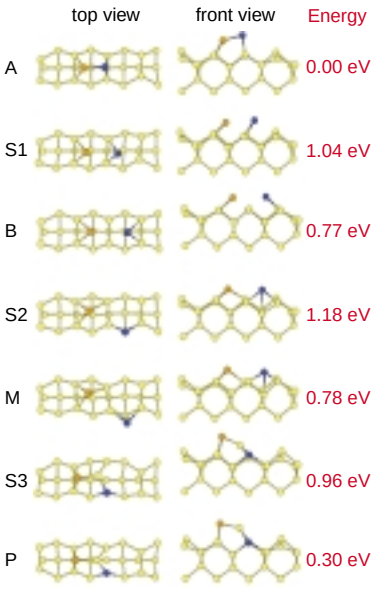
We are examining the roles of surfaces and interfaces in determining the properties of materials through calculations of semiconductor surfaces, metal-semiconductor interfaces, and bulk interfaces such as twin boundaries and grain boundaries.

## COMPUTATIONAL APPROACH

We use a classical molecular dynamics code to obtain a simple description of materials at the atomic level. Due to its simplicity, it is the fastest of our approaches, simulating tens of millions of atoms, but it is often inaccurate in calculating material-specific properties. We therefore use tight-binding molecular dynamics—an approach based on empirical data of the electronic structure—to calculate interatomic forces and, simultaneously, to obtain a simple description of the electronic structure. Finally, our first-principles codes provide efficient non-empirical electronic structure calculations, producing more accurate calculations of energies and structures of atomic interfaces, and allowing us to test and develop better tight-binding parameters.

## ACCOMPLISHMENTS

We have carried out a comparative study of the energetics and dynamics of Si-Si, Ge-Ge, and mixed Ge-Si addimers on top of a dimer row in the Si(001) surface, using first-principles calculations. Results show that the buckling in the addimer observed in scanning tunneling microscopy (STM) experiments is a signature of the mixed Ge-Si addimer. This distinctively different dynamic appearance of a Ge-Si dimer, compared to a Si-Si or Ge-Ge dimer, provides a unique way to identify it using STM.




*Atomic pathway and energies of the lowest barrier exchange process in which the Ge atom (shown in blue) of an adsorbed SiGe dimer is exchanged with a substrate Si atom on the Si(001) surface. The Si atom in the adsorbed dimer is shown in orange. While atomic intermixing is a common dynamic on surfaces, the present system is so far the only system where theoretical calculations can be compared with experimental observations in great detail.*

A recent experiment discovered an interesting reversible intermixing process involving the exchange of the Ge atom in an adsorbed SiGe dimer on the Si(001) surface with a substrate Si atom. We have performed first-principles total energy calculations to study the atomistic mechanisms of diffusion and intermixing in this system. Our calculation suggests that intermixing is triggered by the diffusion of the addimer on the surface. The energy barriers for the diffusion and intermixing events obtained from our calculations are in good agreement with experiment.

We have performed tight-binding molecular dynamics simulations to study the atomic dynamics of diamond surfaces under laser irradiation. Our simulation results suggest that the quality of the laser-treated diamond surfaces is dependent on the length of laser pulse being used. Under nanosecond or longer laser pulses, the diamond (111) surface is found to graphitize via formation of graphite-diamond interfaces, leading to a dirty surface after the laser treatment. By contrast, with femtosecond laser pulses, graphitization of the surface is found to occur layer by layer, resulting in a clean surface after the process. This atomistic picture provides an explanation of recent experimental observations.

We have performed tight-binding calculations to study the atomic relaxation and electronic properties of a stepped Si(111)-(7 × 7) surface. Our studies reveal several new surface bands induced by the step.

## SIGNIFICANCE

The atomic geometry of transition-metal-silicon structures at silicon surfaces and interfaces is a subject of interest both for its technological applications and fundamental theoretical importance. Silicon nanowires, for example, are expected to play important roles both as active components and interconnects in future nanodevices.

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http://cmp.ameslab.gov/

# *Electronic Structure and Simulation Calculations of Reactive Chemical Systems*

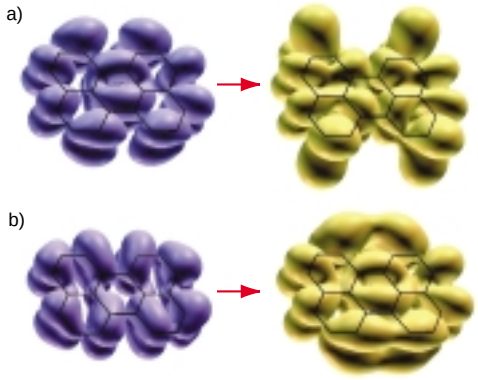
*Martin Head-Gordon and David Chandler,*
*University of California, Berkeley, and Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

Our research centers on the development and application of methods that predict the electronic structure of interesting molecules. We seek to open new classes of chemical problems to study via electronic structure theory.

## COMPUTATIONAL APPROACH

Our approach includes electronic structure methods of the density functional theory type, novel density matrix renormalization group calculations of electronic structure, Car-Parinello *ab initio* molecular dynamics, and transition path sampling methods.




*Perylene radical anion BLYP/6-31+G*//BLYP/6-31G* (a) alpha, and (b) beta electron attachment/detachment densities of the bright $1^2B_{3g} \rightarrow 1^2A_u$ electronic transition.*

## ACCOMPLISHMENTS

We have nearly completed a detailed study of the minima and saddle points of the potential energy surface of $C_3H_2$, corresponding to the reaction between C + acetylene. These results are the highest-level computations yet performed for this system. We have also performed molecular dynamics simulations on the isomerization dynamics of this system.

We have completed two significant time-dependent density functional theory (TDDFT) studies of excited states. The first study was an exploration of excited states of polyenes, in which we showed that the dark excited state, which poses a tremendous challenge for traditional quantum chemical methods, is well treated by TDDFT. This opens the way to applying TDDFT to related systems of biological significance such as carotenoids in the photosynthetic reaction center. The second study was an exploration of the excited states of a novel class of polycyclic aromatic hydrocarbon (PAH) cations which are closed shell. These species have been identified in sooting flames, and may also play a role in interstellar chemistry. However, their visible spectrum has never before been studied either experimentally or theoretically.

The dissociation of a water molecule in liquid water is the fundamental event in acid-base chemistry, determining the pH of water. Because of the short time scales and microscopic length scales involved, the dynamics of this autoionization have not been directly probed by experiment. We revealed the autoionization mechanism by sampling and analyzing *ab initio* molecular dynamics trajectories. We identified the rare fluctuations in solvation energies that destabilize an oxygen-hydrogen bond.

We have devised a novel importance sampling method for nonequilibrium processes. Using results of this sampling, we demonstrated that statistics of the energy gap between a solute's electronic states are Gaussian throughout the dynamics of nonequilibrium solvation in water. However, these statistics do change in time, reflecting linear response that is nonstationary. Discrepancies observed between the dynamics of nonequilibrium relaxation and of equilibrium fluctuations are thus explained. We analyzed a simple Gaussian field theory that accounts for this nonstationary response.

## SIGNIFICANCE

Electronic structure theory has emerged as a valuable counterpart to direct experiments for the study of reactive species that may not be easily characterized (if at all) in the laboratory, yet there are still fundamental challenges remaining. It is in these frontiers of electronic structure theory that our research is focused. Our research on chemical and conformational transformations of biomolecules is beginning to yield a novel microscopic picture of biochemical dynamics. Our results may have significant implications for the general understanding of solvent roles in chemical and biochemical processes.

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http://www.cchem.berkeley.edu/~mhggrp/

# Fluid and Particulate Transport in Self-Affine Fractures

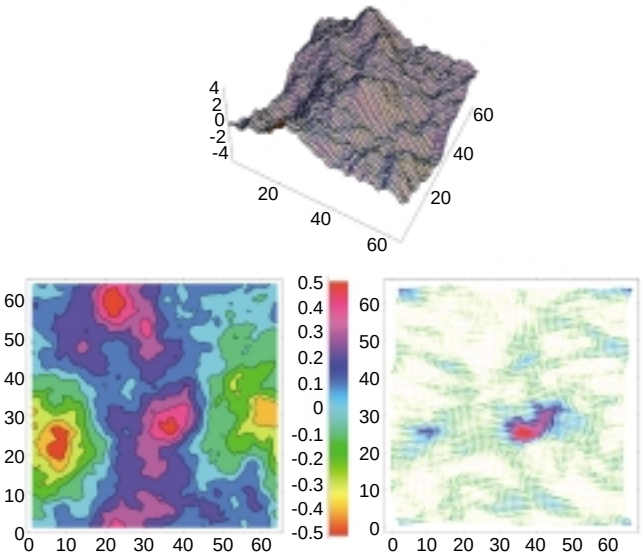
*Joel Koplik, City College of New York*

## RESEARCH OBJECTIVES

(1) Complete our numerical simulations and analytic estimates which aim to relate permeability, dispersivity, and more detailed characterizations of fluid transport to the fractal parameters of the three-dimensional fractured medium. (2) Consider the evolution of the pore space and fracture walls when small colloidal suspended particles in the flow are allowed to deposit along the walls, gradually shrinking the pore space. (3) Consider the dynamics of finite-sized suspended particles, large enough to alter the flow field but still small enough to be sensitive to the surface roughness. (4) Consider flow of fluids containing either passive tracers or suspended particles in fracture junctions, with the aim of understanding how fluids and particulates choose among flow channels, and studying the persistence of correlations between different parts of a fracture network.

## COMPUTATIONAL APPROACH

The computations are based on the lattice Boltzmann method for fluid flows. In this algorithm, fictitious particles move from node to node on a regular lattice with certain rules for collisions, which are designed so that the average motion of the lattice particles reproduce the appropriate solutions of the continuum Navier-Stokes equations. Solid surfaces correspond to nodes from which the particles are reflected, so that walls and particulates may be included. More elaborate rules allow one to simulate non-Newtonian fluids as well.




*Surface elevation plot (top) and contour plot (left) of a typical self-affine fractal surface with Hurst exponent 0.8. The velocity field in a simulated fracture consisting of two such surfaces separated vertically by one-eighth of the lateral size is shown at right; the arrows represent the deviation of the local velocity from the mean.*

## ACCOMPLISHMENTS

We considered the fluid permeability and the dispersion of a passive tracer in a rough-walled fracture, modeled as the gap between two complementary self-affine surfaces rigidly translated with respect to each other. When the mean gap is large compared to the range of the surface height fluctuations, the effect of roughness on permeability is given by a systematic perturbation expansion, whose leading correction is readily expressed in terms of the Hurst exponent characterizing the fracture surface, and which agrees very well with the results of numerical simulations using the lattice Boltzmann method. These results go beyond the common lubrication approximation, because we find that an important ingredient in permeability reduction is the presence of stagnant zones of fluid in the roughness interstices, an effect not allowed for in lubrication.

In the opposite limit of a narrow gap, we began with the two-dimensional case first, where tortuosity effects dominate. Straightforward arguments based on dividing the flow path into decorrelated segments, and supported by numerical simulations, provide a relation between the permeability, the mean aperture, and the fractal exponent of the surface. The ensemble averaged results agree with theoretical scaling predictions for the variation of the effective dispersivity with fracture geometry and transit distance. The dispersivity shows strong anisotropic effects, and furthermore the dispersion front progressively wrinkles into a self-affine curve with a predictable dimension. We then revisited the two-dimensional case and used tortuosity-based arguments to obtain a relation between the surface exponent and the resulting change in dispersivity. Again, lattice-Boltzmann simulations were in agreement with the analytic arguments, but in this case the method required the development of a new concentration boundary condition.

## SIGNIFICANCE

The general goal of this work is to enhance our understanding of the motions of fluids and particles in geological formations, with application to water supply, hydrocarbon production, and waste disposal.

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# *Quantum and Classical Simulations of Clusters, Self-Assembly, Nanoscale Manipulations, Nanotribology, and Biological Processes*

*Uzi Landman, Robert N. Barnett, Charles L. Cleveland, Hannu Hakkinen, and W. David Luedtke, Georgia Institute of Technology*

## RESEARCH OBJECTIVES

This project focuses on development, implementation, and use of quantum and classical modeling and simulation methodologies on high-performance computational platforms for investigating microscopic physical and chemical processes and mechanisms underlying the generation and properties of novel materials in various forms and degrees of aggregation, under equilibrium and nonequilibrium conditions or subject to extreme environments. These investigations aim at discovering and elucidating size-dependent evolutionary patterns of materials properties, bridging the molecular, cluster, and condensed-phase regimes.

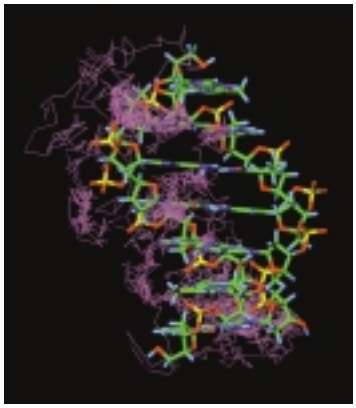
## COMPUTATIONAL APPROACH

We use large-scale classical molecular dynamics (particularly in nanotribology studies) and tested many-body interactions. We also use *ab initio* quantum molecular dynamics (in conjunction with norm-conserving nonlocal pseudopotentials and a plane-wave basis) based on local-spin density functional theory (LSD) with the inclusion of generalized exchange-correlation gradient corrections (GGA). In these *ab initio* simulations, the dynamics of the ions evolve on the concurrently calculated electronic ground state Born-Oppenheimer (BO) potential energy surface, using the BO-LSD-MD method formulated by us, with the codes rewritten for parallel computations with the assistance of Andrew Canning at NERSC.

## ACCOMPLISHMENTS

Investigations of the exactly solvable excitation spectra of two-electron quantum dots with a parabolic confinement, for different values of the parameter *RW* expressing the relative magnitudes of the interelectron repulsion and the zero-point kinetic energy, revealed for large *RW* a rovibrational spectrum associated with a linear trimeric rigid molecule composed of the two electrons and the infinitely heavy confining dot.

The properties of neutral and anionic PdN clusters were investigated with spin-density-functional calculations. The ground-state structures are three dimensional for *N* larger then 3 and magnetic with a spin triplet for *N* larger then 2 and smaller then 7, and a spin nonet for *N* equals 13 neutral clusters. Structural and spin isomers were determined and an anomalous increase of the magnetic moment with temperature is predicted for a Pd7 ensemble. Vertical electron detachment and ionization energies were calculated and the former agrees well with measured values for anionic PdN clusters.



*Trajectory of a sodium counter-ion (in purple) superimposed on a short nucleobase sequence of DNA. The trajectory, taken from a 1.6 nanosecond molecular dynamics simulation at room temperature of DNA in water, illustrates the high mobility of the counter-ions.*

Electron hole (radical cation) migration in DNA, where the quantum transport of an injected charge is gated in a correlated manner by the thermal motions of the hydrated counter-ions, was investigated. Classical molecular dynamics simulations in conjunction with large-scale first-principles electronic structure calculations revealed that different counter-ion configurations lead to formation of states characterized by varying spatial distributions and degrees of charge-localization. Comparative UV light-induced cleavage experiments on native B-DNA oligomers and on ones modified to contain counter-ion ($Na^+$)-starved bridges between damage-susceptible hole-trapping sites (GG steps), show in the latter a reduction in damage at the distal step, indicating a reduced mobility of the hole across the modified bridge in correspondence with the theoretical predictions.

## SIGNIFICANCE

This research is significant both to the formulation and development of computational methodologies and to their employment in investigations of challenging physical and chemical problems in the areas of cluster science, nanostructures, and nanotribology.

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# Quantum Monte Carlo for Electronic Structure of Combustion Systems

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*Alexander Kollias, Lawrence Berkeley National Laboratory*
*Xenophon Krokidis, Accelrys, Inc., Orsay Cedex, France*
*John Harkless, National Institute of Standards and Technology*

## RESEARCH OBJECTIVES

This research is directed principally toward high-accuracy studies to enable the characterization of the reaction pathways (1) leading to the formation of the first aromatic ring in high-temperature environments and subsequent reactions ultimately leading to soot formation, and (b) governing combustion reactions of small organic alcohols.

## COMPUTATIONAL APPROACH

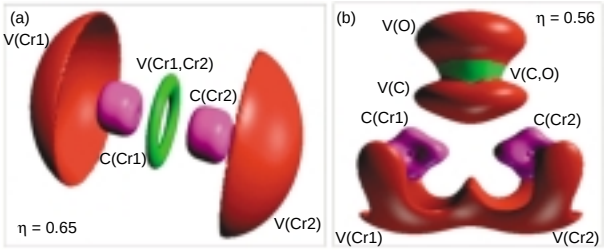
Our dominant computational technique is the quantum Monte Carlo (QMC) method in the diffusion Monte Carlo (DMC) variant. Our version of DMC employs effective core potentials to minimize computational effort. Variational Monte Carlo computations are carried out to test trial functions for DMC constructed as products of independent particle wave functions and correlation functions that depend on interparticle distances. The Schmidt-Moskowitz correlation function based on a functional form introduced by Boys and Handy is used in this work, along with a recently developed wave function optimization method.

## ACCOMPLISHMENTS

The addition of $C_3H_3$ and $C_2H_2$ to form cyclopentadienyl (cpd) radical was investigated using QMC and several density functional theory (DFT) methods. The kinetics of the reaction system were studied using time-dependent solution of the energy-transfer master equations. The computed heat of formation of the cpd radical and the rate of its thermal decomposition compare favorably with available experimental data.

We carried out QMC and DFT computations to identify and quantitatively characterize the ground-state reaction pathways for completion of chlorine plus methanol. Prior to the present calculations, only the reaction leading to methoxy radical had been identified. Using DFT and Fukui function procedures, we were able to identify a previously unknown direct reaction pathway leading to the formation of hydroxymethyl radical, which explained recent experimental data.

Elucidation of reaction pathways and associated rates for the formation of aromatics in high-temperature pyrolysis and oxidation of hydrocarbons is one of the most active areas of research in gas phase chemical kinetics. The primary focus is on the formation of the first aromatic ring from small aliphatics, because this step is perceived to be rate-limiting in the reaction sequence leading to larger aromatics and eventually soot. A critical aspect of the associated analysis is the stability of the normal (n) and iso (i) isomers at high temperature. QMC calculations of the energy differences in $C_4H_3$ and $C_4H_5$ isomers have determined greater stability for both types of isomers and enhanced stability of the n isomers relative to the i isomers.




*This figure displays the electron localization function (ELF) for the interaction of CO with two chromium (Cr) atoms at a separation corresponding to the lattice spacing of Cr(110). The isosurfaces in panels (a) and (b) correspond to different values of ELF, η = 0.65 and 0.56, respectively. The Cr1-Cr2 and C-O bonds are represented by green basins; the carbon, oxygen and chromium valence basins are red; while the cores are magenta. Panel (a) shows the localization domains of a two-Cr cluster before interaction with CO. Panel (b) displays the perpendicular binding mode of CO adsorbed on the surface. (Figure by O. El Akramine, X. Krokidis, and A. Kollias)*

## SIGNIFICANCE

With elementary reactions determined to ~1 kcal/mol, uncertainties in reaction paths can be resolved, removing ambiguity in mechanisms for the formation of successively larger precursors to soot formation. The ultimate goal is full characterization of the mechanism of soot formation, which will provide valuable insight on how to reduce a major pollution source. The methods developed in this research will also be applicable to molecular systems important in catalysis and other application areas.

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# First-Principles Catalyst Design for Environmentally Benign Energy Production

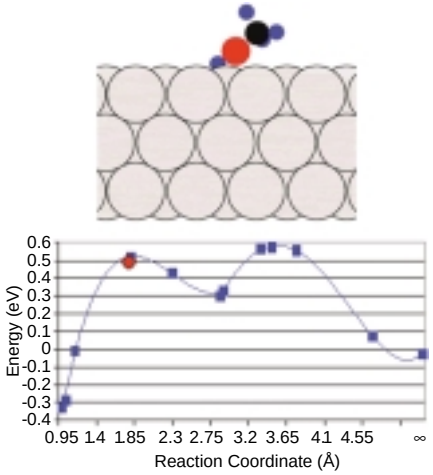
*Manos Mavrikakis, Jeff Greeley, Ye Xu, Jaco Schieke, and Amit Gokhale, University of Wisconsin, Madison*

## RESEARCH OBJECTIVES

We are developing a first-principles approach to the atomic-scale design of novel catalytic materials, tailored to perform specific reactions with the desired activity and selectivity. The thermochemistry of reactions, atomic and molecular diffusion barriers, and activation energy barriers for chemical reactions are calculated. Trends and discontinuities characterizing the behavior of metals can be clearly identified. These trends can be used as a guiding principle for the design of new catalysts.

## COMPUTATIONAL APPROACH

We use a fully parallelized and efficient planewave total energy density functional theory (DFT)-based code for modeling elementary reaction steps on transition metal surfaces and alloys. The total energy of a given system is minimized by using a variety of alternative algorithms, depending on the potential energy surface characterizing the physics of the system treated. The Nudged Elastic Band algorithm is implemented for determining the detailed reaction path and the corresponding components of the reaction coordinate for the elementary reaction steps.




*One-dimensional potential energy surface along the reaction coordinate for partial oxidation of methanol on a model Pt(111) surface. Only the first two elementary reaction steps are shown in the chart, and the transition state of the first step is illustrated. First, the methanol molecule loses its hydroxyl hydrogen (H, shown in blue) to yield a methoxy intermediate (red = oxygen, black = carbon, gray = Pt surface). Another H atom is subsequently removed from methoxy to yield a formaldehyde molecule on the Pt surface. Further H abstraction will lead to CO formation, which poisons the Pt catalyst, a typical problem for direct methanol fuel cells.*

## ACCOMPLISHMENTS

*Methanol decomposition on Cu(111) and Pt(111) surfaces:* Analyzing methanol decomposition on Cu(111) has offered many new insights for the microscopic reverse reaction, namely the synthesis of methanol from CO + $H_2$. We have found that methoxy is a key reaction intermediate, which is tilted on the Pt(111) surface, as opposed to what we found on the Cu(111) surface, where methoxy binds to the surface in a perpendicular configuration. We have also found that methanol decomposition is highly endothermic on Cu(111) and highly exothermic on Pt(111). Methanol decomposes very easily on Pt(111), yielding hydrogen and CO. CO binds on Pt(111) at least twice as strongly as it does on Cu(111), which is direct evidence of the CO poisoning effect.

*Molecular oxygen adsorption and dissociation (oxygen reduction) on Cu(111), Ir(111), Au(111) and Au(211) surfaces:* $O_2$ adsorbs strongly on Cu(111) and Ir(111) as a molecule, whereas it adsorbs only weakly on stretched Au(111) and stepped Au(211) surfaces. $O_2$ dissociates rather easily on Cu(111) and Ir(111) surfaces, whereas the dissociation is highly activated on stretched Au(111) and stepped Au(211) surfaces. The effect of steps and strain had been postulated as the reason for the remarkable low temperature CO oxidation activity of finely dispersed gold particles. Our calculations provide the first direct quantitative proof of these speculations.

## SIGNIFICANCE

Industrial methanol synthesis, a multibillion-dollar industry, is performed on supported Cu catalysts. Methanol decomposition on Pt(111) is directly connected with the chemistry happening at the anode of direct methanol fuel cells (DMFCs), and the CO poisoning effect is the single most important technological problem in the implementation of DMFCs. Oxygen reduction is the first step towards numerous industrial catalytic oxidation reactions, and is the reaction happening at the cathode of most fuel cells. Oxygen interaction with metals is also directly relevant to the corrosion process. Our work on $O_2$ adsorption and dissociation on Ir(111) is technologically relevant, as iridium has been proposed and used as a component of the three-way car-exhaust catalysts.

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http://www.engr.wisc.edu/che/faculty/mavrikakis_manos.html

# Electron-Atom and Electron-Molecule Collision Processes

*C. William McCurdy, Daniel A. Horner, Zhiyong Zhang, and*
*Wim Vanroose, Lawrence Berkeley National Laboratory*
*Thomas N. Rescigno, Lawrence Berkeley National Laboratory and*
*Lawrence Livermore National Laboratory*
*Mark Baertschy, University of Colorado/JILA*
*William Isaacs, Lawrence Livermore National Laboratory*

## RESEARCH OBJECTIVES

This project seeks to develop theoretical and computational methods for treating electron collision processes that are currently beyond the grasp of first-principles methods.

## COMPUTATIONAL APPROACH

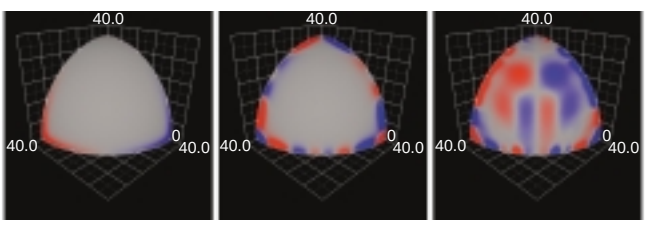
Our approach builds on the algebraic variational formalisms (the Complex Kohn variational method) we have been developing to study electron-atom and electron-molecule scattering. These approaches have now been extended to include complex optical potential interactions, a scattered-wave/flux operator formalism, and a variety of techniques based on analyticity. These techniques allow us to treat a broad range of problems, from low-energy electron-molecule collisions using elaborate variational wave functions to direct solutions of the Schrödinger equation for simple atomic targets that provide detailed ionization cross sections.

## ACCOMPLISHMENTS

We developed a new procedure for computing impact ionization amplitudes that provides a direct and efficient route to computing the breakup cross sections. This provided an independent check on the fundamental correctness of the results we had initially obtained by numerically extrapolating the quantum mechanical flux. The computational approach we have developed has, to date, provided the only complete solution to the quantum mechanical three-body Coulomb at low collision energies.

We have also developed a new technique for computing the scattered wave function that does not require the solution of large systems of complex linear equations. This is accomplished by writing the scattered wave function as the Fourier transform of a time-propagated initial state that can be computed using a discrete variable representation in conjunction with a split-operator method.

We have completed the second phase of our work on electron-$CO_2$ scattering, exploring resonant vibrational excitation in the 4 eV energy region and carrying out time-dependent wavepacket studies in three dimensions. This study represents the first time that all aspects of an electron-polyatomic collision, including not only the determination of the fixed-nuclear electronic cross sections but also a treatment of the nuclear dynamics in multiple dimensions, has been carried out entirely from first principles.




*Wave functions for a quantum mechanical system of a charged particle colliding with a model two-electron atom. The vertical axis represents the coordinate of the incident particle, and the other two axes are the electron coordinates. In the left panel, the collision energy is lower than the breakup threshold; in the center panel, the collision energy is sufficient to singly ionize the atom; in the right panel, the energy is sufficient to cause complete fragmentation of the system.*

## SIGNIFICANCE

Electron collision processes are central to the problems of interest to DOE, playing a key role in such diverse areas as fusion plasmas, plasma etching and deposition, and waste remediation. Electron-molecule collisions play a central role in the plasma processing of silicon chips, but the understanding and modeling of these low-temperature plasmas is severely hampered by the lack of a database of electron-molecule collision cross sections; this project will significantly add to that base of knowledge. In mixed radioactive waste, the primary radioactive decay events produce showers of secondary electrons which initiate the chemistry that produces a mixture very different from the one that was present originally. The tools we are developing will make it possible to understand and model this kind of electron-initiated chemistry. Central to understanding plasma formation are the fundamental studies of electron and positron impact ionization of simple atoms. We developed the first complete method for treating electron-impact ionization of atoms from first principles, solving a fundamental problem in atomic physics that had resisted solution for more than 40 years. We are now working extensions of the computational approach that will allow us to study systems containing more than two electrons.

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www.lbl.gov/cs/amo_theory

# *Semiclassical Molecular Reaction Dynamics: Methodological Developments and Applications to Complex Systems*

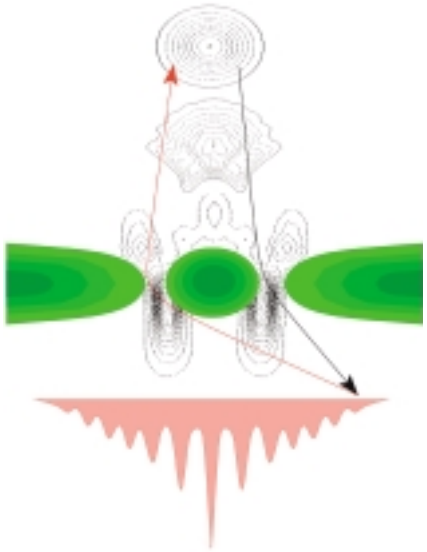
*William Miller, University of California, Berkeley*

## RESEARCH OBJECTIVES

This project continues the methodology development of the semiclassical initial value representations and their practical application to complex molecular systems: reactions in solutions, protein complexes, DNAs, and on surfaces. The main effort of this project is to include quantum effects (tunnelings, interferences, etc.) into classical molecular dynamics simulations, and to address complex problems that are beyond any other existing quantum dynamical methods. Specific studies are grouped in three main areas: (1) methodological developments to extend the capability of the current semiclassical initial value representation (SC-IVR) algorithms, (2) SC-IVR to study the reaction dynamics in complex systems, and (3) *ab initio* potential surface and quantum and molecular mechanics (QM/MM) development

## COMPUTATIONAL APPROACH

Implementation of the SC-IVR is based on classical molecular dynamics (MD) simulation but invoking the quantum superposition principle in gathering the dynamical information. Monte Carlo phase space average is usually carried out over a large number of degrees of freedom. Importance sampling techniques as well as various filtering methods are used to evaluate the high-dimensional integrals efficiently. Quantum effects are finally obtained from the phase information uniquely defined in semiclassics (but missing in traditional classical MD simulations). We plan to adopt the QM/MM method in our SC-IVR algorithms to evaluate the potential surface "on the fly" during dynamical simulations. This enhances our capability to study bond-breaking/forming processes in biological systems.



*Schematic representation of a forward-backward trajectory for the double-slit experiment: quantum interference is reproduced by the superposition of forward and backward trajectories that cross the obstacle through different slits.*

## ACCOMPLISHMENTS

(1) Application of the forward-backward initial value representation (FB-IVR) to the study of quantum coherence effects and their quenching in complex systems. (2) The development of the generalized forward-backward initial value representation (GFB-IVR) to study complex systems. (3) Application of the SC-IVR and the Meyer-Miller mapping technique to describing tunneling effects for chemical reactions. (4) Application of the SC-IVR to the study of nonadiabatic dynamics for multiple electronic state problems. (5) The development of a new powerful filtering method, the generalized Filinov transformation technique, to practically solve the sign problem in an SC-IVR calculation. (6) Application of the generalized Filinov transformation method to evaluating thermal rate constants for proton transfer reactions in the condensed phase.

## SIGNIFICANCE

SC-IVR is the only practical tool for accurately obtaining quantum dynamical effects for complex systems, which is a major improvement over the traditional classical molecular dynamics methods and goes beyond current rigorous quantum mechanical method (only capable of treating few-body problems). The accuracy and efficiency of SC-IVR have been demonstrated in many publications from our group and others. With our methodological developments, we are treating much more complex systems than previously reported in the literature, including applications that break the 100-degrees-of-freedom boundary for the first time in SC-IVR calculations.

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# Magnetic Materials: Bridging Basic and Applied Science

*G. Malcolm Stocks, Oak Ridge National Laboratory*
*Bruce N. Harmon, Ames Laboratory, Iowa State University*
*Michael Weinert, Brookhaven National Laboratory*
*David P. Landau, University of Georgia*

## RESEARCH OBJECTIVES

Our goal is understanding the magnetic properties of real materials by developing a comprehensive multi-length-scale modeling capability. Using this capability, we will study the magnetic structure of systems including disordered alloys, nanoparticles, nanowires, interfaces in multilayers, and quantum corrals, and to study domain walls and their interaction with structural defects.

## COMPUTATIONAL APPROACH

First-principles density functional theory (DFT) methods are applied to calculating fundamental magnetic properties including magnetic moments, exchange interactions, and magneto-crystalline anisotropy. First-principles spin dynamics is used to treat the spin degrees of freedom at finite temperature and in the presence of external fields, and to find complex ground states using relaxation techniques. Tight binding methods based on fits to first principles are being developed to implement spin dynamics at an intermediate level (systems containing several thousands of atoms) between first-principles techniques and extended Heisenberg models.

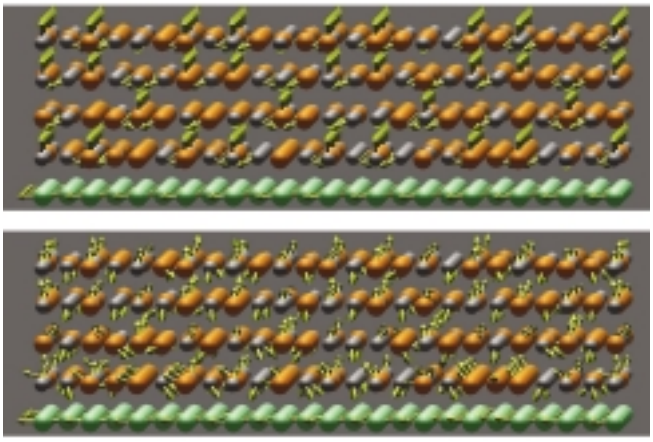
## ACCOMPLISHMENTS

We have performed first-principles calculations of the magnetic structure of gamma-FeMn based on large cell models (up to 2,048 atoms) of the disordered alloy and have discovered a new ground state magnetic structure. The calculations are based on the constrained local moment model and use of first-principles spin dynamics to obtain the ground state orientational configuration.

We have made the first calculations of the magnetic ground states of iron inclusions embedded in fcc copper using first-principles calculations. Our calculations show that, depending on whether the chains of magnetic atoms are embedded in copper along the 100 or 110 directions, the ground state orientation of the magnetic moments on the iron sites can be either parallel or perpendicular to the chain.

In *ab initio* calculations of the reorientation transition for overlayers of Fe on Cu(111), we find that the direction of the magnetization is perpendicular to the surface for films up to two monolayers thick, and it is oriented in-plane for larger thicknesses, in complete agreement with recent experiments.

The order-N locally self-consistent multiple scattering (LSMS) method has been extended to treat relativistic systems. The fully relativistic method, in which solution of the Schrödinger equation is replaced by the solution of the Dirac equation, is capable of treating systems comprising ~2,000 atoms on currently available machines.



*An ab initio spin dynamics calculation has been performed on the FeMn/Co(111) system to understand properties of this interface, a candidate to be used in magnetic read heads. Top: Section of the FeMn/Co interface showing the initial configuration of the magnetic moments. The visualization shows the Co layer and four FeMn layers closest to the interface. The Co layer is initialized in a ferromagnetic state, and the FeMn layers are initialized in the 3Q structure. Gold spheres represent the Fe and gray the Mn atoms. Bottom: Section of the FeMn/Co interface showing the final configuration of the magnetic moments for the same five layers as shown for the initial configuration. This calculation involved 2,016 nodes on the IBM SP to achieve 2.3 teraflop/s performance.*

## SIGNIFICANCE

The goal of this project is to develop modeling tools capable of integrating atomic-level understanding of magnetic properties and interactions with structure and microstructure. Such a capability would enable the science-based understanding and prediction of technologically relevant magnetic properties and the design of improved permanent magnets and magneto-electronic devices, such as magnetic recording media, read heads, and MRAM.

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# Computational Semiconductor Physics

*Alex Zunger, Paul Kent, Gabriel Bester, Marco Califano, Priya Mahadevan, and Cetin Kilic, National Renewable Energy Laboratory*

## RESEARCH OBJECTIVES

Our calculations allow us to predict in detail the effect of nanoscale atomic structure on the electronic and optical properties of semiconductor systems. Using atomistic models in conjunction with quantum mechanical methods, we are able to interpret excitonic spectra, provide feedback to experiment, and predict new properties to be engineered and investigated. Our studies focus on both one-body electronic structure and many-body (configuration interaction) treatments.

## COMPUTATIONAL APPROACH

Our computational approach is based on accurate quantum mechanical calculations for the electronic, optoelectronic, and thermodynamic properties of semiconductor nanostructures using detailed fully relaxed atomistic models of semiconductor nanostructures. We use a combination of methods to bridge the length and computational cost scales from the 100–1000 atom microstructural scale, where we obtain thermodynamic information, and compute fully relaxed geometries of complex structures such as impurity complexes and surfaces, to the 100,000–1,000,000 nanostructure regime, where the optoelectronic properties are determined by the near gap conduction and valence states.

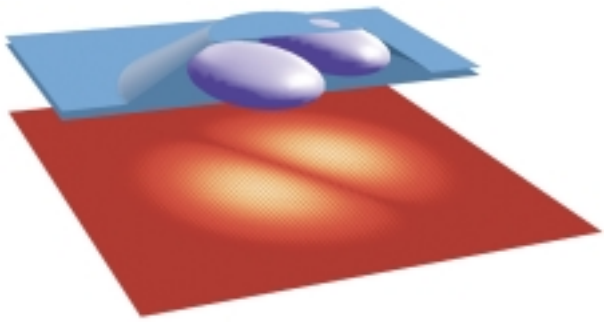
We use local density approximation (LDA) density-functional methods for small systems; for large-scale nanostructures, we use empirical pseudopotential methods, such as the folded spectrum method (FSM), as well as the linear combination of bulk bands method. Our pseudopotential methods are optimized for application to nanostructures, and allow us to study million-atom systems with quantum mechanical accuracy, without the approximations and pathologies inherent in conventional nanostructure calculation approaches such as k.p.

## ACCOMPLISHMENTS

In FY2001 we successfully studied several classes of nanostructure systems:

*Quantum dots:* We extended our theory of lens and pyramidal-shaped embedded InGaAs quantum dots to include composition variation, and utilized the spectroscopic signature of current grown dots to accurately determine their size, shape, and composition profile.

*Nitride alloys and alloy microstructure:* In dilute nitride alloys, we demonstrated how small nitrogen clusters result in below band-gap cluster states, drastically altering these materials' optical properties. In the related InGaAsN system, we established a quantitative theory of spatial correlation, where ordering leads to significant changes in the optical properties and electronic localization.



*The second electron state of an InGaAs quantum dot (blue), calculated using the empirical pseudopotential method (EPM). Shown in purple is the wavefunction obtained by more approximate methods, while a cross section of the EPM wavefunction is shown in red, revealing the rich and phenomenologically important atomistic detail.*

*Metal alloys:* We developed our first-principles theory of brass (Cu-Zn), predicting the low-temperature ground states, finite-temperature phase diagram, and short range order.

## SIGNIFICANCE

The electronic, optical, transport, and structural properties of semiconductor nanostructures (films, quantum dots, and quantum wires) and microstructures in alloys are important because of the novel physical properties exhibited by these systems (state localization, Coulomb blockade, quantum confinement, exchange enhancement, and shape-dependent spectroscopy) and because of their application to lasers, sensors, photovoltaics, and new novel quantum devices. These structural features occur on distance scales of ~100–500 Å, thus encompassing $10^4$–$10^5$ atoms. Ours is the only available pseudopotential-based theory which can address this size scale. Understanding the underlying physical phenomena in these systems is essential to designing nanoscale devices with custom-made electronic and optical properties.

## PUBLICATIONS

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# Low Frequency Climate Variability: Natural and Forced Responses

*Tim Barnett, David Pierce, and Niklas Schneider,*
*Scripps Institution of Oceanography*
*Lai-Yung (Ruby) Leung, Pacific Northwest National Laboratory*

## RESEARCH OBJECTIVES

Our objectives are to examine the physical causes and potential predictability of two aspects of low-frequency climate variability: natural, unforced variability in the North Pacific/American sector, and forced variability in this region associated with changing levels of anthropogenic gases in the atmosphere.

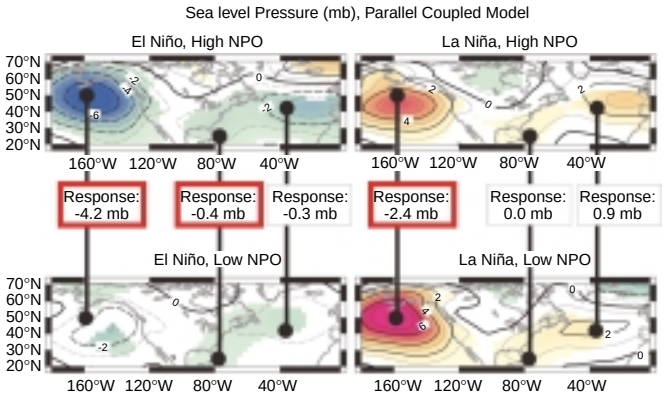
## COMPUTATIONAL APPROACH

We use the Parallel Coupled Model (PCM), a sophisticated coupled general circulation model that includes the ocean, atmosphere, land surface, and sea ice. The individual ocean and atmosphere components from this model are also used separately. The resolution of the atmospheric component of the models is T42, while that of the ocean components varies from about 0.5° to 1°, depending on the latitude and longitude.

## ACCOMPLISHMENTS

The work of Gershunov and Barnett (1998) showed the possible role of North Pacific Ocean sea surface temperatures (SSTs) in modulating the effects of the El Niño/Southern Oscillation (ENSO) over North America. Using forced model runs with tropical SST patterns corresponding to El Niño or La Niña joined to extratropical SST patterns of either the positive or negative decadal phase, we tested the predictive ability of North Pacific SSTs. We found that the modulation effect is arising from internal atmospheric variability, and is not forced by North Pacific SSTs.

Our evaluation of climate response in the Pacific/North American sector to anthropogenic forcing ($CO_2$ and sulfates) is ongoing under the auspices of the DOE's Accelerated Climate Prediction Initiative (ACPI) pilot program.




*Sea level pressure (SLP) anomalies, in millibars, from the Parallel Coupled Model (PCM), for four cases: El Niño with a high North Pacific Oscillation (NPO), El Niño with a low NPO, La Niña/high NPO, and La Niña/low NPO. Values in the boxes show the difference between the SLP seen in the high NPO state and the low NPO state. Red boxes indicate a statistically significant difference at the 95% level. It can be seen that during El Niño, the state of the NPO is associated with significant differences in SLP over the Aleutian low region and the southeast U.S. During La Niña, there is a significant difference over the Aleutian low region. These model responses are similar to observations, and allow us to examine the reason for this link between El Niño and the NPO in the model.*

## SIGNIFICANCE

Natural variability on the decadal time scale presents one of the biggest complications in the detection of anthropogenic climate signals, so determining the levels of natural decadal variability, and being able to understand the physical processes responsible for this natural noise, are a clear requirement of any attempt to make an early detection of human impact on climate. Thus our research of decadal climate research has a direct contribution to climate change research at time scales beyond a decade. Also, examining the large-scale, hemispheric links between the monsoon, ENSO, and North Pacific might increase the forecastability of any of this climate variability.

In the broader scientific sense, this exploration attempts to determine how forced changes in a complicated, nonlinear system (the climate) relate to intrinsic patterns of unforced variability in that same system. It is possible that all the forced changes lie outside of the realm of natural variability, or that all the forced changes are associated with changes in the probability density function of the natural climate modes. The real climate is likely somewhere between these two endpoints, and our investigations will help determine where. The answer will have payoff for prediction of future forced climate variability as well as for anthropogenic change detection strategies.

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http://www.pnl.gov/atmos_sciences/Lrl/ACPI.html

# Simulating Ocean Carbon Sequestration

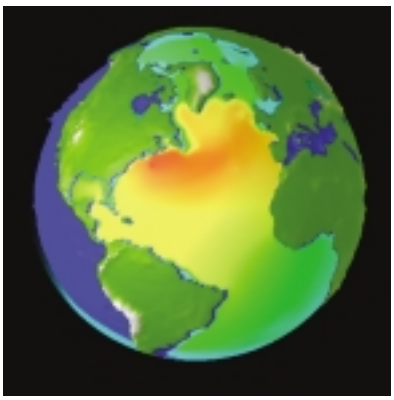
*Kenneth Caldeira, Lawrence Livermore National Laboratory*
*James K. B. Bishop, Lawrence Berkeley National Laboratory*
*Jim Barry, Monterey Bay Aquarium Research Institute*
*Kenneth Coale, Moss Landing Marine Laboratory*
*Paul Falkowski, Rutgers University*
*Howard Herzog and Sallie Chisholm, Massachusetts Institute of Technology*
*Russ Davis, Scripps Institution of Oceanography*
*Gerard Nihous, Pacific International Center for High Technology Research*

## RESEARCH OBJECTIVES

The research objectives of the DOE Center for Research on Ocean Carbon Sequestration are (1) to understand the efficacy and impacts of various strategies proposed for ocean carbon sequestration; (2) to focus research of other groups on the key uncertainties and/or deficiencies in ocean physics and biogeochemical models; (3) to develop the best numerical simulations of ocean carbon sequestration, both with regard to biological fertilization and direct injection of $CO_2$ into the deep ocean, by incorporating the research of other groups into an improved model of ocean physics and biogeochemistry.

## COMPUTATIONAL APPROACH

For our ocean physics model, we initially used the Lawrence Livermore National Laboratory version of the Geophysical Fluid Dynamics Laboratory's MOM, with a later transition to Los Alamos National Laboratory's POP model. Some modifications to the POP code were made to improve the numerics of handling point sources with high spatial concentration gradients. Because some ocean sequestration strategies involve point sources, and the numerics of the models assume relatively small spatial concentration gradients, we explored a number of techniques for handling these large gradients within the model, including testing various tracer advection schemes and using results from a high-resolution regional model (run at MIT) to initialize the global General Circulation Model.



*Simulation of ocean carbon sequestration via direct injection of $CO_2$ at 700 m depth near New York City. This figure represents results from the highest-resolution global simulation of direct injection yet performed. Shown on the figure is the vertically integrated concentration of injected $CO_2$, known as column inventories, after 100 years of continuous injection at the rate of 0.1 PgC per year. At 700 m there is considerable leakage to the atmosphere, but injections at 1500 m or below effectively store the carbon in the ocean for many hundreds of years.*

## ACCOMPLISHMENTS

We achieved the highest-resolution-ever global simulations of direct injection of $CO_2$ into the oceans. These simulations indicate that direct injection of $CO_2$ into the ocean is an effective carbon sequestration strategy. Approximately 80% of the injected carbon remains in the ocean permanently. The approximately 20% of the carbon that leaks back to the atmosphere does so on a time scale of several hundred years. Hence, direct injection of $CO_2$ into the ocean could play a potentially important role in diminishing anthropogenic climate change. We are now studying our simulation results to better understand possible biotic consequences of adopting this sequestration strategy. Initial results indicate that far-field effects (i.e., hundreds of km from the injection point) may be similar to the effects of $CO_2$ absorbed passively from the atmosphere. Near-field effects (i.e., < 1 km from the $CO_2$ source), however, may be acute and significantly impact marine biota in a relatively restricted area.

## SIGNIFICANCE

We must understand the options available to us to slow the rapid accumulation of $CO_2$ in the atmosphere and reduce its environmental impacts. It is the primary goal of this research to advance the science necessary to understand the efficacy and impacts of various strategies to sequester carbon in the oceans and away from the atmosphere.

## PUBLICATIONS

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http://esd.lbl.gov/DOCS

# Computational Studies of Protein Folding and Enzymatic Catalysis of Beta-Lactamases

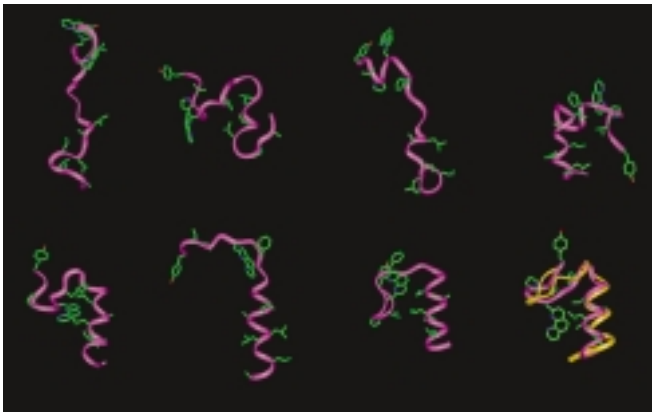
*James Caldwell, University of California, San Francisco*

## RESEARCH OBJECTIVES

(1) To study the early stage of the folding processes of small proteins. (2) To identify important folding intermediates by limited folding simulations using locally enhanced sampling (LES). (3) To refine and evaluate the free energy of structure predictions for small proteins. (4) To elucidate the mechanisms of the enzymatic catalysis for beta-lactamases classes A and C as well as inhibition mechanisms of penicillin-binding proteins by beta-lactam antibiotics.

## COMPUTATIONAL APPROACH

We use the AMBER6 molecular mechanics simulation program suite and Gaussian98 quantum mechanical calculation packages. The AMBER suite was developed by our group and enjoys a large user community.



*A series of early folding events of BBA1 protein domain.*

## ACCOMPLISHMENTS

We have significantly improved both the single-CPU and parallel performance of the molecular dynamics module (Sander) of AMBER. Currently for periodic systems, our parallel performance is of the order of 170/256 on the Cray T3E. We have also made significant progress in speeding up the more complex particle mesh Ewald version of Sander as well.

We have recently completed microsecond scale simulations of the folding motion of the small proteins villin headpiece and BBA1. These simulations marked the beginning of the ability of theory to directly simulate the initial stages of protein folding.

We have successfully reproduced the inherent structure of a heptapeptide which has been implicated as a folding nucleation peptide in folding of SH3 domains. Our calculations not only find it stable on a multinanosecond scale, but the calculated NMR spectra of the peptide over the trajectory is in excellent agreement with available experiments.

The quantum mechanical-free energy method that has been under development here is also yielding exciting insights into the nature of enzyme catalysis for the beta-lactamases.

## SIGNIFICANCE

Elucidation of the mechanism of protein folding has remained a scientific challenge for decades. Molecular dynamics simulation with full representation of solvent possesses a unique advantage to study protein folding due to its atomic-level resolution and accuracy. This method and associated simulation parameters (i.e., the force field) have been tested and refined thoroughly using smaller systems in comparison with many experimental results, although the results of our research may also offer a further critical test of their accuracy. Most proteins take milliseconds to seconds to fully fold, much longer than typical simulation scales, which are presently on the order of nanoseconds. Many methods have been proposed to circumvent this difficulty, including high temperature unfolding, efficient sampling such as LES, and long time dynamics using massive parallelism. These approaches are mutually complementary and cover different parts of the folding process. A combination of these methods can be extremely powerful.

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http://www.amber.ucsf.edu/amber

# Simulations of Global Climate Using a High-Resolution Atmospheric Model

*Philip Duffy, Bala Govindasamy, Jose Milovich, and Starley Thompson, Lawrence Livermore National Laboratory*

## RESEARCH OBJECTIVES

Our goal is to perform global climate simulations using a very high-resolution model of the atmosphere, thus improving the realism of the model and the quality of predictions on both global and regional scales.

## COMPUTATIONAL APPROACH

We run the CCM3 global atmospheric model at spectral truncations of T170 and T239. The corresponding grid cell sizes are ~75 km and ~50 km, respectively. This is in contrast to a grid size of ~300 km in typical global climate simulations. We use a version of this model known as CCM 3.10.11 (366physics), which achieves distributed memory parallelism using a combination of MPI-based message passing and multiple threading using OpenMP. The model physics were tuned to give good results at high resolution in collaboration with the model developers at the National Center for Atmospheric Research (J. Hack et al.).

## ACCOMPLISHMENTS

Using NERSC's IBM SP and supercomputers at Lawrence Livermore National Laboratory, we ran a global climate simulation at 50 km resolution, the highest spatial resolution ever used for a global climate simulation. Compared to a typical global climate simulation, this 50 km simulation has 32 times more grid cells and takes roughly 200 times longer to run. Our goal for the 50 km simulation is to evaluate how well the model simulates the present climate at this resolution. Thus far we have run about five simulated years; preliminary analysis of the results seems to indicate that the model is very robust to a large increase in spatial resolution.

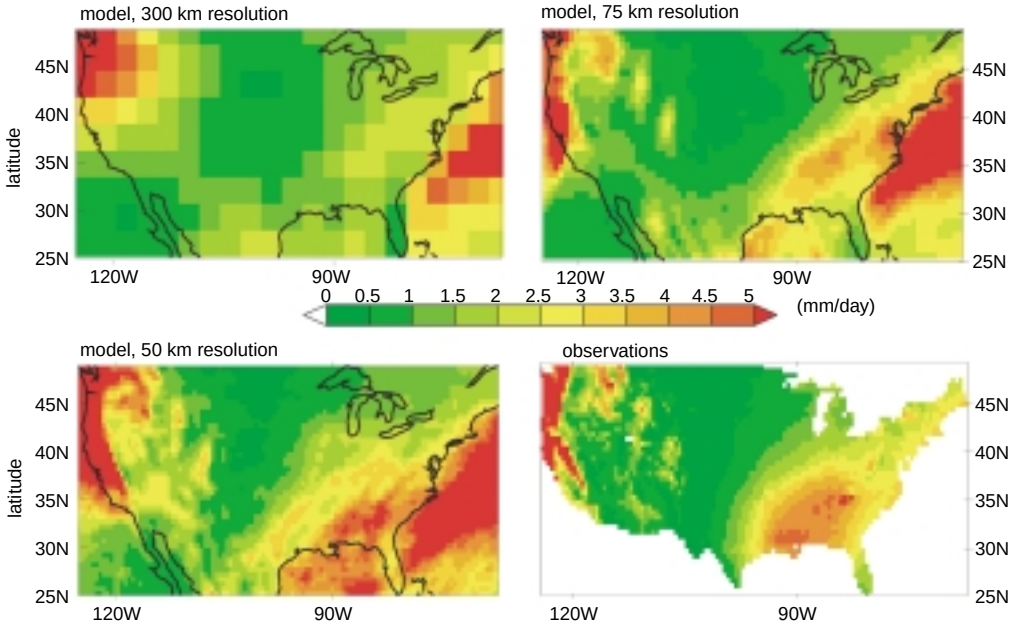
## SIGNIFICANCE

Global climate simulations are typically performed on a latitude-longitude grid, with grid cell sizes of about 300 km. Although simulations of this type can provide useful information on continental and larger scales, they cannot provide meaningful information on regional scales. Thus, coarse-resolution global climate simulations cannot provide information on many of the most important societal impacts of climate change, such as impacts on water resource management, agriculture, human health, etc. By using much finer spatial resolution, we hope to improve the realism of the models and produce better predictions of future climate, specifically of anthropogenic climate change, on both global and regional scales.

## PUBLICATIONS

P. B. Duffy, B. Govindasamy, J. Milovich, S. Thompson, and M. Wehner, "Simulation of global climate using a high resolution atmospheric general circulation model" (in preparation).

http://en-env.llnl.gov/cccm/




*Wintertime precipitation in the U.S. as observed and as simulated by our climate model at three different resolutions: 300 km, 75 km, and 50 km. As the model resolution becomes finer, the results converge towards observations.*

# Theoretical Study on Catalysis by Protein Enzymes, Ribosome, and Molecular Motors

*Martin Karplus, Harvard University*

## RESEARCH OBJECTIVES

This project's goal is to develop a greater understanding of the mechanisms involved in enzyme catalysis and related protein functions. We are studying the protein enzymes chorismate mutase, flavoxireductase, and aminopeptidase, and a nucleic acid enzyme, the hammerhead ribosome. We are also studying another class of enzymes known as molecular motors, which play important roles in bioenergy transduction and gene replication.

## COMPUTATIONAL APPROACH

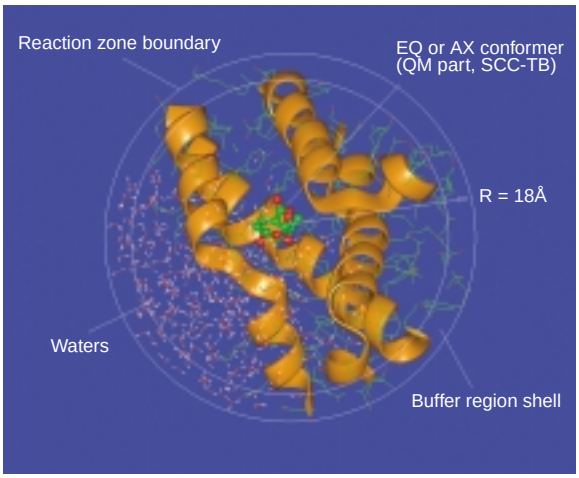
For active-site models in the gas phase, Gaussian98 and NWChem are used for *ab initio* or density functional calculations. To determine the catalytic mechanism in the presence of the enzyme environment, the CHARMM program (developed by the Karplus group) is used for a combined quantum and molecular mechanics (QM/MM) approach.

## ACCOMPLISHMENTS

We studied the role of tunneling for two proton transfer steps in reactions catalyzed by triosephosphate isomerase (TIM). The effect of tunneling on the reaction rate is less than a factor of 10 at room temperature; the tunneling became more important at lower temperatures. The imaginary frequency mode and modes having large contributions to the reaction path curvature were localized on the atoms in the active site, within 4 Å of the substrate. This suggests that only a small number of atoms close to the substrate and their motions directly determine the magnitude of tunneling.

In horse liver alcohol dehydrogenase (LADH) proton and hydride transfers, proton transfers proceeded in a virtually concerted fashion before hydride transfers. The catalytic efficiency of LADH was low for a pH below 5.5, and the hydride transfer was hardly affected for a pH between 5.5 and 8.1. Perturbation analysis of the QM/MM energies suggests a number of charged residues close to the active site as well as the phosphate groups in $NAD^+$ make important contributions to the energetics of proton and hydride transfer reactions.

Chorismate mutase (CM) acts at the first branch-point of aromatic amino acid biosynthesis and catalyzes the conversion of chorismate to prephenate. Two nonreactive conformers of chorismate were found to be more stable than the reactive pseudo-diaxial chair conformer in solution. When these inactive conformers were bound to the active site, they rapidly converted to the reactive chair conformer. This suggests that the enzyme binds the more prevalent nonreactive conformers and transforms them into the active form in a step prior to the chemical reaction.




*The model protein-substrate system used in the QM/MM molecular dynamics simulation of chorismate mutase (CM) based on the X-ray structure of yeast CM. During the molecular dynamics simulation, it was found that the inactive conformers were rapidly converted into the reactive chair conformation through the motion of active site residues; such a conversion was not observed in solution. Thus the results highlight the importance of enzyme dynamics in catalysis.*

## SIGNIFICANCE

Despite the growing availability of enzyme crystal structures, details of the chemical mechanisms employed by enzymes to achieve their catalytic efficiency remain elusive. This is mainly because the chemical events of bond formation and cleavage that define the reaction are exceedingly short and currently inaccessible to direct experimental measurement. It is also very difficult to probe directly the coupling between chemical events and conformational transitions with atomic details, which remains a major obstacle for understanding the working mechanism of molecular motors. Theoretical studies, therefore, are of great value for providing insights into these mechanisms.

## PUBLICATIONS

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# Computational Analysis of Genomic Sequence Data

*Daniel Rokhsar, Lawrence Berkeley National Laboratory and Joint Genome Institute*

## RESEARCH OBJECTIVES

We are developing, implementing, and applying parallel code for the assembly of whole genome shotgun sequence data, including constraints placed by the availability of paired end sequence. Genomes to be assembled include *Fugu rubripes*, the Japanese pufferfish, which has a 400 million base-pair (Mbp) genome; the 200 Mbp *Ciona intestinalis* genome; and the 2.6 billion base pair (Gbp) mouse genome. Other large animal, plant, and fungal genomes will be assembled in the future. We will then use parallel implementations of BLAST and other sequence comparison codes for the high-throughput analysis of genomic and other sequence data. Further development will include rapid parallel searches for short conserved elements.

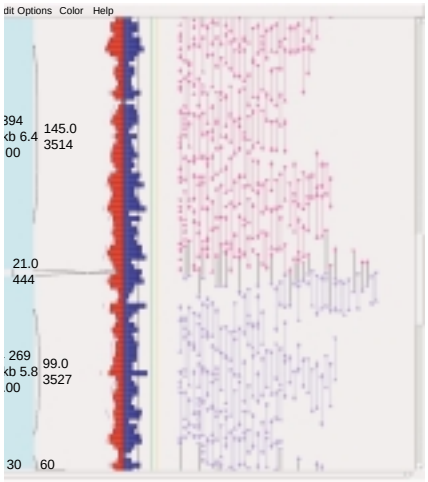
## COMPUTATIONAL APPROACH

We use custom parallel code to accomplish genome assembly. The overall plan has three phases: (1) rapid identification of overlaps between pairs of sequence fragments, (2) the construction of a linear layout of these fragments that is consistent with overlaps and pair-end information, and (3) the conversion of this layout into a consensus sequence. Based on the sequence coverage goals of the Joint Genome Institute sequencing effort, contigs of 50,000 bases or more are expected. Phase 1 is the most time consuming part of the project, and has been parallelized using MPI and tested on a 3× coverage mouse dataset. Phase 2 is memory intensive; it can be completed on a single IBM SP node, threaded over 16 processors, but requires large RAM. Phase 3 is embarrassingly parallel. We have developed a second large-scale assembler with an alternative Phase 2/3 division of labor, and we expect to use both implementations as needed depending on detailed aspects of datasets.

Sequence comparison will be carried out using an implementation of parallel BLAST ported to the IBM SP. Since 5,000 to 10,000 contigs are expected, these comparisons can be distributed across multiple processors in an embarrassingly parallel fashion. Similarly, comparisons of microbial genomes with one another can be straightforwardly parallelized.

## ACCOMPLISHMENTS

We have used the IBM SP to develop and test our newly developed large-scale genome assembly system, JAZZ, which reconstructs contiguous genome sequences by overlapping the short subsequences that can be determined using modern DNA sequencing technology. JAZZ self-consistently uses pair-end information in the construction of contigs, and produces ordered and oriented sequence scaffolds as output. An initial mouse genome assembly has been carried out. The test dataset consisted of mouse sequence fragments that, on average, cover each base of the mouse genome three times—a total of 14 million sequence fragments. We assembled these fragments into approximately one million 3,000-base-pair contiguous sequences. This assembly required over 100,000 hours of processor time, primarily for the fragment comparison step. We are now prepared to assemble future mammalian genome datasets, enabling public whole genome sequencing efforts.




*On the right, each line segment represents a genomic fragment whose sequence has been determined at each end (arrows). On the left, blue rectangles represent contiguous stretches of reassembled sequence. This visualization tool allows rapid inspection of the automated assemblies produced by JAZZ. The genome shown is that of the white rot fungus Phanerochaete chrysosporium.*

## SIGNIFICANCE

The availability of genomic sequences for a wide range of organisms allows unprecedented access to the fundamental parts-list-and-instructions for constructing these organisms, and allows comparison of these lists to uncover essential pathways for various bacterial and eukaryotic processes related to energy, the environment, and human susceptibilities. For example, the human and fish lineages diverged nearly 400 million years ago; direct comparison of their genomic sequence will reveal conserved (and therefore presumably functional) elements defining coding and regulatory sequences. Relatively small-scale comparisons of this sort have proven useful for identifying human genes; we expect the comparison of the human genome with that of a more distant vertebrate will highlight these conserved elements on a genomic scale.

## PUBLICATIONS

http://www.jgi.doe.gov

# Terascale Spectral Element Climate Dynamical Core

*Stephen Thomas, Richard Loft, and John Dennis,*
*National Center for Atmospheric Research*

## RESEARCH OBJECTIVES

The purpose of this project is to develop a scalable dynamical core for atmospheric general circulation models (GCMs).

## COMPUTATIONAL APPROACH

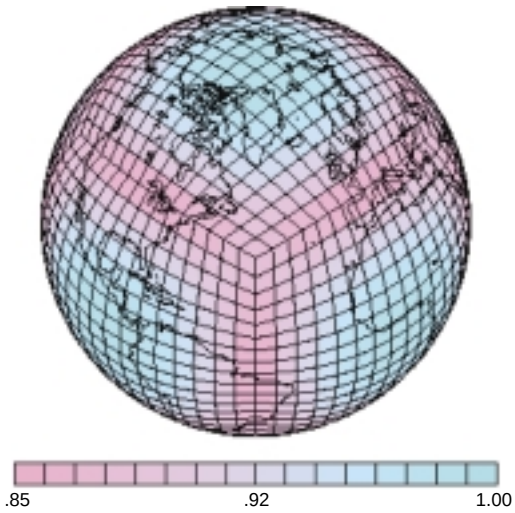
We are building a 3D primitive equations dynamical core for an atmospheric GCM. The time-discretization employs either a fully explicit or semi-implicit scheme. We hope to also implement a semi-Lagrangian advection scheme for tracer transport and possibly the full dynamics. The horizontal discretization is based on spectral elements, and the vertical uses a hybrid pressure coordinate with an energy and angular momentum conserving finite difference scheme.

## ACCOMPLISHMENTS

Traditionally, climate model dynamical cores have been based on the spectral transform method because the global spherical harmonic basis functions provide an isotropic representation on the sphere. In addition, it is trivial to implement semi-implicit time-stepping schemes, as the spherical harmonics are eigenfunctions of the Laplacian on the sphere, and the resulting Helmholtz problem is embarrassingly parallel in spectral space. Despite the lack of exploitable parallelism at relatively low climate resolutions, spectral models have exhibited high performance on parallel vector architectures. Achieving high simulation rates on microprocessor clusters at these resolutions has proven difficult due to the communication overhead required by data transpositions and the lack of cache data locality.

As an alternative numerical method, spectral elements maintain the accuracy and exponential convergence rate exhibited by the spectral transform method. Spectral elements also offer several computational advantages on microprocessors. The computations are naturally cache-blocked, and derivatives may be computed using nearest-neighbor communication. An explicit version of a spectral element atmospheric model has demonstrated linear scaling on a variety of parallel machines. Unfortunately, the explicit model suffers from severe time-step restrictions.

We have developed an efficient semi-implicit formulation of this spectral element model. Numerical innovations include a weak formulation of the governing equations and a block-Jacobi preconditioned conjugate gradient solver that is latency tolerant. The parallel implementation is a true hybrid MPI/OpenMP code, and the entire model time-step is threaded over elements using an SPMD parallel region. Cache-blocking in combination with looping over model layers between thread synchronizations for MPI calls results in a per node execution rate that is 25% of peak. We have achieved 361 Gflop/s sustained performance for this model on the NERSC IBM SP, qualifying us as finalists for the 2001 Gordon Bell award.




*Cubed-sphere spectral element grid.*

## SIGNIFICANCE

Scientific progress in climate modeling depends more on accelerating the integration rate than the resolution. A major goal of our work is to demonstrate that a climate simulation rate of over 100 years per wall clock day is possible on microprocessor-based clusters. This simulation rate is an order of magnitude faster than existing climate models and would represent a major advance in geophysical fluid dynamics.

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S. J. Thomas and R. D. Loft, "Parallel spectral element atmospheric model," in *Proceedings of Parallel CFD 2000 Conference, Trondheim, Norway, May 22–25, 2000*, pp. 331–337 (Elsevier North-Holland, 2001).

http://www.scd.ucar.edu/css/staff/thomas

# Coupled Climate/Carbon Cycle Modeling on Massively Parallel Computers

*Starley Thompson, Philip Duffy, Jose Milovich, Bala Govindasamy, Peter Eltgroth, and Art Mirin, Lawrence Livermore National Laboratory*
*Aaron Herrnstein, University of California, Davis*
*Christine Delire, University of Wisconsin*

## RESEARCH OBJECTIVES

Our overall goal is to produce the first comprehensive coupled climate/carbon cycle model in the U.S. This research will allow better predictions of future climate, because feedback effects of climate change on absorption of carbon by the ocean and terrestrial biosphere—which are ignored in present U.S. climate models—will be taken into account. This model will be more useful to policymakers than present climate models because it will use $CO_2$ emission rates, rather than atmospheric $CO_2$ concentrations, as the fundamental input.

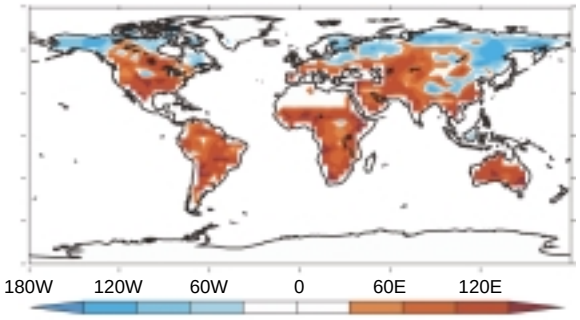
## COMPUTATIONAL APPROACH

All the computational models we employ use a Eulerian discretization approach. The POP ocean model uses finite differences on a structured 3D mesh. Its discretization allows the use of any locally orthogonal horizontal grid, which, for example, allows the Arctic ocean to be resolved without the standard problems of convergence of meridians at the North Pole. The CCM3 atmospheric model implements a spherical harmonics-based spectral formulation with a latitude/longitude transform grid and uses a terrain-following coordinate in the vertical dimension. We are currently using two ocean biogeochemistry (OBGC) models, the LLNL OBGC model and the PICSES OBGC model, as well as the IBIS terrestrial biospheric model.

## ACCOMPLISHMENTS

*High-resolution global climate simulations:* We are running three experimental simulations at very high spatial resolution. The first is a simulation of the period 1979–1989 performed at T239 spectral truncation (50 km resolution). This is the highest-resolution long-term global climate simulation ever attempted. The second is a pair of simulations at slightly coarser resolution (T170 truncation; 75 km resolution) for a doubled-$CO_2$ climate and a control simulation of the present climate. These are the highest-resolution runs ever performed of anthropogenic climate change. Preliminary results show that in simulations of the present climate, some features become more realistic as spatial resolution becomes finer; but the simulated increase in temperature in response to a given increase in atmospheric $CO_2$ does not seem to be sensitive to model resolution.

*Coupled climate and terrestrial biosphere simulations:* The Community Climate Model 3 (CCM3) coupled to the Integrated Biosphere Simulator (IBIS 2) was used to perform a 16-member ensemble of present day simulations with observed sea surface temperatures (SSTs) for the period 1979–1992. Simulated interannual variations in terrestrial carbon uptake have good positive correlation with inferred uptake from observations. Nearly 65% of interannual variability is caused by unforced climate variability not related to variations in SSTs. This unforced interannual variability in the uptake is caused primarily by the unforced variability in net primary productivity, which is driven by variability in precipitation and temperature.




*The correlation between interannual variations in carbon dioxide uptake by vegetation and interannual variations in precipitation as simulated by a coupled model of climate and terrestrial ecosystems. Carbon uptake is enhanced in wet years (red areas) since most of the world's vegetation is water-limited. Only in cold regions do thermal limitations dominate (blue areas).*

## SIGNIFICANCE

A comprehensive coupled climate/carbon cycle model will allow us to directly assess the climatic impact of specified rates of burning of fossil fuels, because it will use $CO_2$ emission rates (not atmospheric $CO_2$ concentrations) as its fundamental input variable. The model will also allow us to improve our fundamental understanding of the coupling between climate change and Earth's carbon cycle, since it is known that both the marine and terrestrial components of the carbon cycle are sensitive to climate change.

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http://www-pcmdi.llnl.gov/cccm/

# Climate Change Prediction with New Generation Models: Moderate and High Resolution Studies

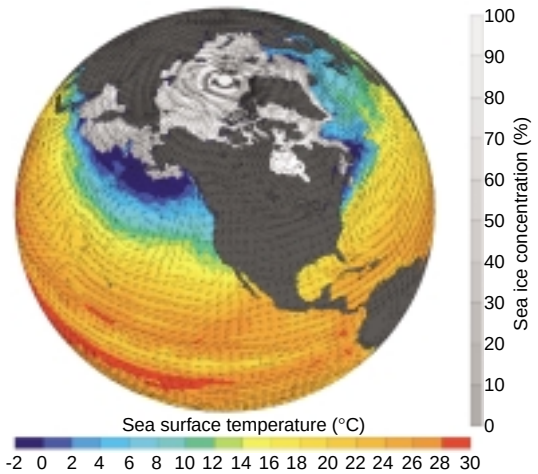
*Warren Washington and Gerald Meehl, National Center for Atmospheric Research*
*Bert Semtner, Naval Postgraduate School*
*John Weatherly, U.S. Army Cold Regions Research and Engineering Laboratory*

## RESEARCH OBJECTIVES

The main purpose of this research is to use the Parallel Climate Model (PCM) and the Community Climate System Model version 2 (CCSM2) for studies of anthropogenically forced climate change simulations with higher resolution and more detailed model components. Because it is difficult to separate anthropogencic climate change from natural climate variability, it is necessary to carry out ensembles of simulations in order to find the statistically significant climate change signal.

## COMPUTATIONAL APPROACH

(1) With collaborators, we have developed an ocean component that uses the finite difference Parallel Ocean Program (POP) with a displaced North Pole. This model was modified from the original average resolution of 2/3° latitude and longitude to allow increased latitudinal resolution near the equator of approximately 1/2°. (2) The sea ice model component is entirely new. The thermodynamic part of the model uses the physics from C. Bitz's University of Washington ice model. It allows for five or more ice thickness categories and elaborate surface treatment of snow and sea ice melt physics. The elastic-viscous-plastic physics uses the E. Hunke and J. Dukowicz approach to the solution of the ice dynamics. (3) The atmospheric component is the massively parallel version of the NCAR Community Climate Model version 3 (CCM3). This model includes solar and infrared radiation, boundary physics, and precipitation physics. (4) The coupler's design allows the component models to execute concurrently as separate executables, or sequentially within a single executable, with the information exchange achieved by message passing (MPI). Since the component grids are different, there is an interpolation scheme for passing information between the atmosphere component grid and the ocean/sea ice grid, which has been designed to run efficiently on distributed memory architectures. Chris Ding and collaborators at NERSC have improved the performance of the coupler on parallel computers.




*This figure depicts a short simulation from the Parallel Climate Model (PCM). For the atmosphere, the figure shows vectors depicting the winds in the lowest model layer, and shows the sea level pressure as lines of constant pressure. The surface temperatures are shown in color, and the sea ice is shown in grayscale. (Illustration: Gary Strand, NCAR)*

## ACCOMPLISHMENTS

During this past year, we completed many climate change simulations. Some of the simulations are of "business as usual" scenarios, in which there are no constraints on the use of greenhouse gases and aerosols. We have also performed various stabilization simulations. In both cases we completed five simulations that have different initial conditions. Using an ensemble is essential for evaluating the natural variability and to separate the climate change signal from the climatic noise. The societal interest is increasingly on regional changes.

## SIGNIFICANCE

The DOE Climate Change Prediction Program is focused on developing, testing and applying climate simulation and prediction models that stay at the leading edge of scientific knowledge and computational technology. The intent is to increase dramatically both the accuracy and throughput of computer model-based predictions of future climate system response to the increased concentrations of greenhouse gases. The PCM and CSM simulations have been highlighted in many parts of the latest report from the Intergovernmental Panel on Climate Change (IPCC).

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http://www.cgd.ucar.edu/pcm

# Sources of Variability in Coupled General Circulation Models

*Michael Wehner, Justin J. Hnilo, James Boyle, Benjamin D. Santer, Karl Taylor, and Balasubramanian Govindasamy, Lawrence Livermore National Laboratory*

## RESEARCH OBJECTIVES

In the Atmospheric Model Intercomparison Project (AMIP), an atmospheric general circulation model (AGCM) is forced with observed sea surface temperatures (SSTs) and sea ice in the hopes that the model will mimic observed atmospheric behavior. Results from participant modeling groups in AMIP I and II show that these prescribed boundary conditions appear to be sufficient in supplying enough information to an AGCM to allow it to reasonably represent recent atmospheric behavior. Some concerns have been raised about the use of prescribing SSTs in a model integration. For example, the specified SSTs might alter the spatial or temporal variability of the simulation compared to a coupled run and presumably reality. This effect is expected to be most prominent in the mid to high latitudes.

This research directly addresses this issue by using the SSTs from the Coupled System Model (CSM) run, which is a fully coupled Ocean-Atmosphere General Circulation Model (OAGCM), as boundary conditions to force the identical atmospheric component alone. Quantifiable differences between the two runs will be attributable in part to the use of prescribing SSTs (as a representation of the ocean) versus using a fully coupled (OAGCM) run. A simple yet important question that we can quantify and answer is "Does the ocean component in this model act to diminish or enhance atmospheric variability when compared to a prescribed SST run and observations?" This research will highlight variables and regions of greatest magnitude and variability changes.

## COMPUTATIONAL APPROACH

This model is a spectral transform atmospheric general circulation model. One-dimensional message passing, although simple, limits its scalability to 64 processors at the resolutions we are interested in. We are using the Community Climate Model (CCM 3.6.6), the state of the art in general circulation models.

## ACCOMPLISHMENTS

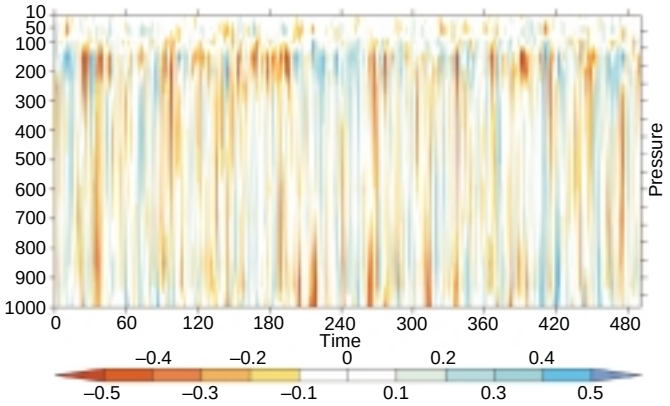
We completed assembly of four 41-year, T42 resolution ($128 \times 64 \times 17$) CSM SST-driven AMIP II style integrations. Monthly data have been rewritten and archived on HPSS. Boundary condition SSTs for model continuations for the next 40+ years have been processed. A new resolution version (T239) of this atmospheric model has been ported to the IBM SP and has been shown (in some preliminary runs) to be stable. We look forward to using this new version in continuing research.

## SIGNIFICANCE

The National Center for Atmospheric Research's coupled model known as CSM is the de facto national climate model. In the Program for Climate Model Diagnosis and Intercomparison (PCMDI) at LLNL, a major thrust is being undertaken to diagnose this model. Currently, only the atmospheric portion of the model, known as CCM3, runs on moderately parallel computing systems. Hence, in addition to our activities in analyzing the CSM runs made at NCAR, we wish to augment these data with studies of its atmospheric component.

The studies on atmospheric variability relate directly to the variability obtained in the fully coupled model. It is vital to our understanding of climatic change to characterize a model's natural variability. This study will contribute to our knowledge of the sources of both observed and modeled variability.

Higher resolution models (T239) offer one the unique opportunity to resolve, as an example, the California central valley, allowing for unprecedented levels of large to regional scale model diagnostics. The results of these model diagnostics will help modelers understand the limitations of certain parameterizations and lead to next-generation model improvements.




*Time series of the differences in global temperature anomalies from an uncoupled to a coupled mode (AMIP–CSM). Global values between –0.1 and +0.1 are not colored to allow for ease of comparison; values are derived over 491 months.*

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M. F. Wehner, "Determination of the sampling size of AGCM ensemble simulations," Climate Dynamics **16**, 321 (2000).

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http://www-pcmdi.llnl.gov/mwehner/amip2/amip2_n.html

# Numerical Tokamak Turbulence Project (Plasma Microturbulence Project)

*B. Cohen, A. Dimits, G. Kerbel, D. Shumaker, and W. Nevins, Lawrence Livermore National Laboratory*
*W. Lee, G. Hammett, and Z. Lin, Princeton Plasma Physics Laboratory*
*J. N. Leboeuf and R. Sydora, University of California, Los Angeles*
*V. Lynch, Oak Ridge National Laboratory*
*Y. Chen, S. Parker, and C. Kim, University of Colorado*
*P. Snyder, R. Waltz, Y. Omelchenko, and J. Candy, General Atomics*
*W. Dorland and S. Novakovski, University of Maryland*
*D. Ross, University of Texas*

## RESEARCH OBJECTIVES

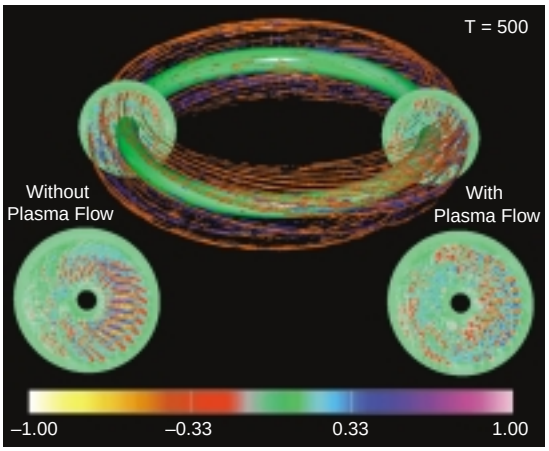
The primary research objective of the Plasma Microturbulence Project (PMP, a follow-on to the Numerical Tokamak Turbulence Project, NTTP) is to develop a predictive ability in modeling turbulent transport due to drift-type instabilities in the core of tokamak fusion experiments, through the use of three-dimensional kinetic and fluid simulations and the derivation of reduced models.

## COMPUTATIONAL APPROACH

We utilize three main classes of simulation algorithms to study core tokamak microturbulence: gyrokinetic particle-in-cell (GK PIC), 5D Eulerian gyrokinetic (EGK), and to a lesser extent gyro-Landau-fluid (GLF). In each case, the simulation domain can be either global or annular (flux tube). (1) The GK PIC simulations are based on PIC methods for the self-consistent solution of Poisson's equation (or Maxwell + Poisson in electromagnetic extensions) and plasma equations of motion, and domain decomposition methods to run efficiently in parallel. (2) The EGK algorithm solves for the 5D distribution function and Maxwell's equations on a mesh that includes two velocity space coordinates (energy and magnetic moment). (3) The GLF algorithm is most similar to conventional fluid dynamics approaches, since a set of fluid moments of the gyrokinetic equation are solved together with Maxwell's equations.

## ACCOMPLISHMENTS

There has been significant progress in two areas of code development: developing efficient simulation algorithms for electromagnetic simulations with kinetic electrons, and developing a global continuum Vlasov model. Our flux-tube continuum Vlasov code has undertaken simulations of both electron and ion temperature gradient instability with electromagnetic effects, and this code has a growing user community. We have developed a toroidal electromagnetic code with kinetic electrons that works well at low plasma $\beta$, and a hybrid fluid electron/gyrokinetic ion code that works well at finite $\beta$. We have continued global gyrokinetic simulations of DIII-D plasma discharges that emulate the correlation reflectometry diagnostic in the experiment with good success. We have extended our database of flux-tube gyrokinetic simulations quantifying the dependence of the transport of ion thermal flux on magnetic shear, safety factor, E × B velocity shear, and toroidal velocity shear. Flux-tube gyrokinetic simulations and a continuum Vlasov simulation have revealed the inadequacy of the approximate rule that shear in the E × B flow equal to the typical linear growth rate is needed to stabilize drift-type instabilities.




*Global simulation of ion-temperature-gradient turbulence in a tokamak showing the influence of sheared flow on moderating the turbulence. Contours of density fluctuations. (Figure by Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang, and R. B. White, Princeton Plasma Physics Laboratory)*

## SIGNIFICANCE

NTTP/PMP simulations are having increasing success in agreeing with experiments and are leading to a deeper understanding of anomalous transport in current experiments. Since controlling the energy transport has significant leverage on the performance, size, and cost of fusion experiments, reliable simulations can lead to significant cost savings and improved performance in future experiments.

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http://www.er.doe.gov/production/cyclone/

# Simulation of Heavy Ion Fusion and Particle Accelerators

*Ronald Davidson, W. Wei-li Lee, Hong Qin, and Edward Startsev, Princeton Plasma Physics Laboratory*

## RESEARCH OBJECTIVES

This project will enable us to perform realistic particle simulations for collective processes and instabilities, such as stable beam oscillations and electron-ion two-stream instabilities, in high-intensity particle beams. Utilizing the large-scale computing power provided by the IBM SP computers, we will be able to carry out 3D multi-species nonlinear particle simulations based on the self-consistent Vlasov-Maxwell equations. The newly developed beam equilibrium stability and transport (BEST) code will be used and will be further developed to include more numerical capabilities and physics contents.

## COMPUTATIONAL APPROACH

We use a 3D multi-species nonlinear perturbative particle simulation method to simulate the collective processes and instabilities in high-intensity particle beams. The perturbative particle simulation method used in the BEST code solves the fully nonlinear Vlasov-Maxwell equations and offers a significantly reduced noise level for the problems being studied. The BEST code advances the particle motions using a leapfrog method, and solves Maxwell's equations in cylindrical geometry. For those fast particle motions which require much larger sampling frequency than the frequency of the mode being studied, the code uses an adiabatic field pusher to advance the particles many time steps without solving for the perturbed fields.

## ACCOMPLISHMENTS

In FY 2001 we carried out large-scale particle simulations for the two-stream instability and pressure anisotropy instability. The IBM SP provided the necessary computing power to simulate these instabilities for realistic accelerator parameters. For example, we were able to push $4 \times 10^{11}$ particle steps to simulate the electron-proton two-stream instability for the Proton Storage Ring at Los Alamos National Laboratory. Our simulation results agreed with the experimental results in terms of eigenmode structures, eigenfrequencies, and growth rates. Our simulations also suggested possible approaches to avoid the instability so that higher proton beam intensity can be achieved.

## SIGNIFICANCE

High-intensity particle beams have a wide range of applications, ranging from basic scientific research in high energy and nuclear physics, to applications such as heavy ion fusion and spallation neutron source. Of particular importance at the high beam currents of practical interest are the collective processes and instabilities. Because the governing equations, the nonlinear Vlasov-Maxwell equations, are intrinsically difficult to solve analytically, our understanding obtained from large-scale computer simulations directly impacts on the quality of the high-intensity particle beams and thus the success of the scientific efforts mentioned above.

## PUBLICATIONS

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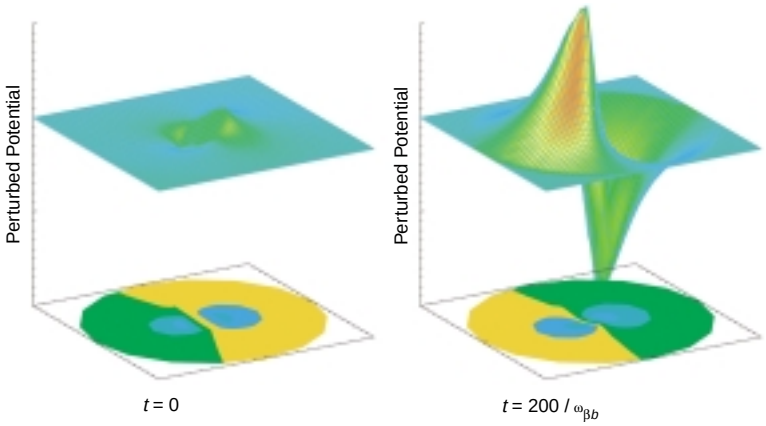
http://w3.pppl.gov/~nnp/best.htm




*Nonlinear δf simulation of electron-proton two-stream instability for the Proton Storage Ring at LANL. When a background electron component is introduced, the l = 1 dipole mode can be destabilized for a certain range of axial wavenumber and a certain range of electron temperature. Simulation results showed that the instability growth rate increases with increasing beam current and decreases with increasing momentum spread. In the simulation, electrons, protons, and self-fields were self-consistently followed for $4 \times 10^{11}$ particle time-steps.*

# University of Maryland Fusion Energy Research

*Parvez Guzdar, Bill Dorland, James Drake, Adil Hassam, Robert Kleva, and Sergei Novakovski, University of Maryland*

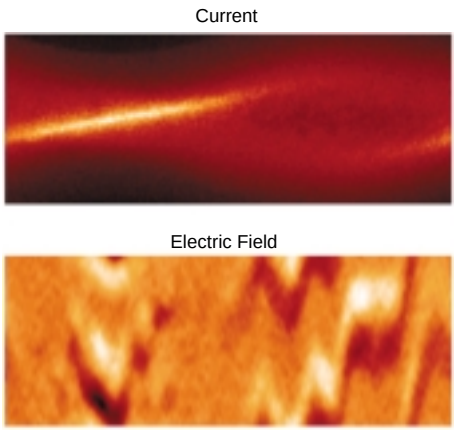
## RESEARCH OBJECTIVES

The Maryland Theory and Computational Physics Magnetic Fusion Energy Program focuses on (1) 3D simulation of particle, ion, and electron energy transport in the core and edge region of tokamak plasmas using the two-fluid Braginskii code Edge3D and the electromagnetic gyrokinetic code GS2; (2) 3D simulation of high-$\beta$ disruptions and sawtooth crashes for tokamak plasmas using the toroidal resistive magnetohydrodynamics (MHD) code TORMHD; (3) 2D and 3D simulations of novel centrifugal confinement devices using MHD codes; and (4) 2D and 3D full-particle, hybrid, and two-fluid simulations of magnetic reconnection.

## COMPUTATIONAL APPROACH

The GS2 code is based on a continuum treatment of the gyrokinetic equations. The second-order accurate algorithm is comprised of an implicit treatment of the linear dynamics, an explicit, pseudo-spectral treatment of the nonlinear terms, and an Adams-Bashforth integrator in time. The gyrokinetic problem involves the usual 3D spatial grid, as well as a 2D velocity space grid, for a total of five dimensions. The Edge3D code is suitable for exploring transport in the colder edge regions of fusion plasmas. It is based on a fourth-order finite difference scheme with a trapezoidal leapfrog scheme for time stepping.

The TORMHD code solves the MHD equations on a toroidal grid. The basic computational scheme is the same as in Edge3D.




*Results of a 3D particle simulation of magnetic reconnection using 670 million particles. The top panel shows the strong electron current (in the out-of-plane direction) generated during reconnection. The bright region cuts across the magnetic x-line. The bottom panel shows the intense electric fields self-generated by the plasma in a plane perpendicular to that in the top figure and cutting through the region of strongest current. The adjacent regions of positive and negative polarity of the electric field are the signature of double layers, which are localized regions of intense electric field which scatter and heat electrons. Such layers are expected to be a prolific source of energetic electrons during magnetic reconnection in fusion and astrophysical plasmas.*

The P3d code has been developed to explore magnetic reconnection or other nonlinear plasma phenomena. P3d can be run as a two-fluid, hybrid (particle ions and fluid, finite-mass electrons) or a full (particle electrons and ions) model. The full-particle version has been run with up to 1 billion particles to explore 3D collisionless magnetic reconnection.

## ACCOMPLISHMENTS

The nonlinear gyrokinetic finite-$\beta$ studies of electron temperature gradient driven instabilities have established the existence of long radial "streamers" which strongly enhance the transport from these short-wavelength instabilities over what had been previously predicted. Simulations of tokamaks with toroidal flows have demonstrated that these flows have a stabilizing influence on sawteeth.

The release of magnetic energy during magnetic reconnection in nature and also in some laboratory experiments (sawteeth in tokamaks) is typically much faster than can be explained by resistive MHD models. We have shown that at the small spatial scales where magnetic reconnection occurs, the MHD model breaks down. At these scales, whistler and kinetic Alfvén waves dominate the dynamics. The dispersive property of these waves causes reconnection to remain fast, consistent with observations, even when the out-of-plane magnetic field is large and/or the system size is very large. The new model resolves the long-standing discrepancy in the energy release time between magnetic reconnection models and observations.

## SIGNIFICANCE

The goal of building an efficient fusion reactor is best served by understanding what processes control confinement in present-day devices and then proposing techniques for improving confinement properties. Work on magnetic reconnection and anomalous transport has spin-off applications in space and astrophysical plasma applications.

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http://www.ireap.umd.edu/Theory/research.htm

# 3D Extended MHD Plasma Simulation with Multiple Levels of Physics

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## RESEARCH OBJECTIVES

The M3D (Multilevel 3D) Project consists of a multilevel comprehensive plasma simulation code package and applications of various levels of the code to increasingly more realistic fusion problems. M3D is capable of describing the nonlinear behavior of large-scale instabilities in most every magnetic fusion energy confinement configuration, including tokamaks, spherical tokamaks, stellarators, spheromaks, reversed field pinch, and field-reversed configuration. Many phenomena of interest require a plasma description that includes some kinetic effects, and thus the need for the multi-level description.

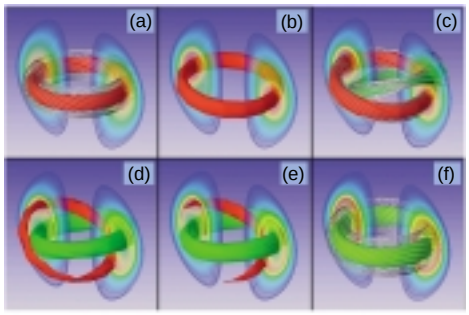
## COMPUTATIONAL APPROACH

The M3D code is basically a magnetohydrodynamics (MHD) code which implies a fluid description of the plasma. However, it is well known that the fluid model of a plasma leaves out many important effects, for example, due to the long-mean-free-path particle orbits and some wave-particle resonant effects. For more realistic simulations, the key factor that determines the degree of realism and also the corresponding computational requirements is the phase-space resolved in the simulation. Thus, the M3D multilevel physics code package has options to resolve increasingly larger phase-spaces, which are thus increasingly more realistic. To resolve velocity space, and hence kinetic effects, we use the $\delta f$ particle method, rather than a Vlasov phase-space fluid model, since as the dimensionality increases, the former becomes much more efficient than the latter model.

## ACCOMPLISHMENTS

*Internal disruption events in spherical tokamaks:* We have demonstrated that the spherical tokamak will be unstable to a catastrophic internal instability when the current is too broad and when the central safety factor passes through unity. There is another regime involving double tearing that can also be unstable during current ramp-up. These simulation results show good agreement with recent National Spherical Torus Experiment (NSTX) results.

*Flux surfaces and ballooning modes in stellarators:* The M3D code has been extensively applied to the quasi-axisymmetric National Compact Stellarator Experiment (NCSX) stellarator design. Resistive simulations, initialized with VMEC equilibria, allow the magnetic field to reconnect and develop islands. Comparisons with equilibria generated with the PIES code are under way, as are studies showing the nonlinear evolution of ballooning modes once the linear stability threshold is exceeded.




*Time sequence of a simulated "reconnection event" in the NSTX at PPPL. Red and green iso-surfaces of constant pressure are shown. Some frames also show select magnetic field lines before, during, and after the reconnection process. The initial (red) high pressure region has been expelled from the center and replaced by a (green) lower pressure region in this spontaneous, self-regulating event.*

*Pressure tensor effects on the stability of tearing modes:* It was shown that anisotropic pressure effects strongly influence the dynamics and stability of toroidally confined plasmas through the parallel viscous stresses. Inclusion of these effects in the plasma description was shown to greatly influence the stability and evolution of resistive modes.

*Nonlinear kinetic stabilization of tilting modes in the field reversed configuration:* The global stability of the field-reversed configuration (FRC) has been investigated using fluid electron and kinetic ion simulations. It was shown that the resonant interaction of the tilting mode with ions for which the Doppler-shifted wave frequency matches the betatron frequency is essential for describing the saturation of that mode.

## SIGNIFICANCE

The M3D code is one of two major extended MHD codes in the nation, the other being NIMROD. Extended MHD goes well beyond the standard MHD model to greatly improve the realism of plasma model by using increasingly more realistic physics models, including various levels of hybrid particle/fluid models. In a few years, the realism is expected to reach such a level that the fundamental device-scale nonlinear dynamics of magnetized plasma configurations with parameters close to fusion-relevant regimes can be simulated.

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http://w3.pppl.gov/~wpark/pop99

# 3D Gyrokinetic Particle Simulation of Turbulence and Transport in Fusion Plasmas

*W. W. Lee, Z. Lin, W. M. Tang, J. L. V. Lewandowski, W. Wang, and S. Ethier, Princeton Plasma Physics Laboratory*

## RESEARCH OBJECTIVES

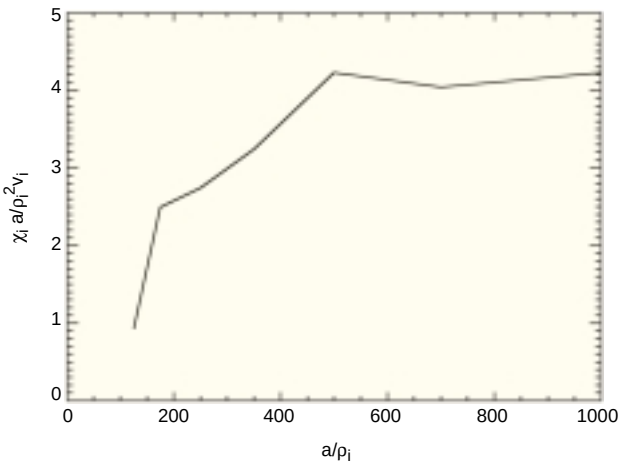
Our objective is improvement of the existing 3D Gyrokinetic Toroidal Code (GTC) by using split-weight $\delta f$ and hybrid schemes for the electrons for studying the trapped particle and finite-$\beta$ effects. The improved GTC code will be used for studying neoclassical and turbulent transport in tokamaks and stellarators as well as for investigating hot-particle physics, toroidal Alfvén modes, and neoclassical tearing modes.

## COMPUTATIONAL APPROACH

The basic approach for transport studies in tokamaks and stellarators is the gyrokinetic particle-in-cell method. GTC, in general geometry with 3D numerical equilibria, is written in Fortran 90 with MPI/OpenMP and is scalable on MPP platforms. The inclusion of the vital electron dynamics makes the code computation-intensive because of the mass disparity between the electrons and the ions.

## ACCOMPLISHMENTS

We have carried out gyrokinetic particle simulation studies on turbulent transport using GTC and have gained substantial understanding of the zonal flow physics. For example, the interplay between the ion temperature gradient (ITG) driven turbulence, zonal flow generation, and the collisional effects in the simulation is shown to rise to the bursting behavior observed in Tokamak Fusion Test Reactor (TFTR) experiments. A full-torus simulation of turbulent transport in a reactor-sized plasma indicates a more favorable scaling of transport driven by ITG modes as the size of the plasma increases. Gyrokinetic calculations of the neoclassical radial electric field in stellarator plasmas have also been carried out with the GTC code, which is part of the PPPL's effort for designing the next generation of stellarators. In addition, we have developed several versions of the split-weight schemes for the electrons to account for the trapped-particle and finite-$\beta$ effects.




*A full-torus simulation of turbulent transport scaling shows that transport driven by microscopic-scale fluctuations (ITG modes) in present devices can change character and transition from Bohm-like scaling ~ $(\rho_i v_i)$ to Larmor-orbit-dependent "gyro-Bohm" scaling ~ $(\rho_i v_i)(\rho_i/a)$.*

## SIGNIFICANCE

A key issue in designing a fusion reactor is the realistic assessment of the level of turbulent transport for reactor-grade plasma conditions. Up until very recently, this has been done by extrapolating to larger reactors the transport properties observed in smaller experimental devices. This approach relies on models of transport scaling that have often stirred debates about reliability. Taking advantage of the power recently accessible in new supercomputer capabilities, we have been able to take a major step forward in understanding turbulent transport behavior in reactor-sized plasmas by using direct numerical simulations. These advanced simulations have just become feasible because of the recent development of better physics models and efficient numerical algorithms, along with the newly available 5 teraflop/s IBM SP at NERSC.

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# NIMROD: Extended Magnetohydrodynamic Modeling for Fusion Experiments

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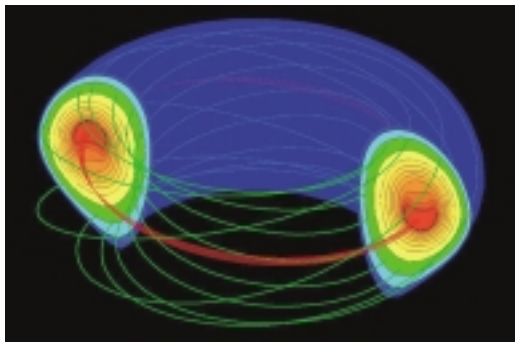
*Carl Sovinec, University of Wisconsin, Madison*
*Rick Nebel and Tom Gianakon, Los Alamos National Laboratory*
*Charlson Kim and Scott Parker, University of Colorado, Boulder*
*Eric Held, Utah State University*

## RESEARCH OBJECTIVES

The goal of this research is to develop a code which provides both flexibility in the physics, by using two-fluid or magnetohydrodynamic (MHD) models with analytic or gyrokinetic closures, and flexibility in the geometry, allowing for studies of any axisymmetric fusion concept, no matter how complicated the geometric configuration.

## COMPUTATIONAL APPROACH

The NIMROD code uses the extended MHD model to simulate the electromagnetic plasma behavior. The code has a time-split, semi-implicit advance and a combined finite element/Fourier series spatial representation. A major advance in the past year has been the generalization of the NIMROD code to use higher-order Lagrangian elements. This algorithm has been designed to run on massively parallel computers, while being able to handle the extreme stiffness of MHD problems in fusion plasmas. Normal modes of the system propagate across the domain in times that are orders of magnitude smaller than the time scales of the instabilities that we wish to study. Therefore, we have paid particular attention to avoiding numerical dissipation in the part of the algorithm associated with wave propagation. We have also paid considerable attention to ensure that truncation errors do not lead to unphysical coupling of compressional and shear waves.



*Simulation of a sawtooth crash that occurred during DIII-D shot 86144. NIMROD solves the time-dependent resistive MHD equations. Both pressure contours and magnetic field lines are shown. The field lines are color coded with the pressure value. The nonlinear simulation was carried out with a Lundquist number of $S = 10^7$. Calculations of this type demonstrate significant progress toward performing numerical simulations with experimentally realistic values of important parameters.*

## ACCOMPLISHMENTS

Extensive simulations of spheromak formation using NIMROD show that the spheromak does not have large regions of closed flux surfaces, but rather is chaotic over most of its domain. Results of the simulations agree well with many experimental observations. Simulations of the stabilization of tearing modes using NIMROD show that an important aspect of stabilization is the localization of the rf current source. Because realistic current sources cannot be perfectly localized, their effectiveness may not be as great as analytic theory predicts. Simulations with NIMROD show that a new heuristic model for the electron and ion stress tensors gives many of the effects analytic theory predicts, yet avoids many of the numerical problems that more rigorous closures give. The new closure allows for more realistic simulations of neoclassical tearing modes to be performed.

We are in the process of incorporating energetic particle effects into nonlinear MHD simulations. This has involved development of a finite element formulation of $\delta f$ particle-in-cell simulation. We now have $\delta f$ particles evolving in the time varying NIMROD fields and are calculating the energetic perturbed pressure. As an intermediate step, we are running a linear eigenmode in NIMROD and using the energy exchange between the particles and the MHD eigenmode to determine linear growth or damping. This is done by scaling the MHD field quantities by an appropriate factor, each time step representing the energy exchange between the particles and the MHD fields.

## SIGNIFICANCE

The NIMROD code is designed to do nonlinear, initial-value simulations of long-wavelength phenomena in fusion-reactor-relevent plasmas. These phenomena severely constrain the operating regime of fusion experiments, and improved understanding should lead to a better approach to providing fusion energy. Our development initiatives represent a consensus based on community feedback, especially feedback from the experimental community.

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http://www.nimrodteam.org

# Plasma Confinement, Stability, Heating, and Optimization in Stellarators and Tokamaks

*Donald A. Spong, Vickie Lynch, Steven Hirshman, Ben Carreras, Phil Ryan, and Wayne Houlberg, Oak Ridge National Laboratory*

## RESEARCH OBJECTIVES

The ORNL Fusion Theory Group is addressing the major scientific issues relating to the magnetic confinement of hot plasmas in both axisymmetric (tokamak) and non-axisymmetric (stellarator) devices. Specific areas of research include stellarator optimization and physics, toroidal plasma turbulence, anomalous transport, rf antenna design, and physics databases for future burning plasma experiments.

## COMPUTATIONAL APPROACH

(1) *Stellarator optimization:* The plasma optimization uses a Levenberg-Marquardt algorithm. The control variables are the coefficients of a Fourier expansion for the shape of the outermost closed magnetic flux surface. The coil optimization uses the minimization of the normal magnetic field component on the outer magnetic plasma surface as a target. We are currently merging the plasma and coil optimizations into a single code. (2) *Stellarator transport and heating:* Collections of particles are followed by solving coupled ordinary differential equations in time on parallel processors. The time integration is periodically stopped and random changes made in the particles' velocities to simulate inter-particle collisions. (3) *Stellarator drift kinetic solver:* This model uses a variational procedure to obtain upper and lower bounds on the entropy production rates for plasmas confined in 3D configurations. This project is developing new representations for the pitch angle dependence of the distribution function (B-splines instead of Legendre polynomials) and also converting over to band and iterative matrix solvers in place of the currently used Thomas algorithm. (4) *Plasma turbulence models:* We follow the motion of tracer particles and use several of the diagnostics that we have used in the case of sandpile models. We calculate the different moments of particle positions and consider their time evolution. The use of the nonlinear Lyapunov number approach has been very useful for such determination. We have successfully tested this method in sandpiles and simple turbulence systems and we are planning to make a more extensive application of this method to 3D plasma turbulence models.

*Quasi-Poloidal Stellarator (QPS) optimized stellarator plasma surface with magnetic field line (white) superimposed.*

## ACCOMPLISHMENTS

An optimized compact stellarator QPS (quasi-poloidal stellarator) has been developed and passed through a successful physics validation review, and will be proposed as a future experiment at Oak Ridge National Laboratory. Some specific accomplishments in stellarator were neoclassical transport studies of the QPS device, Monte Carlo studies of neutral beam heating and alpha particle confinement in the National Compact Stellarator Experiment (NCSX) and QPS concepts, development of scenarios for access to second ballooning stability in both the QPS device and its reactor embodiment, and synthesis of coilsets for the QPS and NCSX devices that accurately preserve flux surface integrity.

We have investigated the transport properties of a 3D pressure-gradient-driven turbulence. This system was characterized by subcritical transport by avalanches when a noise source was introduced in the equations. Similar properties of avalanche transport are found in the supercritical regime. The use of particle tracers in this system has allowed us to characterize through different diagnostics the transport properties of the tracers in such systems. The main result is that the transport is superdiffusive with a transport exponent of 0.88. There is no change of the exponent, within the error bars, in going from subcritical to supercritical transport. Several of the methods used in calculating this exponent lead to the same result.

## SIGNIFICANCE

The development of new compact stellarators allows larger volume plasmas to be designed at a fixed cost. Larger volume plasmas are less edge-dominated, lose less energy from charge exchange, and as a result allow better science to be carried out. Compact plasmas could also lower the development costs and allow smaller, more modular devices to be built. If successful, this could significantly improve the economics of fusion power.

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http://www.ornl.gov/fed/Theory/theory.htm

# Equilibrium, Stability, and Transport Studies of Toroidal Magnetic Confinement Systems

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*A. M. Garofalo, Columbia University*
*E. J. Kinsey, Lehigh University*

## RESEARCH OBJECTIVES

The aim of this research is fourfold: (1) Provide support calculations for the DIII-D National Fusion Facility, including experimental predictions and analysis and interpretation of data. (2) Establish an improved theoretical and computational scientific basis for the physics of fusion plasmas. (3) Optimize presently known Advanced Tokamak configurations for high performance and identify potential new Advanced Tokamak configurations. (4) Explore and optimize alternative magnetic confinement configurations, and elucidate the relationships between these and tokamak configurations.

## COMPUTATIONAL APPROACH

The principal codes used are EFIT and TOQ (equilibrium); GATO, TWIST-R, MARS, BALOO, DCON, NIMROD, and BOUT (MHD stability); GLF23, GYRO, BALDUR, TRANSP, ONETWO, CORSICA, MCGO, and P2D (transport and fuelling); CQL3D, CURRAY, and TORAY (current drive); and UEDGE and DEGAS (edge physics). New computational tools are also being developed and tested, especially linearized MHD stability codes (ELITE, TWIST-R) and the new highly parallelized simulation codes GYRO, GRYFFIN, and FORTEC.

## ACCOMPLISHMENTS

Considerable progress was achieved in understanding the physics of rotating wall-stabilized plasmas and in increasing DIII-D performance. Stability calculations were used in conjunction with improvements in DIII-D experiments to show that rotational stabilization can be maintained with $\beta$ values up to twice the limit attainable without wall stabilization. Calculations were also used to model the intelligent shell realization for active control used in the DIII-D experiments. These calculations are being incorporated into designs for an extension of the active control system on DIII-D.

New insight into how the fundamental processes determining the size and field strength scaling of confinement can be obtained from dimensionally similar tokamak discharges was gained through analysis of numerical results and experiments. The transport bifurcation from L- to H-mode and internal transport barriers, as well as the edge confinement improvement in the DIII-D VH-mode, can be explained by a theory based on E × B rotational shear driven by changes in the diamagnetic flows at the plasma edge.

Theory-based transport modeling is providing new understanding of the fundamental transport processes in high-$\beta$ plasmas. Gyrofluid nonlinear ballooning mode flux tube methods developed for numerically simulating 3D homogeneous turbulence in toroidal geometry were applied to determine the dependence of transport on shear, safety factor, toroidicity, and sheared E × B rotation. Parallel electromagnetic gyrofluid simulations using the GRYFFIN code showed that microturbulence takes on an electromagnetic character even at low values of $\beta$; significant electromagnetic effects on turbulent transport were found, such as a reduction in heat transport at low $\beta$ and a significant increase in heat transport as the MHD $\beta$ limit is approached.

## SIGNIFICANCE

Recent progress in fusion has been accelerated as a result of a renewed emphasis on scientific understanding of tokamak plasmas, which has been brought about by a strong coupling between theory, computation, and experiments. It is therefore important to pursue more theoretical investigations in areas such as macroscopic stability, microinstabilities, and turbulence.

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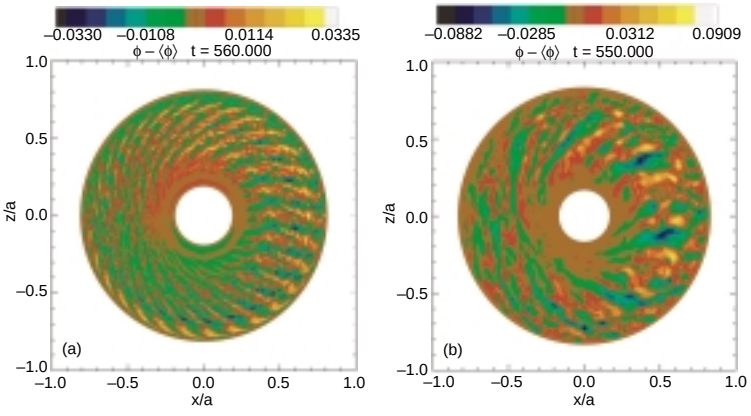
http://fusion.gat.com




*Contour plots of density perturbations in the poloidal plane for ion temperature gradient mode turbulence, comparing (a) $\rho_* = 0.0025$ (240 ion gyroradii) and (b) $\rho_* = 0.0075$ (80 ion gyroradii) simulations with moderate profile variation and an adaptive source to maintain equilibrium profiles. The diffusion is in a gyroBohm scaled regime. Cases closer to threshold with more rotational velocity shear show Bohm, scaled diffusion.*

# Lattice Boltzmann Simulations for Plasmas

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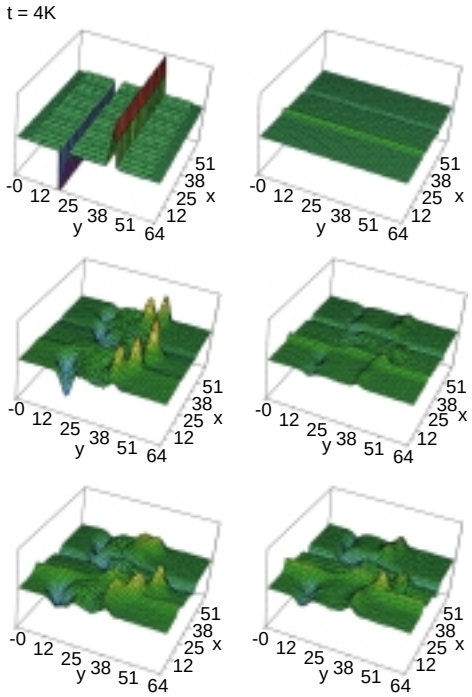
*Mary Linda Vahala, Old Dominion University*
*Pavol Pavlo, Institute of Plasma Physics, Czech Academy*

## RESEARCH OBJECTIVES

Thermal lattice Botlzmann modeling (TLBM) is an ideal MPP computational tool to study nonlinear macroscopic systems. In the tokamak divertor regime, where the neutral collisionality varies from very collisional (fluid) to weakly collisional (Monte Carlo), TLBM can give a unified framework, and thus avoid the difficult problem of coupling UEDGE to Monte Carlo. Energy-dependent lattices are being examined, and preliminary runs have attained higher Reynolds and Mach numbers of 0.5. We are also investigating LBM for 2D magnetohydrodynamics, using octagonal lattices.

## COMPUTATIONAL APPROACH

TLBM discretizes the Bhatnagar-Gross-Krook (BGK) kinetic equation to solve the system on a particular lattice. The level of lattice symmetry has important consequences on the numerical stability of TLBM codes. An explicit numerical scheme involves summations at each spatial node (all local information), followed by Lagrangian streaming that shifts information to neighboring spatial nodes. Domain decomposition is used, with MPI required to distribute information streamed across the boundaries allocated to each PE. To attain greater numerical stability, more complicated streaming algorithms are being investigated, such as energy-dependent streaming.




*Turbulence in the lighter gas (left hand plots) induces nonlineaerities in the heavier gas (right hand plots) with the resulting vorticity equilibration between the gases.*

## ACCOMPLISHMENTS

TLBM, because of the increase in dimensionality over computational fluid dynamics (CFD) solvers, is of interest only for massively parallel platforms. Because of the discretization of phase space velocity, the BGK relaxation distribution function cannot be Maxwellian and at the same time ensure that no discrete symmetry effects plague the final Chapman-Enskog-derived moment equations. As a result, TLBM codes are somewhat schizophrenic: collisions drive towards Maxwellians, but Maxwellians must be excluded. We have been investigating some preliminary methods to increase the solution space that can be attained by TLBM. In particular, instead of the customary streaming from node to node, we have incorporated a local streaming distance that is proportional to the temperature at that spatial node. To then extract moment information on a given spatial node, we invoke an allocation scheme that always preserves the conserved quantities. With this algorithm, we can attain jet flows up to Ma = 0.6. This algorithm is now being extended to permit the full energy equation to be solved.

## SIGNIFICANCE

The accurate resolution of the nonlinear convective derivatives that arise in the macroscopic conservation equations can take over 30% of the CPU in standard CFD. In TLBM, one avoids the Riemann problem by embedding the system into higher dimensional phase space. For highly collisional regimes, one can utilize the linear BGK collision operator. This approach is ideal for parallel processors. TLBM is somewhat similar to multiscale perturbation theory in its ability to solve singular problems in applied math and physics.

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# The Nearby Supernova Factory

*Gregory Aldering, Saul Perlmutter, Peter Nugent, and Stewart Loken, Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

The Nearby Supernova Factory (SNfactory) is an international collaboration between astrophysicists at Lawrence Berkeley National Laboratory and three institutions in France: Laboratoire de Physique Nucléaire et de Haute Énergies de Paris, Institut de Physique Nucléaire de Lyon, and Centre de Recherche Astronomique de Lyon. The aim of the collaboration is to discover nearby supernovae and to study them in detail so that they can be used more effectively as cosmological distance indicators.

## COMPUTATIONAL APPROACH

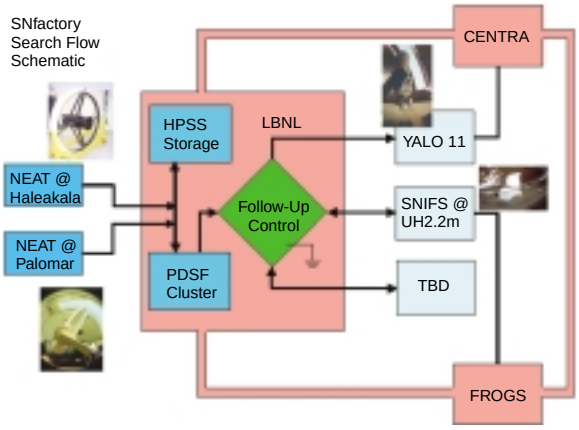
Discovering supernovae as soon as possible after they explode requires imaging the night sky repeatedly, returning to the same fields every few nights, and then quickly processing the data. The most powerful imager for this purpose is the CCD (charge-coupled device) camera built by the Jet Propulsion Laboratory (JPL). This camera delivers 100 MB of imaging data every 60 seconds, and an upgraded version of the camera will more than double this. The new images are compared to images of the same field archived on HPSS using digital image subtraction to find the light of any new supernovae. This digital image subtraction involves numerous steps to align the images and account for blurring by the Earth's atmosphere. Because the amount of data is so large (50 GB per night), the image archive even larger (presently 8 TB and growing), and the computations so extensive, it is critical that the imaging data be transferred to a large computing center (in this case NERSC) as quickly as possible (see figure).

## ACCOMPLISHMENTS

During the past year we worked to automate the Nearby Supernova Factory image subtraction pipeline. We also began archiving data from the Near Earth Asteroid Tracking (NEAT) team, who built and operate the current JPL camera at Palomar as well as a camera on Haleakala in Hawaii. These efforts have recently come to fruition with the discovery of our first probable supernova from this most recent effort. (Note that in spring 1999 we lead a similar effort which used similar techniques to find over 40 confirmed supernovae.)

## SIGNIFICANCE

In the past few years, measuring distances to Type Ia supernovae at very high redshifts has allowed astrophysicists to measure the rate of expansion of the Universe over the last 8 billion years. (The Universe is now believed to be about 14 billion years old.) Since all known matter in the Universe is pulled together by gravity, it was expected that these measurements would show that the expansion of the Universe has been slowing down. However, the Type Ia supernova measurements indicate that within the last few billion years, this expected slowdown has been reversed. The cause for this reversal is unknown—it may be related to Einstein's famous Cosmological Constant—and so has been dubbed "dark energy." This discovery, named the most important scientific discovery of 1998 by the journal Science, has revolutionized cosmology. Understanding the physical cause for the dark energy requires more precise measurements, and this should be possible with large numbers of accurately measured Type Ia supernovae. Understanding gained from this project will contribute to the design of future experiments, such as the Supernova/Acceleration Probe (SNAP).




*Data flow for the SNfactory search and follow-up. Left: Supernovae are discovered on images obtained by the NEAT team at JPL using telescopes on the summits of Haleakala, Hawaii and Palomar Mountain, California. Those images are transferred to LBNL via the Internet. Center: Once at LBNL, the images are archived onto HPSS. They are processed using the PDSF cluster and compared to archived processed images taken a week earlier to look for the light of new supernovae. Right: Follow-up spectroscopic and imaging data are obtained for these new supernovae using the Yale/Lisbon/Ohio (YALO) telescope on the summit of Cerro Tololo, Chile, and the University of Hawaii's 2.2-m telescope on the summit of Mauna Kea, which will have a new instrument—the SuperNova Integral Field Spectrograph (SNIFS)—specifically optimized for the study of supernovae. The search and follow-up flow will be monitored across the SNfactory collaboration, indicated by the salmon-colored "ground-plane." (CENTRA is the Centro Multidisciplinar de Astrofisica at the Instituto Superior Tecnico, Lisbon. FROGS is the French Observing Group for Supernovae.)*

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http://snfactory.lbl.gov

# Phenomenology with O(a) Improved Lattice QCD

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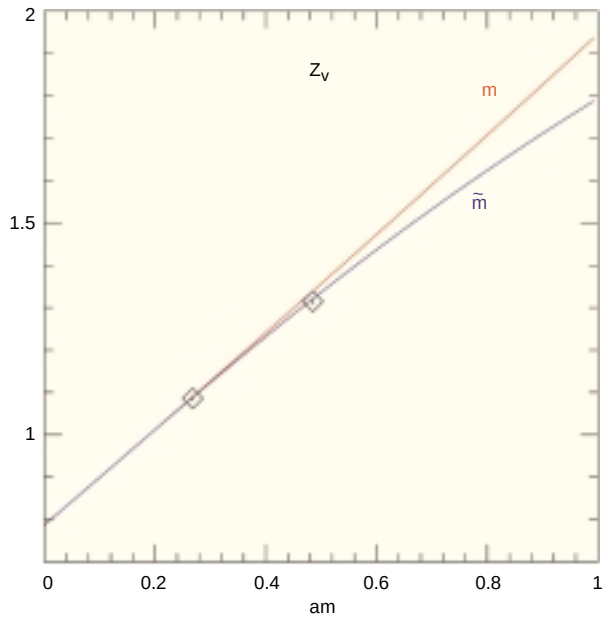
*Los Alamos National Laboratory*
*Stephen Sharpe, University of Washington*
*Gregory Kilcup, The Ohio State University*

## RESEARCH OBJECTIVES

Our goal is to calculate $B_K$, the matrix element that gives rise to charge parity (CP) violation in kaon decays, using three flavors of dynamical quarks. Our analyses show that this is best achieved using improved staggered fermions.

## COMPUTATIONAL APPROACH

Our lattice QCD simulations involve five steps: (1) Generation of a statistical sample of background gauge configurations which provides an accurate representation of the functional integral. This is done by Monte Carlo methods and using molecular dynamics evolution with the *R* algorithm. (2) Calculation of quark propagators by inversion of a very large but sparse matrix, using a BiCGstab iterative solver. (3) Calculation of correlation functions, which is done by tying together the gauge links and quark propagators. (4) Calculation of improvement constants and normalization factors. (5) Analysis of the correlation functions to extract desired masses of hadrons and matrix elements within these states.




*The mass dependence of the renormalization constant for the vector current $Z_V$ extracted from lattice simulations near the strange quark mass. The two functional forms, shown as red and blue lines, differ by higher order discretization errors. By comparing with measurements at two much heavier values of quark mass, we are able to ascertain that the fit corresponding to the blue line works better when extrapolating up to the charm quark mass.*

## ACCOMPLISHMENTS

In FY 2001 we completed our study of $O(a)$ improvement of quenched Wilson fermions. Calculations of the renormalization and improvement constants for quark bilinears were carried out at three values of the coupling, $\beta$ = 6.0, 6.2, 6.4. A scaling analyses of the residual discretization errors has been carried out. We have also completed the theoretical analyses required to extend the calculation to dynamical quarks. This analyses shows that all but a few unimportant constants can be determined, but the calculation will be extremely CPU time intensive. In view of the CPU requirements, and on comparing this cost against improved staggered fermions, we conclude that for the proposed calculation of $B_K$ with three dynamical flavors of quarks, it is better to use improved staggered fermions. With this in view, we have already begun quenched staggered calculations to develop improved operators.

## SIGNIFICANCE

Our proposed calculation of $B_K$ will have significant impact on the phenomenology of CP violation. Current phenomenology uses quenched lattice estimates of $B_K$, and we propose to remove the largest remaining uncertainty due to quenching. This is estimated to be a 5–10% effect, and removing it will pin down this important parameter, leading to a better estimate of the Cabibbo-Kobayashi-Maskawa matrix.

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# Lattice QCD Monte Carlo Calculation of Hadron Structure

*Keh-Fei Liu, Terrence Draper, and Shao-Jing Dong,*
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## RESEARCH OBJECTIVES

The proposed numerical study of nucleon structure will produce results to be compared with experimental results already obtained and to be obtained from the DOE-supported nuclear and high energy labs.

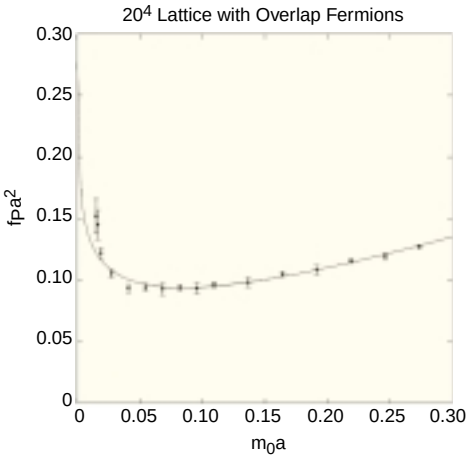
## COMPUTATIONAL APPROACH

The new overlap fermion action involves a matrix sign function. We approximate the square root of the matrix by the optimal rational fraction approach, and we invert the matrix with conjugate gradient with multiple mass algorithm. To speed up the convergence, we project out some of the smallest eigenvalues and treat the sign function of these states exactly. The overall inversion of the quark matrix to obtain the quark propagator is also done with conjugate gradient with multiple quark masses.

## ACCOMPLISHMENTS

We have carried out a production run on a quenched $20^4$ lattice with lattice spacing at 0.15 fm. The size of each direction is thus 3 fm, which is about the largest volume that any lattice calculation has attempted. We have also pushed the pion mass to as low as ~ 200 MeV, which is also a record. We found many interesting features of chiral symmetry at such a low mass and large volume. First of all, we found that the zero mode contribution to the pion propagator is not negligible at small time region, and its contamination needs to be avoided when extracting pion properties such as the pion mass and decay constant. We found that after nonperturbative renormalization, the pseudoscalar meson decay constant is very constant in the range between the strange and up/down quark mass. In view of the fact that it has a very small statistical error (less than 2% with only 63 gauge configuration), it is a physical quantity free of quenched chiral log, and is thus an ideal quantity to set the lattice scale. On the other hand, we have clearly observed the quenched chiral log in the pseudoscalar matrix elements at small quark masses, and it is in agreement with the prediction based on the $U(1)$ anomaly with the $\eta'$ mass.

We have computed the $a_0$ (isovector-scalar) and $a_1$ (isovector-axial) masses. We found that the propagator of $a_0$ becomes negative in the large time separation when the quark mass becomes small and that of $a_1$ flattens off. We understand them as the quenched artifacts due to decays to the $\eta'\pi$ and $\eta'\eta'\pi$ respectively. We have calculated one- and two-loops in the effective meson theory to help fit them and extract the $a_0$ and $a_1$. This is clear and concrete evidence for the quenched artifacts which people have been expecting to see.




*Pseudoscalar decay constant of the pseudoscalar meson is plotted as a function of the quark mass. The calculation is done on the quenched $20^4$ lattice at lattice spacing a = 0.148 fm with the overlap fermion. At sufficiently small quark mass, the decay constant appears to diverge. This verifies the quenched chiral log behavior predicted from the quenched chiral perturbation theory.*

## SIGNIFICANCE

With the advent of Neuberger's overlap fermion, which has the promise of exact lattice chiral symmetry for finite lattice spacing, it is time to calculate the fundamental quantities such as the quark condensate, chiral logs in hadron masses, light quark masses, decay constants, and nucleon form factors with this new action. Besides the continuum and large volume limits, this new action allows an extrapolation and perhaps interpolation to the physical quark mass region, one of the last frontiers in lattice QCD in the quenched approximation. With the guidance of chiral symmetry, physical observables which are sensitive to this symmetry should be calculated much more reliably than before, and they can be compared with experiments more readily and directly.

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http://www.pa.uky.edu/~liu

# Core Collapse Supernova Simulations in Multidimensions with Boltzmann Neutrino Transport

*Anthony Mezzacappa, Oak Ridge National Laboratory*

## RESEARCH OBJECTIVES

We will take a major step forward in simulating core collapse supernovae in two and three dimensions with Boltzmann neutrino transport by implementing ray-by-ray Boltzmann transport. Ray-by-ray simulations capture much of the transport realism in multidimensional models by performing independent calculations of the radiation transport along each radial direction. This neglects only contributions from lateral neutrino transport, which will likely only be important below the neutrinospheres in the proto-neutron star, where the neutrinos and matter are strongly coupled and the flow may be highly nonspherical. Nonetheless, ray-by-ray simulations will mark a major advance in multidimensional supernova models, particularly when the flow of neutrinos along each ray is handled using multigroup Boltzmann transport, a much more sophisticated approach than the transport used in past multidimensional supernova simulations. This is an intermediate step towards completing simulations with true multidimensional Boltzmann transport and continues our effort to develop scalable radiation (in our case, neutrino) transport on MPP platforms.

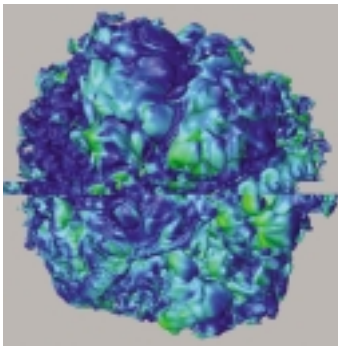
## COMPUTATIONAL APPROACH

Our 2D and 3D supernova simulations with ray-by-ray neutrino transport will couple our multidimensional PPM hydrodynamics code, VH-1, with our existing 1D Boltzmann neutrino transport code, BOLTZTRAN. BOLTZTRAN will be used to perform independent transport calculations along each radial ray, allowing us to achieve a high degree of parallelism.

## ACCOMPLISHMENTS

We have developed the RadHyd framework that will allow us to merge disparate hydrodynamics, transport, and nuclear physics codes in a modular fashion, both for use in the ray-by-ray simulations and for future work. Adaptations made by Calder and Mezzacappa to a prior version of VH-1 have been integrated into the newer, MPI-based massively parallel version of VH-1. In addition, we have added the capability to track nuclear composition, and we have generalized the handling of equations of state. Using the enhanced VH-1module, RadHyd has been extensively validated, in one and two dimensions, against a number of known hydrodynamics test problems. For use in the ray-by-ray simulations, our existing Boltzmann neutrino transport code for spherically symmetric flows, BOLTZTRAN, has been integrated into the RadHyd framework to calculate the neutrino transport, providing an exact transport solution along each ray.

We have tested the combination of BOLTZTRAN and EVH-1 through a series of spherically symmetric core collapse simulations to allow the comparison of RadHyd to our previous results, and have completed our first 2D ray-by-ray simulations.



*This visual rendering of data output from a 3D supernova simulation shows a surface of constant temperature below the supernova shock wave. The green areas show regions of fluid overturn, and the blue areas show regions of fluid inflow or outflow. Combined, the blue and green regions depict the turbulent environment beneath the supernova shock wave. (Figure by Anthony Mezzacappa and Ross Toedte, Oak Ridge National Laboratory, and John Blondin, North Carolina State University)*

## SIGNIFICANCE

Our goal is to understand the mechanism by which core collapse supernovae explode. A signal of the demise of a massive star and the birth of a neutron star or black hole, core collapse supernovae are among the brightest events in the Universe and create many of the chemical elements that make up our solar system. They are the key link in our chain of origins from the Big Bang to the present. To reach this goal we must develop scalable radiation hydrodynamics, which will enable a new class of multidimensional supernova models and will have broad implications for a variety of applications, such as combustion modeling, climate modeling, and nuclear medicine.

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# Exploration of Hadron Structure Using Lattice QCD

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*Robert Edwards, Thomas Jefferson National Accelerator Facility*
*Thomas Lippert, Hartmut Neff, and Klaus Schilling, University of Wuppertal*

## RESEARCH OBJECTIVES

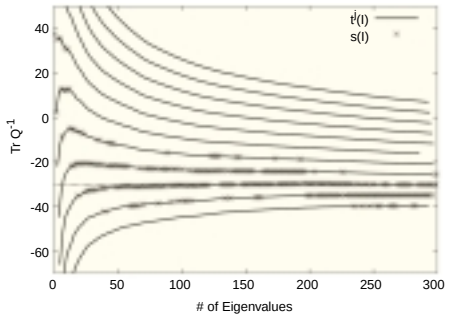
The major focus this work is on understanding the role of instantons and their associated quark zero modes in nucleon structure, and using the quark zero modes to calculate the sea quark content of the nucleon.

## COMPUTATIONAL APPROACH

We calculate the low eigenmodes of the Dirac operator using the Arnoldi method, which has compelling advantages for our work. One advantage is that since it works in a fixed dimension space, there is no degradation of orthogonality and corresponding loss or duplication of modes. A second advantage, when applied to the non-hermitian Dirac operator, is its insensitivity to the quark mass, which makes it extremely useful near the chiral limit of low pion mass. We have two complementary implementations. One is an exploratory code in which we can control the region of eigenvalues at will. The other uses the robust and well optimized PARPACK package from ORNL combined with Chebyshev acceleration.

## ACCOMPLISHMENTS

NERSC resources enabled us to calculate on 400 configurations the low eigenmodes of the hermitian Dirac operator, which is $\Gamma_5$ times the standard Dirac operator. This showed that, contrary to our original expectation, at the large quark masses relevant to current unquenched calculation, the eigenmode expansion of the hermitian Dirac operator has superior convergence properties to that of the standard operator. An unfortunate property of the hermitian Dirac operator, however, is the need to calculate new eigenmodes at each quark mass, in contrast to the standard operator, for which a single set of eigenmodes applies for all masses. Hence, the computational needs of the project have increased relative to our original expectation in order to calculate eigenmodes at several masses.




*Because topological properties of QCD are associated with zero modes of the Dirac operator, properties such as the topological susceptibility and the mass of the η′ meson can be calculated most efficiently by calculating the low eigenmodes of the Dirac operator. This figure shows how, in a space of 1.57 million states, the lowest 300 eigenmodes already give a precise determination of the topological charge of a gluon configuration. Using extensive calculations at NERSC, this truncated eigenmode expansion has recently been used to calculate the mass of the η′ meson with unprecedented statistical precision.*

## SIGNIFICANCE

Ever since the discovery of quarks in the nucleon, tremendous experimental effort and resources have been devoted to the measurement of the detailed quark and gluon structure of the nucleon, and theorists have sought to understand this structure from first principles. In a clever and difficult series of experiments at Bates and Jefferson Lab which are now finally coming to fruition, experimentalists have used the interference between parity-conserving and parity-violating electron scattering amplitudes to measure the contributions of strange quarks to electric and magnetic form factors. Given the investment of effort and resources in these fundamental experiments, it is extremely important to develop the means to calculate the strange quark content of the nucleon reliably using lattice QCD. We are developing a new method which can attain a higher level of statistical accuracy than existing methods, and will provide the essential quark zero modes necessary for these calculations. In addition to elucidating the physics for timely parity-violating electron scattering experiments, this new method should also enable the evaluation of the disconnected diagrams encountered in deep inelastic electron scattering.

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http://www-ctp.mit.edu/~negele/

http://www.fz-Juelich.de/nic/Forschungsgruppen/Elementarteilchen/

# Spectrum Synthesis of Supernovae

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*Edward Baron, University of Oklahoma*
*Peter Hauschildt, Jason Aufdenberg, Christopher Shore,*
*Andreas Schweitz, and Travis Barman, University of Georgia*

## RESEARCH OBJECTIVES

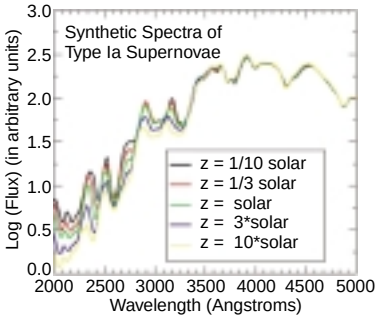
Using astrophysics techniques developed in the LBNL Physics Division's Supernova Cosmology Group, we have begun to measure the fundamental parameters of cosmology that shape our current understanding of particle physics through the observation of very distant Type Ia Supernovae. Our goals are: (1) Completion of spectrum synthesis calculations for both distant and nearby supernovae to look for any systematic differences which might bias the cosmological parameters we measure. (2) Development of an objective classification scheme for SNe~Ia to accurately describe their age and luminosity through their spectral features. (3) Creation of a grid of synthetic supernova spectra which will be used to understand the supernovae discovered via LBNL's Supernova Factory and prepare for the Supernova/Acceleration Probe (SNAP) satellite through a comprehensive set of simulations. (4) Detailed study of core-collapse supernovae and their use for determining the cosmological parameters and nucleosynthesis products.

## COMPUTATIONAL APPROACH

We use a MIMD approach utilizing Fortran 90 and the MPI message passing interface.

## ACCOMPLISHMENTS

We analyzed spectra from SN 1997ff, the most distant Type Ia supernova discovered to date. This widely publicized event, which strongly confirmed the existence of "dark energy," argues against the notion that observations of distant Type Ia supernovae may be systematically distorted by intervening gray dust or the chemical evolution of the universe.




*SN 1999be at the edge of the galaxy CGCG 089-013 in the constellation Cancer was one of almost 40 supernovae found by the Supernova Cosmology Project in 1999 as part of a project to improve our understanding of these objects as tools for cosmology. The graph shows a series of synthetic spectra produced on NERSC's IBM SP which aim at understanding the influence of the progenitor's metallicity on the spectra of supernovae such as 1999be.*

We have run numerous models of Type IIP supernovae which will be extremely useful for determining the extragalactic distance scale (and determining the nature of the dark energy) independently of Type Ia Supernovae.

Two complete advanced model grids were calculated to analyze observations of very low mass stars and brown dwarfs. Normally it takes a few months to run such a grid, but NERSC's IBM SP took about four days. We included the calculation of very detailed radiation fields that are needed by people that try to observe stellar occultations or planetary transits. The models include the latest physics and detailed spherical radiation transport (never before done for this type of model). The grid will be used to analyze observed spectra and to better understand the physics behind these objects.

## SIGNIFICANCE

This project aims to provide theoretical justification of the empirical results found by the Supernova Cosmology Project, that we live in an accelerating universe. In other words, we want to be able to answer the question "How well do we know the cosmological parameters?" from a theoretical standpoint.

Supernovae are among the largest explosions in the universe, and the elements they eject form the basic building blocks for the stars and planets. Understanding the nature of their explosions and the materials synthesized during this process allows us to probe many different basic question in astrophysics, nuclear and high energy physics.

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http://www.lbl.gov/~nugent/

# STAR Detector Simulations and Data Analysis

*Doug Olson, Lawrence Berkeley National Laboratory*
*John Harris, Yale University*

## RESEARCH OBJECTIVES

The STAR detector (Solenoidal Tracker at RHIC) at Brookhaven National Laboratory is a large acceptance collider detector designed to study the collision of heavy nuclei at very high energy in the laboratory. Its goal is to investigate nuclear matter at extreme energy density and to search for evidence of the phase transition between hadronic matter and the deconfined quark-gluon plasma. The computations carried out at NERSC are focused around analysis of the processed data, comparison of these data with experimental models, and studies of the detector performance and acceptance.

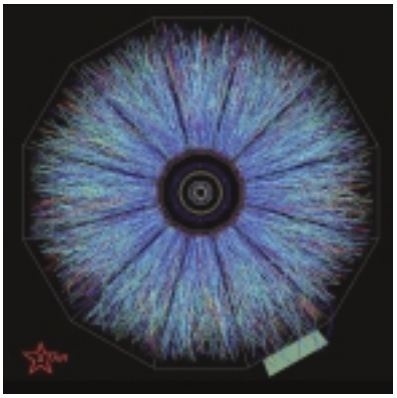
## COMPUTATIONAL APPROACH

Physics results are derived from experimental relativistic heavy ion collisions by carrying out statistical analysis of large numbers of events (collisions of individual atomic nuclei). The theoretical models are implemented as Monte Carlo codes that describe the final state of each of the thousands of particles that are produced in these collisions. We use a number of these theoretical codes (VENUS, HIJING, RQMD, and others) to produce large samples of events. A simulation code called GEANT is used to propagate each of these thousands of particles through the material of the STAR detector and compute the reactions and energy deposition that occurs throughout the detector.

## ACCOMPLISHMENTS

Elliptic flow from nuclear collisions is a hadronic observable sensitive to the early stages of system evolution. STAR reported first results on elliptic flow of charged particles at midrapidity in Au + Au collisions at $\sqrt{s_{NN}}$ = 130 GeV. The elliptic flow signal, $v_2$, averaged over transverse momentum, reaches values of about 6% for relatively peripheral collisions and decreases for the more central collisions. This can be interpreted as the observation of a higher degree of thermalization than at lower collision energies.

Results on the ratio of midrapidity antiproton-to-proton yields in Au + Au collisions show that the ratio is essentially independent of either transverse momentum or rapidity, within the rapidity and transverse momentum range of |y| < 0.5 and 0.4. From a pion interferometry analysis, the multidimensional identical pion correlation functions at midrapidity indicate that the source size grows with event multiplicity. The dependence of the correlations on transverse momentum, reflecting collective transverse flow, is qualitatively similar to that observed at lower energies. Anomalously large sizes or emission durations, which have been suggested as signals of quark-gluon plasma formation and rehadronization, are not observed. These results extend the weak $\sqrt{s}$ dependence of the Hanbury-Brown-Twiss (HBT) parameters established for heavy ion collisions at lower energies.



*Display of a single Au + Au ion collision at an energy of 200 A-GeV, shown as an end view of the STAR detector. Outlines of detector elements are shown as well as the thousands of particle tracks from this one event. This particular event is one of the first of several million events acquired by the STAR experiment in 2001.*

The minimum bias multiplicity distribution and the transverse momentum and pseudorapidity distributions for central collisions have been measured for negative hadrons (h-) in Au + Au interactions. The multiplicity density per participant at midrapidity for the 5% most central interactions increases 38% relative to $p\bar{p}$ collisions at the same energy. The mean transverse momentum is larger than in central Pb + Pb collisions at lower energies. The scaling of the yield per participant is a strong function of $p_t$. The pseudorapidity distribution is almost constant within $|\eta| < 1$.

## SIGNIFICANCE

The existence of the quark-gluon plasma is predicted by lattice QCD calculations, and this state of matter is thought to be important in the dynamics of the early universe and the core of neutron stars. The most violent nuclear collisions at RHIC generate approximately ten thousand secondary particles. STAR detects and characterizes a large fraction of these secondaries in order to reconstruct a meaningful picture of each individual collision.

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http://www.star.bnl.gov/

# Exact Calculations of Light Nuclei Using Realistic Interactions

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*Argonne National Laboratory*

## RESEARCH OBJECTIVES

Our goal is to compute ground-state and low-lying excited-state expectation values of energies, densities, structure functions, astrophysical reaction rates, etc., for light nuclei, neutron drops, and nucleonic matter, using a Hamiltonian that also provides an excellent description of nucleon-nucleon scattering. Such a "standard nuclear model" can then be used, for example, to compute low-energy astrophysical reactions which cannot be experimentally measured.

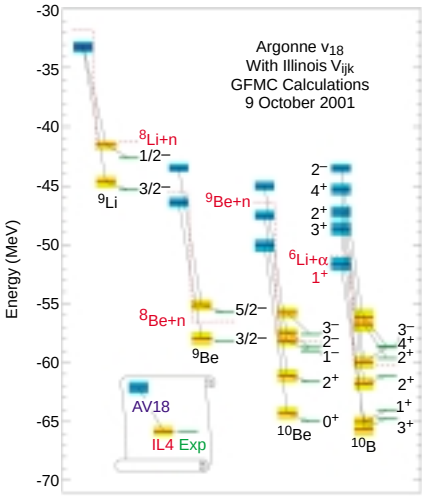
## COMPUTATIONAL APPROACH

This project uses variational (VMC) and Green's function (GFMC) Monte Carlo and coupled-cluster [exp(S)] methods. The variational wave function contains non-central two- and three-body correlations corresponding to the operator structure of the potentials. The GFMC systematically improves these wave functions to give the exact (within statistical errors) energy for the given Hamiltonian. We have demonstrated the reliability of constrained path methods for overcoming the well-known Fermion sign problem. Our Monte Carlo methods are limited to light nuclei; for heavier systems we use the coupled-cluster method. The present implementation of the exp(S) method for finite nuclei is carried out in configuration space. We have shown that we can choose a large enough configuration space in order to achieve convergence despite the relatively hard core of the *NN* interaction.

## ACCOMPLISHMENTS

We made our first calculations of nine- and ten-nucleon systems, the only calculations of such nuclei that use realistic two- and three-nucleon interactions and achieve a reliability of 1–2%. Our $^{10}$B calculations show that one must have a three-nucleon potential to correctly predict the ground-state spin of $3^+$. Using just realistic two-nucleon potentials gives a ground-state spin of $1^+$. We are now making the first calculations of bound unnatural parity states in $A$ = 10 nuclei; these calculations are significantly more complicated than those for the normal parity states. We are also studying the development of nuclear structure in these nuclei as the two-nucleon potential evolves from more simple schematic models to a fully realistic interaction.

For heavier nuclei, we have continued the study of ground-state properties in the *p*-shell using exp(S). We are in the process of carrying out calculations for the spin-isospin saturated nuclei $^{12}$C, $^{14}$C, $^{14}$O, and $^{16}$O. We are also in the process of making exp(S) calculations of Yrast states in neighboring nuclei, and calculating observables of interest to Jefferson Lab, such as the magnetic form factors for $^{15}$N and $^{13}$C.




*GFMC calculations of nine- and ten-body nuclei using just the AV18 NN potential and AV18 + Illinois-4 NNN potential. The negative-parity A = 10 results are preliminary. Note that a three-nucleon potential is necessary to obtain the correct $^{10}$B ground state.*

## SIGNIFICANCE

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. We work in both areas and have made the only calculations of six- through ten-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 JLab), and to compute astrophysical reaction rates, many of which cannot be measured in the laboratory.

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# Advanced Computing for 21st Century Accelerator Science and Technology

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*Salman Habib and Ji Qiang, Los Alamos National Laboratory*
*Viktor Decyk and Warren Mori, University of California, Los Angeles*
*Panagiotis Spentzouris, Fermi National Accelerator Laboratory*
*Alex Dragt, University of Maryland*
*Gene Golub, Stanford University*
*Kwan-Liu Ma, University of California, Davis*
*Esmond Ng, NERSC*

## RESEARCH OBJECTIVES

The primary objective of this project is to establish a comprehensive terascale simulation environment for use by the U.S. particle accelerator community, enabling physicists and engineers to solve the most challenging problems in accelerator design, analysis, and optimization. Terascale simulation will help ensure the success of the next generation of particle accelerators by facilitating design decisions aimed at controlling and reducing cost, reducing risk, and optimizing performance.

## COMPUTATIONAL APPROACH

This project has three main physics-based focus areas: beam systems simulation (BSS), electromagnetic systems simulation (ESS), and beam/electromagnetic systems integration (BESI). The BSS component uses parallel particle-in-cell (PIC) techniques, particle managers, dynamic load balancing, FFT-based Poisson solvers, and techniques from the field of magnetic optics. The ESS component utilizes unstructured mesh generation, domain decomposition, adaptive mesh refinement, finite elements and sparse linear solvers (for eigenmode codes), and unstructured Yee grids (for time-domain codes). The BESI component involving particles in electromagnetic structures will utilize hybrid grids, with a structured mesh in the region of the beam and an unstructured grid near the structure boundaries.

## ACCOMPLISHMENTS

The Omega3P parallel electromagnetic eigenmode solver was run on NERSC platforms to help design and evaluate accelerating structures for the Next Linear Collider (NLC). In particular, simulations of structures comprised of roughly 50 cells were performed, which is close to the planned ~200 cells in an NLC traveling wave structure. Simulations of an alternative standing wave structure, which would be comprised of ~50 cells, have also begun and may hold the key to an improved NLC design. Omega3P was also used to study anomalous heating in the PEP-II B-factory interaction region. The heating has been identified as being caused by a "trapped mode," and methods to deal with this problem are under investigation.

The 3D parallel PIC code IMPACT was used to model the Low-Energy Demonstration Accelerator (LEDA) beam halo experiment, the Spallation Neutron Source linac, and the CERN superconducting proton linac. Extensive simulations were performed on the behavior of nonequipartioned beams, work that is relevant to almost all proposed high-intensity proton linac designs. IMPACT was also used to numerically generate, for the first time, 3D nonequipartioned self-consistent solutions of the Poisson/Vlasov equations for a beam in a constant focusing channel. This work involved a combination of analytical work to mathematically describe the equations governing the self-consistent solutions and large-scale computations (involving a parallel Langevin code) to numerically generate them and study the stability properties. Finally IMPACT was combined with GEANT3 to produce the first parallel simulation of a muon cooling channel.

*Top: Omega3P simulation of the PEP-II interaction region (from crotch to crotch) showing domain decomposition of a portion of the mesh around the interaction point. Bottom: Wall loss distribution of a trapped mode in this region of the vacuum chamber.*

## SIGNIFICANCE

The design of the next generation of accelerators will require a new level of simulation capability as accelerator designers push the boundaries of beam intensity, beam energy, and system complexity. All near- and far-future accelerators have very challenging modeling requirements that require high performance computing.

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# Two-Color QCD at Finite Quark-Number Density and Temperature, and QCD at Finite Isospin and Strangeness Densities and Temperatures

*Donald Sinclair, Argonne National Laboratory*
*John B. Kogut, University of Illinois*

## RESEARCH OBJECTIVES

This project will complete our studies of two-color QCD at finite chemical potential for quark number at zero and finite temperatures, and will study true (three-color) QCD at finite chemical potential for isospin, and at finite chemical potentials for isospin and strangeness, both at zero and finite temperatures. These studies will be performed using the lattice gauge theory simulations, using hybrid molecular dynamics methods to include the dynamical fermions (quarks).

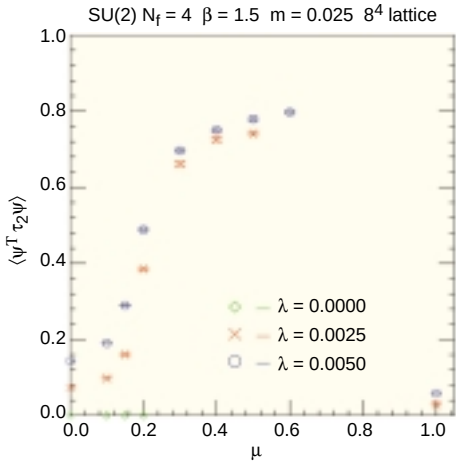
## COMPUTATIONAL APPROACH

Our simulations use the standard hybrid molecular dynamics algorithm with "noisy" fermions. This involves using Gaussian noise for the pseudo-fermion fields which allows us to tune the number of flavors to the desired value. We use the modified updating scheme of Gottleib-Liu-Toussaint-Renken-Sugar which keeps the errors $O(dt^2)$ in the presence of such noisy fermions. The explicit symmetry breaking terms in each case keep the determinant (or Pfaffian) positive, permitting such importance sampling simulations to work. This simulation method requires inverting the Dirac operator for each update. The inversion of this sparse matrix is performed using a simple conjugate gradient algorithm. This inversion dominates the computing requirements of these simulations.

## ACCOMPLISHMENTS

We have simulated two-color, four-flavor QCD on $8^4$ and $12^3 \times 24$ lattices at $\beta = 4/g^2 = 1.5$, which is close to the $\beta$ of the $N_t = 4$ phase transition, and the relatively large quark mass $m = 0.1$. Here we observed clear evidence for a second-order transition to a phase with a non-zero diquark condensate at $\mu = \mu_c$, close to half the pion mass, as expected. The expectation that the condensate merely rotates from a chiral condensate to a diquark condensate, predicted from an effective (chiral) Lagrangian analysis, appears to be a good approximation until the saturation effects of Fermi statistics become important. On the larger lattice we have observed clear evidence for the expected Goldstone mode, and observed that the pseudo-Goldstone mode behaves qualitatively as expected. We are now repeating these analyses at a smaller quark mass $m = 0.025$, where a more quantitative comparison with chiral perturbation theory should be possible, and a richer spectrum of Goldstone and pseudo-Goldstone bosons measured. In addition, the clearer separation of the desired transition from the saturation transition should allow better estimates of the critical exponents at this transition.

In addition, we have simulated this theory at finite temperature on $8^3 \times 4$ and $12^3 \times 6$ lattices. For $\mu > \mu_c$, as we increase the temperature, we eventually reach a temperature at which the quark-number symmetry is restored. These simulations indicate that the restoration occurs at a first-order transition. Further studies of this transition are under way.




*Preliminary measurements of the diquark condensate on an $8^4$ lattice at $m = 0.025$.*

## SIGNIFICANCE

Studies of QCD at finite baryon/quark number density (nuclear matter) have potential relevance to the physics of neutron stars. Studies of QCD at finite density and finite temperature are relevant to the physics of the early universe. In addition, they are expected to be relevant to the physics of relativistic heavy-ion collisions, which are now being observed at Brookhaven National Laboratory's RHIC. Finally, they would greatly enhance our knowledge of the structure of QCD.

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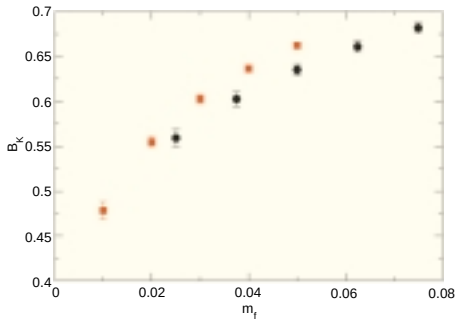
# *K to ππ and ε Calculations with Domain Wall Fermions*

*Amarjit Soni, Brookhaven National Laboratory*

## RESEARCH OBJECTIVES

This research primarily intends to accomplish a calculation of weak matrix elements relevant for $K$ to $\pi\pi$ decays and $K\bar{K}$ oscillations. Since quark masses are fundamental parameters of the Standard Model of Particle Interactions, and their precise calculations are amenable to domain wall quarks, we also intend to pursue their evaluation.




*The (quenched) kaon B parameter computed with two values of the lattice cut-off, corresponding to β = 5:85 (filled circles) (preliminary) and β = 6:0 (filled squares), but with the same physical volume. The physical kaon system corresponds to bare quark mass $m_f \approx 0{:}023$ and 0.018 for β = 5:85 and β = 6:0, respectively, so the non-zero lattice spacing errors appear to be small for these couplings. $B_K$ is important for determining the value of the (CP violating) fundamental parameter $\eta_{CKM}$ of the Standard Model of particle physics. (All calculations at β = 5:85 were performed on the NERSC T3E, and β = 6:0 was calculated on the QCDSP supercomputers at the RIKEN BNL Research Center at Brookhaven National Laboratory and at Columbia University.)*

## COMPUTATIONAL APPROACH

The basic innovation being used in these renewed attempts to solve some very old problems in hadron weak decays is called "domain wall fermions" (DWF). These require introducing a fictitious fifth dimension to enable the lattice to preserve important chiral symmetries of the continuum theory. Simulations done at NERSC in 1996–97 showed that this procedure is quite practical, despite the need for the fifth dimension. In fact, to date all studies suggest that scaling behavior is significantly improved, which tends to offset the cost of the extra dimension.

## ACCOMPLISHMENTS

In FY2001 we have collected data at gauge coupling of $\beta = 5.85$ with 200 gauge configurations that will be used to calculate $K$ to $\pi\pi$ amplitudes, $\varepsilon'$, $B_K$, and light quark masses.

## SIGNIFICANCE

This research will enable us to use experimental information on direct and indirect charge parity violation, obtained by extremely expensive experiments performed at DOE-funded facilities, to subject the Standard Model of Elemenatry Particle Physics to stringent tests.

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# High-Temperature QCD with Three Flavors of Improved Kogut-Susskind Quarks

*Doug Toussaint, University of Arizona*
*Claude Bernard, Washington University*
*Tom DeGrand, University of Colorado*
*Carleton DeTar, University of Utah*
*Steven Gottlieb, Indiana University*
*Urs Heller, Florida State University*
*Bob Sugar, University of California, Santa Barbara*

## RESEARCH OBJECTIVES

This project will be a significant step towards an accurate first-principles calculation of the location of the high-temperature phase transition or crossover in high-temperature QCD, including the effects of the strange quark as well as the light up and down quarks. In addition, we will get information about the nature of the high-temperature regime, and will begin to accumulate the results needed to calculate the equation of state.

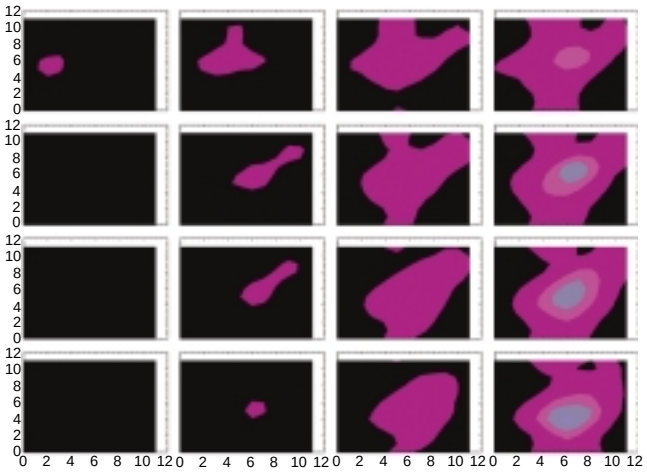
## COMPUTATIONAL APPROACH

The time-consuming part of lattice gauge theory calculations is the computation of the force, or acceleration of the gluon fields, coming from the dynamical quarks. First, this force is non-local, and its computation requires the solution of a sparse matrix problem where the matrix is Hermitian and positive definite. We use the conjugate gradient algorithm to obtain an approximate solution to the sparse matrix problem. Then, for each lattice link included in the quark action, the force on the corresponding gauge field is computed by parallel transporting the source and result of the sparse matrix computation from both ends of the path in the action to the lattice point where the force is being computed, and taking the outer product of these two vectors.

## ACCOMPLISHMENTS

We began a multiyear study of the QCD high-temperature phase transition with our improved action, including the effects of strange quarks. Because our improved action approximates continuum physics so well, our strategy has been to follow as nearly as possible trajectories in the parameter space of the input up, down, and strange quark masses and gauge couplings that fix the output zero temperature hadronic mass ratios. In this way we distinguish effects of temperature variation from effects of quark mass variation. Thus we require a reasonably careful calculation of the zero temperature spectrum of hadron masses at both ends of the temperature range of the thermodynamics study in order to anchor the trajectory in the bare (input) quark masses. We completed an essential study of the zero-temperature spectrum at a lattice spacing $a$ = 0.2 fm, which provided the low-temperature anchor point.

The spectrum studies used $16^3 \times 48$ lattices with the strange quark mass $m_s$ fixed approximately at its physical value throughout and with three values of equal up and down quark masses: 0.2 $m_s$, 0.4 $m_s$, and 0.6 $m_s$. An immediate byproduct of this work was a better understanding of the scaling properties of the zero-temperature light hadron spectrum with our improved action.



*The "chiral density" of one fermionic mode in a lattice simulation. This kind of structure is important in understanding what the QCD ground state, or "vacuum," looks like. The various panels are 2D slices through the 4D lattice.*

## SIGNIFICANCE

At very high temperatures one expects to observe a phase transition or crossover from ordinary strongly interacting matter to a plasma of quarks and gluons. To observe such a crossover, it is important to determine the nature of the transition, the properties of the plasma, including strange quark content, and the equation of state. Lattice gauge theory has proven to be the only source of first-principle quantitative calculation for the phase structure of high temperature QCD away from the limiting cases.

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# The Experimental Mathematician's Toolkit

*David Bailey and Xiaoye Sherry Li, NERSC,*
*Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

This project seeks to develop several easy-to-use, preferably Web-based tools for experimental mathematics, such as high-precision arithmetic constant evaluations, definite integral evaluations, integer relation detection, and others. The numerical code underlying these calculations has already been developed—what remains is to package these tools so that someone other than highly trained numerical analysts can use them.

## COMPUTATIONAL APPROACH

The approach is first to gather together a number of tools that appear to have promise as tools for experimental mathematics. In some cases, some additional development or polishing is needed. Once this is done, they will be placed in a common repository with detailed instructions and examples of usage. A few key items will be provided to users by means of an easy-to-use Web interface. This interface may require developing processes for moving heavier computation to other platforms, including parallel platforms (in order to provide excellent real-time, interactive performance).

## ACCOMPLISHMENTS

In a previous project, we took a major step toward answering the age-old question of whether the digits of pi and other mathematical constants are "normal," which means that their digits are random in a certain statistical sense. Our results indicate that the normality of certain constants is a consequence of a plausible conjecture in the field of chaotic dynamics, which states that sequences of a particular kind are uniformly distributed between 0 and 1—a conjecture we refer to as "Hypothesis A." We have thus translated a heretofore unapproachable problem to a more tractable question in the field of chaotic processes. Previous work on the PSLQ integer relation algorithm was selected as one of ten "Algorithms of the Century" by the publication "Computing in Science and Engineering."

A high-quality software package was completed that provides double-double (128-bit) and quad-double (256-bit) floating-point arithmetic. This package includes translation modules for both Fortran-90 and C/C++, which greatly reduce the programming effort to use these routines. In most cases it is only necessary to change a few type declarations to utilize these facilities. We used the quad-double software to perform a large simulation of a vortex roll-up phenomenon, running on the IBM SP and Cary T3E systems. Using this software, this calculation ran approximately five times faster than with arbitrary-precision software, thus saving thousands of CPU-hours of run time. The resulting calculations confirm that an instability occurs in these situations that had not been observed in previous studies.


*The apparent randomness of pi's digits is represented by a random-walk landscape to illustrate the September 1, 2001 Science News cover story describing David Bailey and Richard Crandall's research into the normality of certain mathematical constants. (Illustration: David V. Chudnovsky and Gregory V. Chudnovsky. Copyright ©2001 Science Service. Reprinted with permission.)*

## SIGNIFICANCE

Although high performance computer technology is now a mainstay in many fields of scientific research, and much of modern computer technology has its roots in pure/applied mathematics, the field of mathematics has not yet benefited much. Several valuable software tools have been developed, including several that were developed at NERSC. But for the most part they remain research codes, typically written in Fortran-90 or requiring parallel platforms, which places them out of range for most mathematicians. This work seeks to bridge this gap, making these tools available to average mathematicians for the first time.

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http://www.nersc.gov/~dhbailey

# Applied Partial Differential Equations

*Center for Computational Sciences and Engineering (CCSE) and Advanced Numerical Algorithms Group (ANAG), Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

The long-term goal of this project is to develop high-resolution adaptive methods for partial differential equations and to implement the resulting methodology into production-quality software tools that are broadly applicable to a number of DOE Office of Science research programs. The current focus applications are magnetic fusion, accelerator design, and turbulent reacting flow. Of these applications, computational reacting flow is the most mature, with a goal of developing a high-fidelity numerical simulation capability for turbulent combustion processes such as those arising in furnaces and engines.

## COMPUTATIONAL APPROACH

The principal computational tools for this project will be based on the adaptive mesh refinement algorithm developed by CCSE and ANAG. The methodology is based on a block-structured refinement approach that allows computational effort to be focused in regimes of the flow where it is required. For reacting flow simulations, we use a version of this methodology developed for low Mach number combustion. The algorithm uses a fractional step discretization that easily facilitates the inclusion of complex kinetics mechanisms as well as differential diffusion and radiative heat transfer. The key issue in modeling turbulent reactions is the interplay between kinetics and the small-scale turbulent eddies in the flow.

## ACCOMPLISHMENTS

During combustion of coal and biomass fuels, fuel-bound nitrogen compounds are volatized and released with combustible gas, potentially leading to enhanced NOx formation. Laboratory experiments at the Technical University of Denmark are being used to study this phenomenon. In the experiment, ammonia is added to an inflow methane stream to model the effects of fuel-bound nitrogen. To simulate the experiment computationally, we incorporate a set of detailed methane mechanisms describing the nitrogen chemistry, and NO formation in particular. These comprehensive mechanisms contain as many as 65 chemical species and 447 fundamental reactions. We were able to show that by modeling the detailed kinetics in an adaptively refined diffusion flame, we could accurately predict the NO produced by the flame as a function of inlet ammonia.


*Temperature and mole fraction of nitrous oxide from simulation of a methane diffusion flame using comprehensive chemistry. Predicting the formation of pollutants in flames requires detailed modeling of both the carbon chemistry in the flame and nitrogen chemistry that leads to pollutants. These simulations, performed using a parallel adaptive mesh refinement algorithm for low Mach number combustion, use a comprehensive chemical mechanism that models the behavior of 65 species and 447 reactions. The computed results show excellent agreement with experimental data and provide additional insight into the mechanisms of pollutant formation.*

We have begun to study turbulence-flame interaction in three dimensions to determine the effect of the turbulence on the average flame speed and to assess how turbulence modulates flame chemistry. We precomputed a field of isotropic decaying turbulence in the reactant stream. This field was then allowed to convect into the initially steady premixed hydrogen flame. The complete hydrogen mechanism was simulated (9 species, 27 reactions). The adaptive algorithm is set up to track the flame front and regions of strong vorticity, locally refining the base $32 \times 32 \times 64$ grid by up to a factor of 4. We are currently beginning the analysis of these results.

## SIGNIFICANCE

The modeling of turbulent fluid flow, even in the non-reacting case, remains one of the great scientific challenges. For realistic combustion scenarios, the picture becomes more complex, because small-scale turbulent fluctuations modify the physical processes such as kinetics and multiphase behavior. Developing techniques that accurately reflect the role of small-scale fluctuations on the overall macroscopic dynamics would represent a major scientific breakthrough.

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# A Numerical Study of Acceleration-Driven Fluid Interface Instabilities

*James Glimm and Xiaolin Li, State University of New York, Stony Brook*

## RESEARCH OBJECTIVES

We conduct 3D simulations of acceleration-driven fluid mixing, based on the front tracking code FronTier and the untracked TVD/level-set code for comparison. We continue studying two types of mixing: the steady acceleration-driven Rayleigh-Taylor (RT) instability and the shock-driven Richtmyer-Meshkov (RM) instability. In addition, we also use the FronTier code for the study of jet breakup, spray, and efficient diesel engine combustion.

## COMPUTATIONAL APPROACH

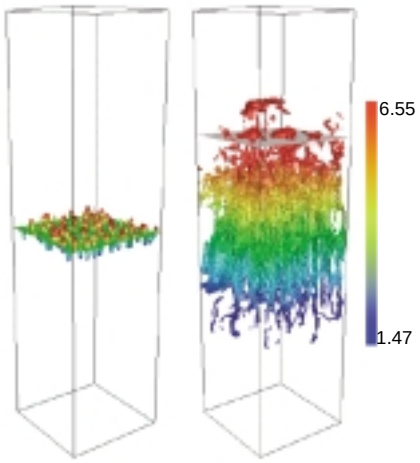
We use the front tracking method to study the RT and RM instabilities. Front tracking features high resolution of physical quantities at the material interface, thus giving a more accurate solution to the physical problem. It eliminates mass diffusion across the interface, reduces mesh orientation effects, and reduces diffusion of vorticity from the interface (where it is deposited by a shock wave in the RM instability) into the interior. Recently, we have implemented a robust grid-based method to handle the interface geometry. This method resolves the interface topology at the level of a single rectangular grid block. It provides a high degree of robustness to the numerical procedures. It reconstructs the interface at every time step and automatically corrects interfacial tangling. The traditional front tracking, known in contrast as grid-free tracking, also has advantages, in controlling the quality of the interface elements (triangles) and refined interface meshing.

A hybrid combination of the two methods will combine the best features of both. It is best suited for study of both the RT and RM instabilities. The use of grid-free tracking at the initial stage of both problems gives an accurate startup of the problem, since any grid-based interface description would require a very fine grid to resolve the fine-scale features and small amplitudes typically used to initialize the simulation studies. Grid-based tracking can handle the late-time chaotic stage of the fluid interface mixing without difficulty.

## ACCOMPLISHMENTS

Experimental values for the RT mixing coefficient $\alpha$ lie in the range of 0.05–0.07. FronTier simulation gives a value at the upper end of this interval, while most simulation codes report values of $\alpha$ outside of this experimental range, for example, $\alpha = 0.03$.

Using diffusion-based renormalization of the diffusive TVD simulation, we obtained agreement for all values of $\alpha$. We studied numerical mass diffusion by comparing the density distributions at horizontal slices drawn from similar penetration distances and heights within the mixing zone. The comparison




*Simulation of Rayleigh-Taylor fluid mixing instability (left, early time; right, late time). The cut plane (right) shows a height level with 5% light fluid. The mixing rate $\alpha = h/Agt^2 \approx 0.07$ falls within the experimental range.*

shows the expected complete absence of mass diffusion for FronTier, and an approximate 50% reduction of density contrast for the TVD simulation. On this basis, we computed a time-dependent reduced effective, or mass diffused Atwood number, and used it to obtain an effective $\alpha_f$ for the TVD simulation. Remarkably, $\alpha_f$ is approximately equal to 0.07.

We have conducted a number of axisymmetrically perturbed spherical pure and multimode RM simulations. A careful validation and numerical study was reported, and the influence of axisymmetry as a statistical bias (due to the "north pole effect") from pure spherical symmetry was observed and studied. FronTier appears to have overcome the problem of mesh orientation dependence which afflicts Eulerian codes.

## SIGNIFICANCE

Acceleration-driven fluid mixing instabilities play important roles in inertially confined nuclear fusion and stockpile stewardship. Turbulent mixing is a difficult and centrally important issue for fluid dynamics, and impacts such questions as the rate of heat transfer by the Gulf Stream, resistence of pipes to fluid flow, combustion rates in automotive engines, and the late-time evolution of a supernova. Our computational study will provide a better understanding of the development of these instabilities.

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J. Glimm, J. Grove, and Y. Zhang, "Interface tracking for axisymmetric flows," SIAM J. Sci. Comp. (submitted).

J. Glimm, J. Grove, X. L. Li, W. Oh, and D. Sharp, "A critical analysis of Rayleigh-Taylor growth rates," J. Comp. Phys. **169**, 652 (2001).

http://www.ams.sunysb.edu/~shock/FTdoc/FTmain.html

# Global Optimization Approaches to Protein Tertiary Structure Prediction

*Teresa Head-Gordon and Silvia Crivelli,*
*Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

We have developed a global optimization strategy that incorporates soft constraints in both a local optimization context and as directives for global optimization approaches. Such a strategy will only succeed if the objective function, or energy model, is sufficiently accurate, and it is through advances in optimization capability that shortcomings in the model generally are revealed.

## COMPUTATIONAL APPROACH

Protein structure prediction by optimization approaches requires effort focused on the following three areas: large-scale global optimization algorithms, construction of accurate energy models of proteins, and large-scale parallel computation. Our team has developed ways for the structure of the problem to be incorporated advantageously into the numerical optimization algorithms. Our global optimization approach draws on patterns and knowledge from biochemistry to provide guidelines and hints for the optimization method without making these hard constraints that limit the solutions that the method can find.

## ACCOMPLISHMENTS

Our group is one of the leaders in developing and assessing water and aqueous solvent models that are vital component of a successful energy model for protein folding. We recently participated in the Critical Assessment of Techniques for Protein Structure Prediction experiment (CASP4) in which hundreds of groups compete in blindly predicting the structures of proteins prior to their public release. Most methods used for CASP4 predictions rely heavily on knowledge about known proteins, whereas our method uses such knowledge only in forming secondary structure, but not in the prediction of overall tertiary structure.

*Global optimization result on phospholipase C β C-terminus, turkey, 242 amino acids. Ribbon structure comparison between experiment (center); submitted prediction (right), our lowest energy submission, which had an RMSD with experiment of 8.46Å; and next generation run of the global optimization algorithm (left). This new run lowered the energy of our previous best minimizer.*

The performance of our algorithm at the CASP4 competition can be summarized as follows: (1) Our method is more effective on targets where less information from known proteins is available. Our method produced the best prediction for one of the most difficult targets of the competition, a new fold protein of 240 amino acids. The method's atom-based energy function and novel solvation function, derived from experiments by our group, apparently did a reasonable job of discriminating misfolds from correct folds. (2) The method produced reasonable results with a very small number of initial configurations (1–10 compared to 1,000–millions in other methods). This suggests that the global optimization algorithm is more effective than the search mechanisms used by the other groups. (3) Our physical method takes a lot of computational time to converge, which makes it considerably more expensive than knowledge-based methods that use more information from the databases. (4) Further data that we developed after the CASP4 conference was the energy ordering of our submitted predictions relative to the experimental structures. We were pleased to find that the experimental structures were as low or lower in energy than the models we submitted to CASP4, verifying that the energy function that includes our unique solvation model is behaving appropriately.

## SIGNIFICANCE

The protein folding problem is one of the fundamental challenges of modern science. It is to predict the three-dimensional structure, or native state of a protein, given its sequence of amino acids. Optimization is one of the promising approaches to solving this problem, because it is believed that in most cases, the native state corresponds to the minimum free energy of the protein.

## PUBLICATIONS

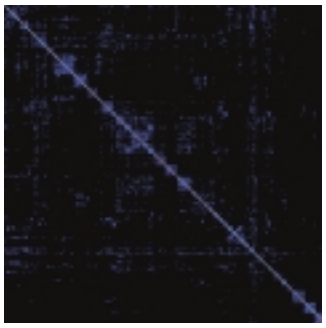
S. Crivelli, E. Eskow, B. Bader, V. Lamberti, R. Byrd, R. Schnabel, and T. Head-Gordon, "A physically based approach to protein structure prediction," Biophysical Journal (in press).

T. Head-Gordon and J. Wooley, "Computational challenges in structural and functional genomics," in Deep Computing in the Life Sciences, B. Robson, J. Coffin, and W. Swope, eds., IBM Systems Journal **40**, 265 (2001).

A. Azmi, R. H. Byrd, E. Eskow, R. Schnabel, S. Crivelli, T. M. Philip, and T. Head-Gordon, "Predicting protein tertiary structure using a global optimization algorithm with smoothing," in *Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches*, C. A. Floudas and P. M. Pardalos, eds. (Kluwer Academic Publishers, Netherlands, 2000), pp. 1–18. http://www.lbl.gov/~thg

# High Performance Sparse Matrix Algorithms

*Esmond Ng, Xiaoye Sherry Li, Chao Yang, and Parry Husbands,*
*Lawrence Berkeley National Laboratory*
*Patrick Amestoy, ENSEEIHT, Toulouse, France*
*Padma Raghavan, Pennsylvania State University*



*The graphic matrix comes from the structural analysis of an automobile body. The black background represents zero entries, while the colors represent the variation of nonzero values in the matrix. The matrix and the finite element discretization came from the PARASOL Project and were generated using the MSC Software.*

## RESEARCH OBJECTIVES

The goal of this research project is to develop and implement highly efficient and scalable algorithms for solving sparse matrix problems on various classes of high-performance computer architectures. Problems to be considered include direct methods and iterative methods for solving sparse linear systems, preconditioning techniques for iterative methods, and sparse eigenvalue problems.

## COMPUTATIONAL APPROACH

Both direct methods and iterative methods will be considered. For direct methods, the approach is based on matrix factorization. The techniques include ordering to preserve sparsity, symbolic factorization to determine structural information, and numerical factorization and solution. For iterative methods, the work will concentrate primarily on preconditioning, which attempts to improve the rate of convergence. Preconditioning based on incomplete factorization will be the focus of the work on iterative methods. In particular, technology that has been proven to be successful for sparse direct methods will be exploited as much as possible to enhance the performance of incomplete factorization. Multilevel incomplete factorization schemes will also be considered. Scheduling and task mapping techniques in the context of sparse matrix computation will be investigated.

Eigenvalue computation research will consider both Lanczos and Arnoldi iterations. Of particular interest is the solution of generalized eigenvalue problems for which the matrices are complex and symmetric. Initial work will focus on adapting PARPACK (parallel version of ARPACK) by incorporating scalable sparse direct linear system solvers to enhance the performance of shift-invert iterations. Approaches based on Jacobi-Davidson iterations will also be considered, in which case preconditioning techniques will be needed for the inner correction step.

## ACCOMPLISHMENTS

In the case of direct methods, we used NERSC computing resources to tune and analyze a general-purpose sparse solver (MUMPS), and then to compare it with the SuperLU code developed by Sherry Li and James Demmel. We have compared their performance characteristics with respect to uniprocessor speed, interprocessor communication, and memory requirements. Our ongoing work includes the improvement of the scalability of the MUMPS solver, the analysis of the impact of point-to-point communication on the performance of sparse solvers, algorithmic development in the continuation of reordering work, and the analysis of the influence of reorderings on the scalability of parallel sparse solvers.

In the case of iterative methods, we studied in detail the scalability of parallel block incomplete Cholesky factorization codes that we developed. Our current work involves developing new strategies to ensure the numerical stability of incomplete Cholesky factorization.

## SIGNIFICANCE

Sparse matrix problems are at the heart of many scientific and engineering applications, including fusion energy, accelerator physics, structural dynamics, computational chemistry, groundwater simulations, etc. The algorithms resulting from this project are expected to have significant impact on the performance of these applications. This research and development is part of the SciDAC project "Terascale Optimal PDE Simulations," and is particularly relevant to a number of SciDAC science applications, including accelerator physics simulation and fusion.

## PUBLICATIONS

John Gilbert, Xiaoye Li, Esmond G. Ng, and Barry Peyton, "On computing row and column counts for sparse QR factorization," BIT (in press).

Esmond G. Ng, Padma Raghavan, and Keita Teranishi, "Scalable preconditioning using incomplete factors," in *Proceedings of the Tenth SIAM Conference on Parallel Processing for Scientific Computing* (2001).

P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li, "Analysis, tuning and comparison of two general sparse solvers for distributed memory computers," Lawrence Berkeley National Laboratory Report LBNL-45992 (2000).

# Mixing Optimization in a Transverse Jet

*Ahmed Ghoniem, Massachusetts Institute of Technology*

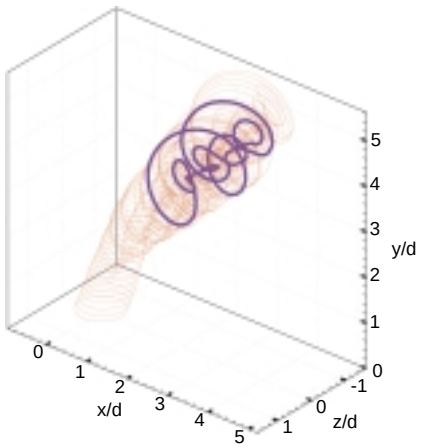
## RESEARCH OBJECTIVES

The goal of this project is to develop strategies for control and optimization of turbulent mixing and combustion—in particular, mixing and combustion at high Reynolds number in complex 3D vortical flows. These flows are typical of the mixing processes employed in almost all combustion-based energy-conversion systems. We intend to use these simulations in an investigation of the effectiveness of feedforward/feedback control of the underlying processes by imparting well-defined time-dependent boundary conditions on the flow.

## COMPUTATIONAL APPROACH

Our computation employs a Lagrangian, grid-free 3D vortex filament method for simulation of the Navier-Stokes equations at high Reynolds number. This method is used to construct a computational model of a spatially evolving transverse jet in which actuations are imposed as time-dependent boundary conditions. Arbitrary pulsation of the jet velocity is allowed, and the jet velocity profile may itself be altered in a time-dependent fashion.

Vortical velocity is obtained by integrating the discrete, desingularized Biot-Savart law along the vortex filaments. The present implementation incorporates a mesh refinement scheme to insure good resolution in the presence of strong flow gradients; core overlap is maintained between neighboring segments of a filament by inserting new nodes as the filament is stretched. To suppress the development of small scales, we employ filament-based hairpin removal algorithms, as introduced by Chorin, which helps curb a computationally overwhelming proliferation of vortex elements.




*Vortex filaments in the near field of the transverse jet. Ring-shaped filaments are introduced at the jet nozzle; as they penetrate into the flow, the downstream side of each filament folds and merges with the upstream side of neighboring vortex rings, as shown in the highlighted (blue) filament. As a result, vorticity is cancelled in a plane normal to the jet trajectory, while vorticity intensifies in two spirals aligned with the jet trajectory. This mechanism of distortion and folding transforms jet vorticity into a counter-rotating vortex pair.*

## ACCOMPLISHMENTS

In FY2001 we developed a code for unsteady 3D vortex-filament-based simulations of the transverse jet. A convergence study was undertaken to ensure the numerical fidelity of the simulation, in particular with respect to the parameters governing the spatial discretization of the vorticity field and the time integration of the flow.

Initial runs have focused on understanding the unforced dynamics of the transverse jet. Our computations have reproduced the key physical features observed in the experimental literature: rollup of the shear layer in the near field of the transverse jet, formation of a counter-rotating vortex pair oriented in the streamwise direction, and matching of the jet trajectory and vortex-pair trajectory with known experimental correlations. The counter-rotating vortex pair (CVP) is an essential coherent structure of the transverse jet and is its primary engine of entrainment and mixing. Earlier studies, both experimental and numerical, have not produced consensus on the formation mechanism of the CVP. Our computations have led us to identify a clear mechanism of CVP formation based on the underlying vorticity dynamics. We will use this mechanistic insight in designing actuation strategies for mixing optimization in the transverse jet.

## SIGNIFICANCE

The mixing and combustion dynamics of the transverse jet are important to a variety of engineering applications. Transverse jets may function as sources of fuel in industrial furnaces, or as diluent jets for blade cooling or exhaust gas cooling in industrial or airborne gas turbines. Other industrial applications include pipe tee mixers and jets of oil and gas entering the flow in oil wells. Transverse jets have also been studied extensively for their relevance to aerodynamics and to environmental problems such as pollutant dispersion from chimneys or the discharge of effluents into the ocean.

## PUBLICATIONS

Y. M. Marzouk and A. F. Ghoniem, "Computational modeling and control of mixing in a transverse jet," *First MIT Conference on Computational Fluid and Solid Mechanics*, Cambridge, MA, June 2001.

Y. M. Marzouk and A. F. Ghoniem, "Mechanism of streamwise vorticity formation in a transverse jet," *40th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, NV, January 2002 (in preparation).

Y. M. Marzouk and A. F. Ghoniem, "Modeling and control of mixing in a transverse jet," *18th International Colloquium on the Dynamics of Explosions and Reactive Systems*, Seattle, WA, August 2001.

http://centaur.mit.edu/rgd

# Information Retrieval Algorithms

*Horst Simon, Chris Ding, and Parry Husbands,*
*Lawrence Berkeley National Laboratory*

## RESEARCH OBJECTIVES

The goal of this research is to use high performance computing to help understand and improve subspace-based techniques for information retrieval, such as LSI (latent semantic indexing). In the past these techniques have been used only on very small data sets. We are developing an environment and scalable linear algebra algorithms where LSI-based information retrieval, for example, can be applied to matrices representing millions of documents and hundreds of thousands of key words and graphs the size of the World Wide Web. The computational power of NERSC systems is required to accomplish this.

## COMPUTATIONAL APPROACH

We continue to explore the use of the singular value decomposition and other low-rank approximations in information retrieval/data mining, not only of pure text collections, but of those augmented with hyperlinks (such as in the World Wide Web). We are investigating the use of link information to augment retrieval, attempting to discover and interpret structure in the Web and see how it can be used to improve retrieval accuracy. We perform both spectral and graph-based analyses of the link matrix on the Web.

## ACCOMPLISHMENTS

We have been able to perform singular value and eigen-decompositions of a site level graph of the World Wide Web. This has allowed us to extract some semantic structure purely from the information contained in the singular/eigenvectors. We have also been able to investigate the graph structure of the Web, confirming earlier observations on the length of paths between various sites.

## SIGNIFICANCE

This project is one of the first to compute decompositions of complete large term-document matrices. Other efforts have had to resort to sampling to keep things computationally tractable. Thus we are in a unique position to study how scale affects subspace-based retrieval techniques. We are also well poised to discover new and interesting features about the structure of the Web.

We believe that the algorithms developed here will be of use not only in text retrieval, but in more complicated settings such as classification of image collections and extraction of images with desired features from large collections. Combining effective search and classification algorithms for image problems with the compute and storage capabilities of future NERSC systems will position Berkeley Lab as a leader when it comes to developing algorithmic techniques for the data and visualization corridors of the next decade.

## PUBLICATIONS

Chris Ding, Parry Husbands, Horst Simon, and Xiaofeng He, "Analysis of hubs and authorities on the Web," Lawrence Berkeley National Laboratory report LBNL-47847 (2001).

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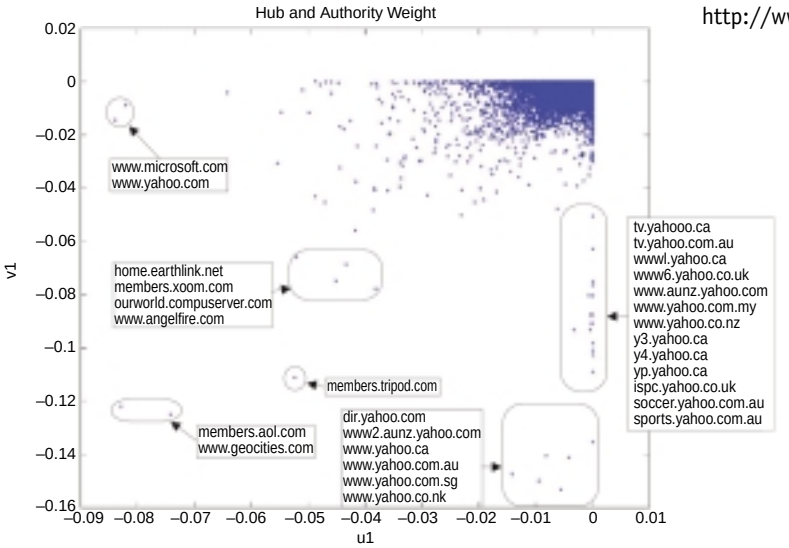
Parry Husbands, Charles Isbell, and Alan Edelman, "MATLAB*P: A tool for interactive supercomputing," in *Proceedings of the 9th SIAM Conference on Parallel Processing for Scientific Computing* (1999).

http://www.nersc.gov/research/SIMON




*Hub weight vs. authority weight for a site level graph of the World Wide Web. "Hubs" point to useful sources of information, while "authorities" are themselves informative sites. The calculation of these weights involves a large singular value decomposition of the adjacency matrix of the Web graph. The hub weights are identified with the first right singular vector (v1), and the authority weights with the first left singular vector (u1). It is interesting to note that some broadly related sites (directories, home page repositories, and other popular sites) can be grouped together using this technique.*

# APPENDIX A *NERSC Policy Board*

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Princeton Plasma Physics Laboratory

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Fermi National Accelerator Laboratory

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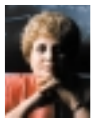

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University of Texas

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Douglas Rotman
Environmental Sciences
Lawrence Livermore National Laboratory

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APPENDIX D

# Supercomputing Allocations Committee

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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***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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Linda Twenty
ASCR Program Analyst

For SciDAC projects, we acknowledge the management support of Steve Eckstrand, Acting Assistant Director for SciDAC (until October 2001); David Bader, Acting Assistant Director for SciDAC (since October 2001); and Kimberly Rasar, Deputy Assistant Director for SciDAC.

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APPENDIX F

# *Advanced Scientific Computing Advisory Committee*

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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# *Index of Researchers*

The researchers listed below produced the scientific results highlighted in this report.

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