NERSC

# 1998 ANNUAL REPORT

National Energy Research Scientific Computing Center

Ernest Orlando Lawrence
Berkeley National Laboratory
Berkeley Lab


# 1998 Annual Report

National Energy Research
Scientific Computing Center


ERNEST ORLANDO LAWRENCE
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LBNL-42920, March 1999

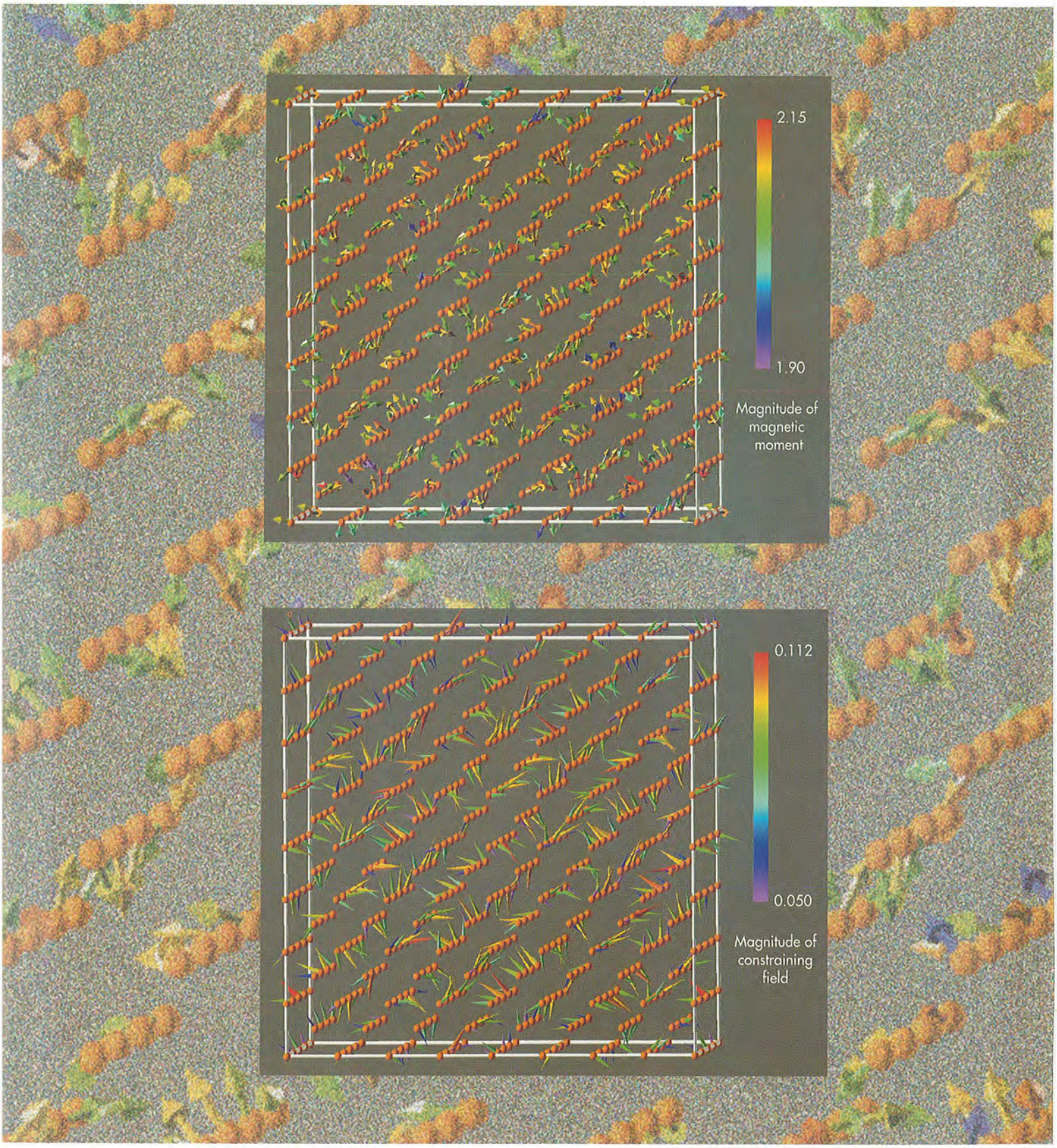
NERSC aspires to be a world leader in accelerating scientific discovery through computation. Our vision is to provide high-performance computing tools to tackle science's biggest and most challenging problems, and to play a major role in advancing large-scale computational science and computing technology. 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.

# Contents

# Director's Perspective



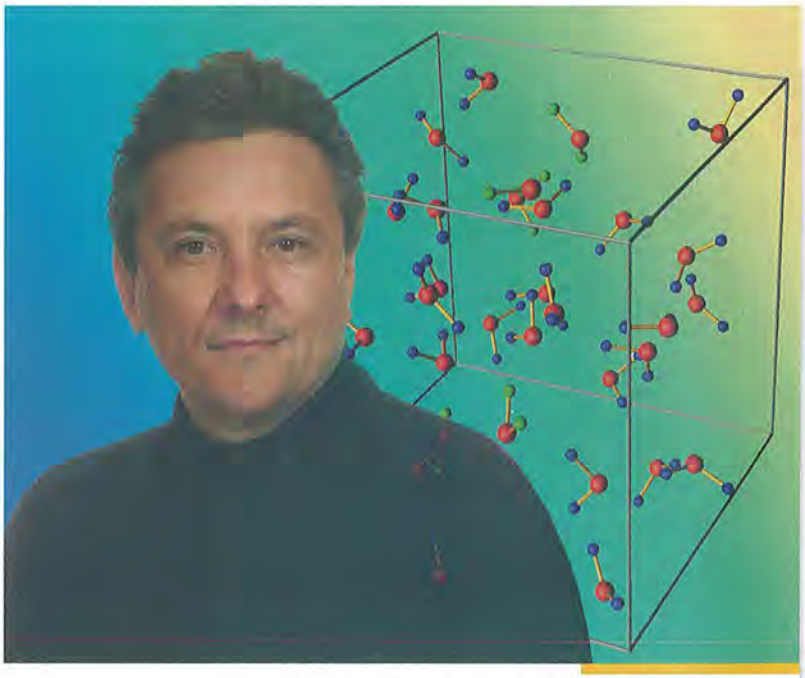

**The 1998 Gordon Bell Prize for best performance of a parallel supercomputer application went to a team of collaborators from DOE's Grand Challenge on Materials, Methods, Microstructure, and Magnetism. Their 1024-atom first-principles simulation of metallic magnetism in iron, with code tested and fine-tuned at NERSC, was the first complete application to break the teraflops barrier. Their performance achievement is discussed on page 6, and their research is described on page 40.**

Looking back, 1998 was another year of positive changes and great achievements for NERSC. When we set out to reinvent NERSC three years ago, our vision was to make NERSC a world leader in high performance computing by balancing excellent services with a first-class research program in computer science and computational science. Our latest accomplishments clearly demonstrate the success of NERSC's vision of a high performance computing center. I have read our annual report with great satisfaction. The report documents not only major progress in all areas at NERSC, but also the accelerated pace of scientific discovery we are enabling in our community of users.

During 1998 we completed our transition to HPSS; combined our two Cray T3Es into a single, 640-processor machine; decommissioned the C90; upgraded the J90 cluster; installed new math and visualization servers; completely overhauled the PDSF; and on top of all this began the procurement process for our next supercomputer. Almost every month there was a major systems change. This rapid pace of innovation was kept without ever dropping our high commitment to quality. A survey of our users confirmed that indeed we are doing extremely well in delivering these resources and services to the DOE Office of Science research community.

We ended the year with a strong showing at SC98, which demonstrated NERSC's intellectual leadership. NERSC researchers brought home the 1998 Sidney Fernbach Award recognizing efforts in computational science, as well as the Gordon Bell Prize for one of our Grand Challenge collaborations between NERSC, Oak Ridge National Laboratory, the Pittsburgh Supercomputing Center, and the University of Bristol. Not only did this team win the prize, but they also were the first to achieve a 1.02 teraflops performance with a real scientific application code producing real scientific results.

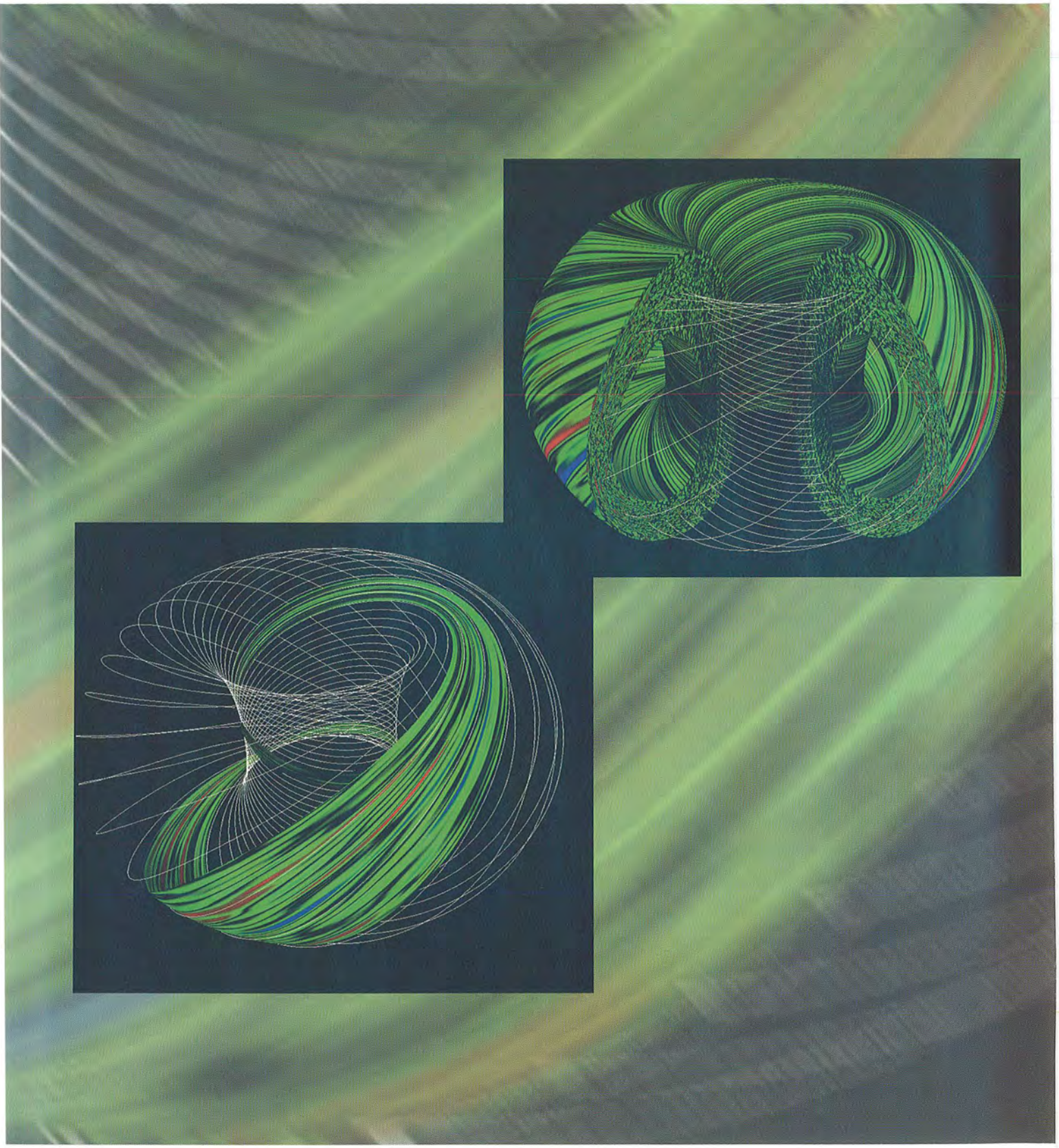
Our fast pace will continue throughout 1999. DOE just announced a new allocations policy for NERSC. This will bring major changes, since NERSC will operate more like other DOE national user facilities, with extensive peer reviews and outside advisory boards. The initial NERSC-3 platform will be online and available for early users within the next few months, and will bring major new challenges. Finally, there is a proposal to significantly increase the level of federal funding for information technology. Congress is considering a significant increase in the DOE Office of Science budget for this new initiative. NERSC is already deeply involved in the planning process, and we expect major new opportunities to arise within a year that will even further enhance our contributions to the DOE Office of Science mission.



**Horst D. Simon, Division Director of NERSC**

With these exciting times ahead of us, I am again grateful to our DOE Office of Science sponsors for their continued endorsement of all of our ambitious plans. I would like to thank our clients, in particular ERSUG and EXERSUG members, for their continued support in transition times, especially for their willingness to collaborate on the new allocation process and their input to the NERSC procurement. My special thanks and congratulations, however, 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



The Numerical Tokamak Turbulence Project, a DOE Grand Challenge, is developing the ability to predict turbulence in tokamak fusion experiments. These images show the results for the perturbed plasma density from a Gryffin gyrofluid ion-temperature-gradient (ITG) instability simulation viewed in noncircular magnetic geometry. The ITG perturbations are shown on a bundle of magnetic flux lines in the lower image. See page 30 for details.

Outstanding achievements in computational science are enhancing the reputation of NERSC and the nationwide community of researchers who use our computing facilities. High performance computing is a field in which real-world results sometimes lag behind technological advances. For several years, NERSC has been working to narrow that gap, making state-of-the-art computing a practical tool for scientific research.

Our success was recognized by our peers in the awards presented to NERSC researchers and staff at SC98 in Orlando (see page 6). But our real reward is the satisfaction we receive from contributing to scientific progress, such as the discovery that the universe is expanding at an accelerating rate, and thus is likely to go on expanding forever (page 8).

As a national facility for scientific research, funded by the Department of Energy, Office of Science (DOE SC), NERSC annually serves about 2,000 scientists throughout the United States (Figure 1). These researchers work in DOE laboratories, universities, industry, and other Federal agencies (Figure 2). 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 (Figure 3 on the next page).

This Annual Report provides a representative (though not exhaustive) sampling of NERSC researchers' scientific accomplishments in 1998.

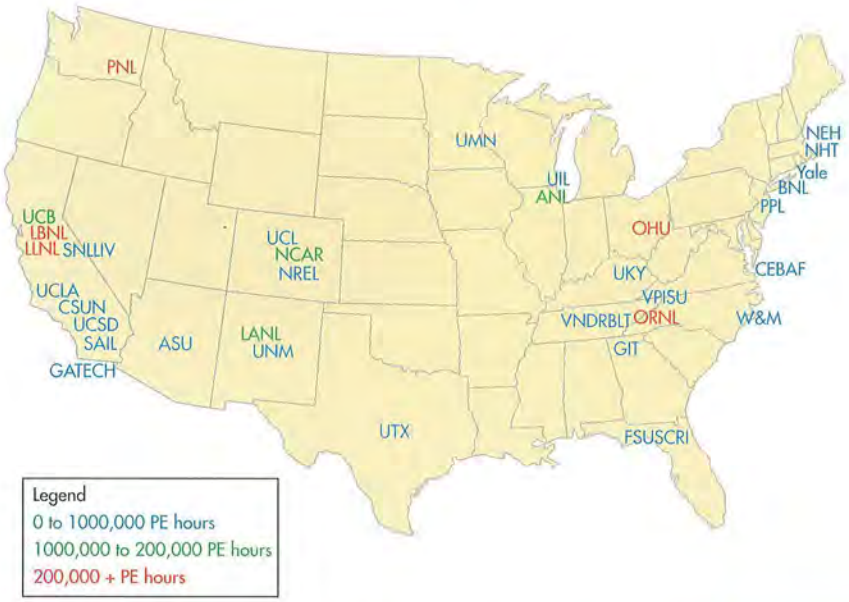
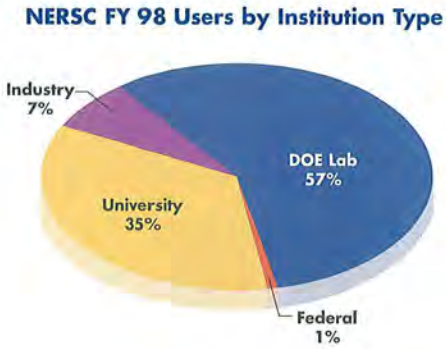



**Fig. 1. Principal locations of U.S. scientists who use NERSC's computing facilities, showing the level of usage at each location.**



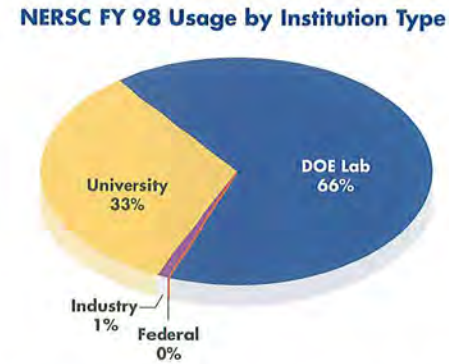




**Fig. 2. Percentage of NERSC users from the four types of institutions where they work (top); percentage of usage (i.e., computing time) from each type of institution (bottom). The zero is a result of rounding.**

## Grand Challenge Breakthroughs

Through its Mathematical, Information, and Computational Sciences (MICS) Division, the DOE Office of Advanced Scientific Computing Research (ASCR) sponsors NERSC as a national facility, and also sponsors eight Grand Challenge projects in which NERSC is a partner. Grand Challenge applications address computation-intensive fundamental problems in science and engineering whose solutions can be

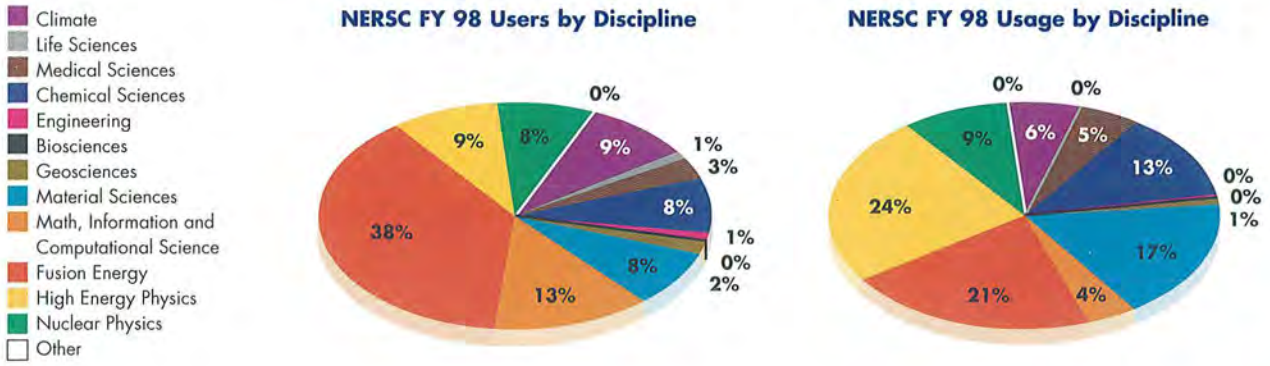
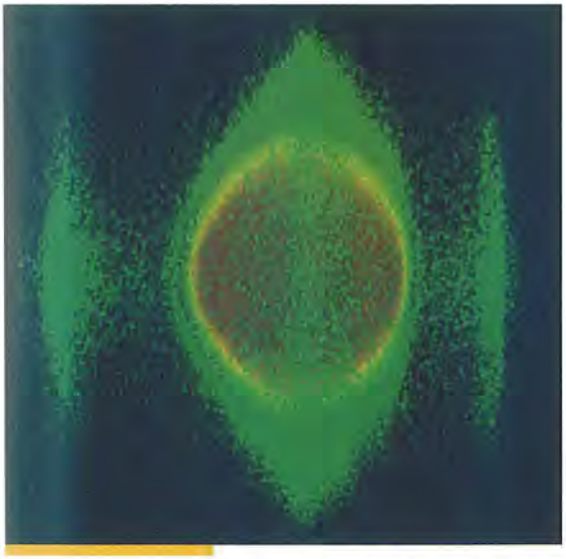



**Fig. 3. NERSC users (left) and usage (right) by scientific discipline; zeros result from rounding.**

advanced by applying high performance computing and communications technologies and resources.

The advanced modeling tools developed in the Computational Accelerator Physics Grand Challenge will allow future particle accelerators to be designed with reduced cost and risk as well as improved reliability and efficiency. During the past year, collaborators parallelized the electromagnetics codes, performed high-resolution calculations for the Next Linear Collider and the Spallation Neutron Source, and performed the largest simulations to date for the Accelerator Production of Tritium project.



**The Computational Accelerator Physics Grand Challenge is working to understand and predict beam halo, a major issue in next-generation high-current linear accelerators. (Details on page 38.)**

In the Computational Chemistry of Nuclear Waste Characterization and Processing Grand Challenge, researchers are developing and applying the methods of relativistic quantum chemistry to assist in the understanding and prediction of the chemistry of actinide and lanthanide compounds. Modeling these heavy-element compounds is essential to modeling the fate and transport of nuclear wastes in the environment, as well as evaluating remediation alternatives. Existing codes are being parallelized for the T3E and extended to enable calculations on larger molecules at higher levels of accuracy.

Several members of the Grand Challenge Application on HENP (High Energy and Nuclear Physics) Data successfully ported the CERNLIB physics software to a parallel architecture—a large and complex task that had been attempted several times before but never completed (see further discussion on page 24). The project also generated over 1 terabyte (TB) of simulated heavy ion collision data, to be used as a testbed for developing data management and analysis tools and algorithms. A cross-country data transfer experiment, from NERSC in Berkeley to Brookhaven National Laboratory on Long Island, achieved transfer rates of 800–900 kB/sec over brief periods, and sustained an average 200 kB/sec over several days.

The High Performance Computational Engine for the Analysis of Genomes Grand Challenge has developed a prototype web-based framework, The Genome Channel,

which shows the current progress of the international genome sequencing effort and allows navigation through the data down to individual sequences and gene annotations. Work in progress also includes developing a CORBA-based analysis framework to facilitate automation of the genome annotation process, developing specialized software and databases for genome analysis, and preparing to utilize the NERSC T3E for production analysis. (For a discussion of NERSC's Center for Bioinformatics and Computational Genomics, see page 15.)

In the Materials, Methods, Microstructure and Magnetism Grand Challenge, researchers are establishing the relationship between magnetism and microstructure based on fundamental physical principles. Understanding this relationship could result in breakthroughs in computer storage as well as power generation and storage, and could enable the design of magnetic materials with specific, well-defined properties. In 1998 the group studied quantum atomic interactions on a scale not previously accessible, and developed a new constrained local moment theory of non-equilibrium states in metallic magnets—in addition to winning the Gordon Bell Prize and breaking the teraflops barrier (see page 6).

Researchers in the Numerical Tokamak Turbulence Project reported a major advance in the computer modeling of fusion plasmas in the September 18 edition of *Science* magazine. Using NERSC's Cray T3E for three-dimensional nonlinear particle simulations of microturbulence in the plasma, they performed calculations involving 400 million plasma particles in 5000 time-steps—the first simulations realistic enough to compare with existing experiments. The Cyclone Project, which compared various models for core transport in tokamaks, was also discussed in both *Science* and *Nature*.

Detailed simulations of the Standard Model of particle physics, developed in the Particle Physics Phenomenology from Lattice QCD Grand Challenge, will help determine some of the fundamental constants of nature. In the past year, researchers successfully computed the decay amplitudes of kaons for the first time, and successfully reproduced the observed "delta I=1/2" effect, in which seemingly similar decay processes proceed at different rates. They established a publicly available "Gauge Connection" archive (http://qcd.nersc.gov), which provides "unquenched" lattice quantum chromodynamics (QCD) configurations that include virtual quarks. A new algorithm being developed will speed up calculations involving virtual quarks.

In the Protein Dynamics and Biocatalysis Grand Challenge, researchers are working to understand the chemical mechanisms in enzyme catalysis, which are difficult to investigate experimentally. Computer simulations can provide the necessary insights, at an atomic level of detail, for a complete understanding of the relationship between biomolecular dynamics, structure, and function. For example, while the class of enzymes known as beta-lactamases are largely responsible for the increasing resistance of bacteria to antibiotics, the precise chemical resistance mechanism used by this enzyme is still unknown. Simulations are critical for further study of this mechanism.

## Advanced Scientific Computing Research

In addition to the Grand Challenges, ASCR/MICS sponsors other computationally intensive research projects. One research team achieved the first direct numerical solution of a quantum mechanical three-body Coulomb problem—specifically, electron-hydrogen ionization. Another group developed an efficient code for stochastic simulation on a parallel computer, which is being used to study magnetic switching. Other scientists are simulating the complex instabilities of fluid mixing layers, which can be found everywhere from supernova explosions to petroleum pipelines. And NERSC's Center for Computational Sciences and Engineering (CCSE) develops and applies advanced computational methodologies to solve large-scale scientific and engineering problems arising in DOE mission areas involving energy, environmental, and industrial technology. (See page 18 for a discussion of CCSE's combustion modeling research.)

# NERSC Staff, Researchers Win Top Computing Awards

Andrew Canning

Phil Colella

Two NERSC staff members and two NERSC clients were honored by the scientific computing community as recipients of top awards at SC98 in Orlando, Florida.

A team of researchers working on the DOE Grand Challenge project Materials, Methods, Microstructure, and Magnetism won the 1998 Gordon Bell Prize for best performance of a supercomputing application. The team won the award for their modeling of 1,024 atoms of a metallic magnet. The model was run on progressively more powerful Cray T3Es, starting with NERSC's 512-processor machine, and won the prize with a top performance of 657 gigaflops on a 1024-processor T3E. Shortly before the prize was awarded, the group was given access to a 1480-processor machine on Cray's manufacturing center floor and achieved 1.02 teraflops performance—the first time a complete application broke the teraflops barrier.

The prize-winning group included Malcolm Stocks, B. Ujfalussy, Xin-Dong Wang, Xiaoguang Zhang, D. M. C. Nicholson, and W. A. Shelton of Oak Ridge National Laboratory; NERSC staff physicist Andrew Canning; Yang Wang of the Pittsburgh Supercomputing Center; and B. L. Gyorffy of the University of Bristol, UK. Andrew Canning's role included testing the code, working with Cray to fine-tune it, obtaining access to the fastest computers, and running the code at record-breaking speeds.

Phil Colella, leader of NERSC's Applied Numerical Algorithms Group, received the 1998 Sidney Fernbach Award "for fundamental contributions in the development of software methodologies used to solve numerical partial differential equations, and their application to substantially expand our understanding of shock physics and other fluid dynamics problems."

Phil's award nomination cited his contributions in high-resolution finite difference methods, adaptive mesh refinement, volume-of-fluid methods for fronts and irregular geometries, and multidimensional shock dynamics.

Another 1998 Gordon Bell prize recognized scientists who achieve the best price/performance level on a computer system. The winning team in this category included Greg Kilcup, a physicist at The Ohio State University. And the SC98 award for Best Applications Paper and Best Overall Paper went to a paper co-authored by Robert Harrison of Pacific Northwest National Laboratory. Kilcup and Harrison are both DOE Grand Challenge researchers and NERSC clients.

Earlier, at the Fifth Copper Mountain Conference on Iterative Methods, Mark Adams from the University of California, Berkeley (a student of UCB/NERSC computer scientist James Demmel) won the best student paper competition for his work on a parallel multigrid solver for unstructured finite element method meshes in solid mechanics.

## Basic Energy Sciences

DOE's Office of Basic Energy Sciences (BES) sponsors research in areas including materials sciences, chemical sciences, geosciences, and engineering. NERSC provides computational support for a large number of BES projects.

Materials science researchers using NERSC systems during the past year clarified how the properties of materials are changed during ion irradiation or cluster bombardment; modeled microstructural pattern formation during the growth of solids; developed the first method for calculating the optical properties of insulators and semiconductors from first principles, which may lead to the synthesis of higher-temperature superconductors; completed the first million-atom simulation of semiconductor quantum dots, a key area of research for atomic-scale computing; and improved the techniques for determining macroscopic mechanical properties from microscopic calculations, which will accelerate the search for ultra-hard materials and protective coatings.

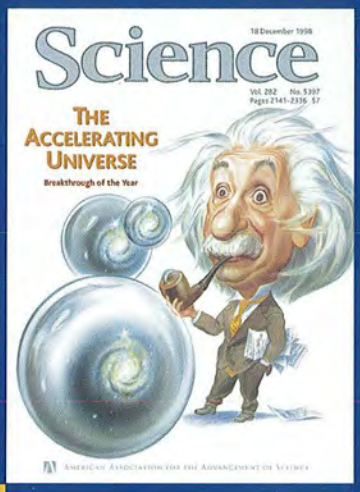
Chemical science researchers studying the molecular basis of complex fluids achieved the first molecular-simulation-based prediction of the viscosity index of a lubricant; this kind of simulation could lead to the creation of more efficient and environmentally benign lubricants and solvents. Other computational chemists characterized the electronic structure of ceramic-metal interfaces, which is important for the development of improved sensors, electronic components, medical prostheses, and high-temperature alloys; worked on first-principles prediction of materials performance for electrolytes and electrodes in batteries and fuel cells, which reduces the need for expensive trial-and-error experimentation; studied electron transfer dynamics at semiconductor-liquid interfaces, which may eventually lead to new or improved alternative energy sources; developed computational procedures for atomic structure calculations that can predict properties such as energy levels, binding energies, and transition probabilities; and applied the molecular theory of matter to metastable liquids, enriching the fundamental understanding of metastability.

**Modeling microstructural pattern formation during the growth of a solid helps determine what the final properties of the fabricated material will be. (Details on page 55.)**

Unlocking the mysteries of combustion through numerical simulations requires a multidisciplinary approach that involves specialists in fields such as computational fluid dynamics and chemical kinetics. In a new approach to simulating chemical kinetics, the solution of ordinary differential equations has been parameterized by a set of algebraic polynomials; this approach has produced accurate simulations in one-tenth the processing time. Researchers are also using NERSC computers to simulate step-by-step chemical reactions in diesel fuel combustion, model turbulent combustion as found in gas burners, elucidate the mechanisms of soot formation, and identify the exact mechanism that determines the formation of polycyclic aromatic hydrocarbons (PAHs), which are potent carcinogens and mutagens formed during incomplete combustion of fossil fuels. (The contributions of NERSC staff mathematicians to simulating the fluid dynamics of combustion are discussed on page 18.)

In the geosciences, researchers are modeling the molecular structure at the surface of hydrated clay minerals, which are important in petroleum production and the containment of environmental contaminants; developing

# NERSC Plays Key Role in Science Magazine's "Breakthrough of the Year"




**Einstein watches in surprise as a universe expands exponentially, its galaxies rushing apart ever faster. Evidence for an accelerating universe resurrects Einstein's discarded idea of a cosmological constant which counteracts gravity and pushes space apart. (Copyright © 1998 by the American Association for the Advancement of Science. Used with permission. Illustration: John Kascht. Albert Einstein™ represented by the Roger Richman Agency, Inc., Beverly Hills, CA.)**

The discovery that the universe is expanding at an accelerating rate, and thus is likely to go on expanding forever, was named Science magazine's "Breakthrough of the Year for 1998." The international Supernova Cosmology Project, headed by Saul Perlmutter of the Berkeley Lab Physics Division, calculated how fast the universe was expanding at different times in its history by comparing the distance of Type Ia supernovae with the redshifts of their home galaxies. To analyze the data from 40 supernovae for errors or biases, the cosmology team used the Cray T3E at NERSC.

Perlmutter's team used ground-based telescopes plus the Hubble Space Telescope and the T3E to determine the universe's rate of expansion. The discovery was confirmed by the High-z Supernova Search Team in Australia, who shared the magazine's honor. In addition to showing that there is not enough mass in the universe for gravitation ever to stop the expansion, the discovery implies that an unknown property of space, called the cosmological constant and first proposed by Albert Einstein, is acting to expand space itself.

To analyze the supernova data for errors or biases, the Supernova Cosmology team used the Cray T3E-900 to simulate 10,000 exploding supernovae at varying distances, given universes based on different assumptions about cosmological values; these were then plotted and compared with real data to detect any biases affecting observation or interpretation.

To make meaningful comparisons of nearby and distant Type Ia supernovae—in other words, to confirm their usefulness as "standard candles," objects whose intrinsic brightness is the same wherever they are found—the light measurements from the more distant supernovae, with larger redshifts, were compared with the redshifts of closer ones. These measurements were then altered slightly to examine the effects of dust along the line of sight, and to test slightly different explosion scenarios. These simulations were compared with the team's observations to make sure the data matched their theoretical calculations.

The T3E was also used to make sure that the error bars presented in the research were reasonable. In addition to chi-square fitting, researchers employed bootstrap resampling of the data. Here they plotted the mass density of the universe and the vacuum energy density based on data from 40 supernovae. Then they began resampling the data, taking random sets of any of the 40 supernovae and finding and plotting the minimum value for each parameter. The resampling procedure was repeated tens of thousands of times as an independent check on the assigned error bars.

next-generation wave propagation and hydrodynamics codes for computational geophysics; and developing high-resolution geophysical imaging software that will be an essential tool for DOE projects involving oil, gas, coal, geothermal energy, and geophysical exploration, as well as environmental restoration of contaminated sites and nuclear waste.

Engineering problems involving slurries, fluidized beds, hydraulic fracturing, and many other applications will benefit from the first parallel numerical software that can directly simulate solid particles moving in a viscoelastic fluid.

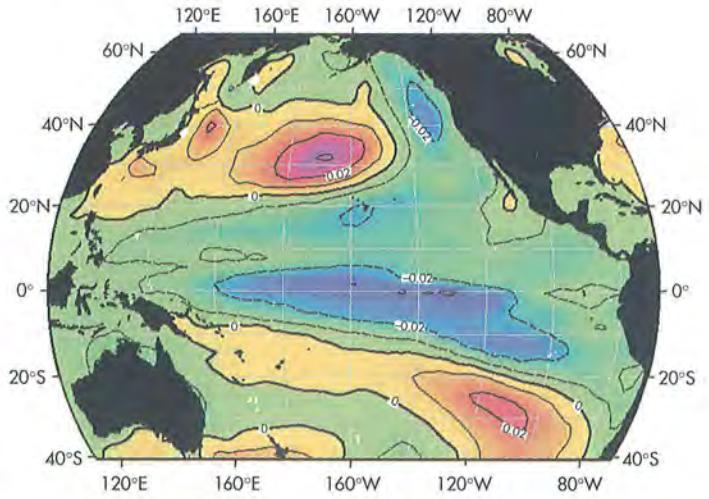
## Biological and Environmental Research

Computational simulations are now playing a crucial role in biological and environmental research, particularly in the areas of climate modeling and genomics.

NERSC's high performance computers are being used by researchers nationwide for global climate change simulations and other atmospheric studies, as well as investigations of pollutant formation, energy use, and other environmental issues.

A team led by the National Center for Atmospheric Research (NCAR) used the new high-resolution Parallel Climate Model (PCM) to produce a climate simulation for the 1990s which will be used as the control experiment for future climate change scenarios. The NCAR/NERSC collaboration has achieved the fastest climate modeling performance in the nation. Using 256 processors on NERSC's Cray T3E, it takes less than a half hour to simulate one model year with PCM; the same one-year simulation would take more than 10 hours on the older Cray C90.

Collaborators at NERSC and the National Oceanic and Atmospheric Administration's Geophysical Fluid Dynamics Laboratory (GFDL) are adapting GFDL's Modular Ocean Model (MOM) so that it will run efficiently on massively parallel computers for high-resolution, century-long ocean simulations. In the first phase of the project, portions of the code are running 15 to 50 times faster.



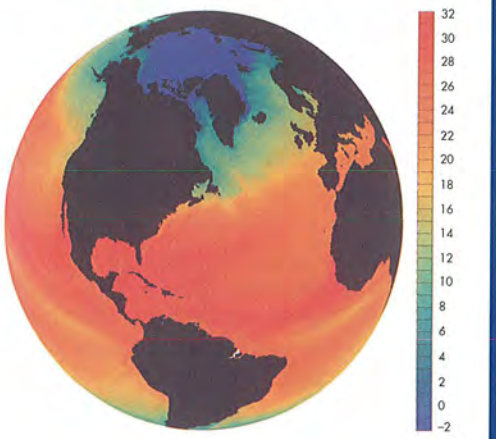

**The similarity of this simulation to observed conditions shows that the coupled ocean/atmosphere general circulation model faithfully captures the large-scale patterns of low-frequency climate variability. This pattern is associated with changes in winter temperature and precipitation over much of North America. (Details on page 71.)**

Another GFDL team working with an atmospheric general circulation model has found that increased vertical resolution produces far more realistic simulations of winds in the tropical middle atmosphere. This important discovery opens up the possibility of alleviating one of the most serious and widespread problems in atmospheric simulation—the absence of the Quasi-Biennial Oscillation (QBO).

Researchers at the Scripps Institution of Oceanography are working on a coupled ocean/atmosphere model to determine the predictability of century-long precipitation and temperature patterns. At various DOE laboratories, scientists are making seasonal hydroclimate predictions for the western U.S.; developing a global tropospheric/stratospheric model to assess the impacts of energy-related emissions on tropospheric ozone; and investigating the effects of albedo (atmospheric reflection of light) due to sulfate aerosol emissions. A team of researchers from NCAR and academia are using simulations to study the effects of gravity waves on the atmosphere.

The Human Genome Project is producing an enormous database of amino acid sequences. To understand what

# Parallel Processing Allows Faster, More Detailed Climate Modeling




**This image depicts the sea surface temperature from a coupled simulation with PCM. Note the Gulf Stream meander pattern and the cooler tropical Pacific and Atlantic surface temperatures caused by upwelling of cold water. Also depicted is the cold water under the Arctic and East Greenland sea ice.**

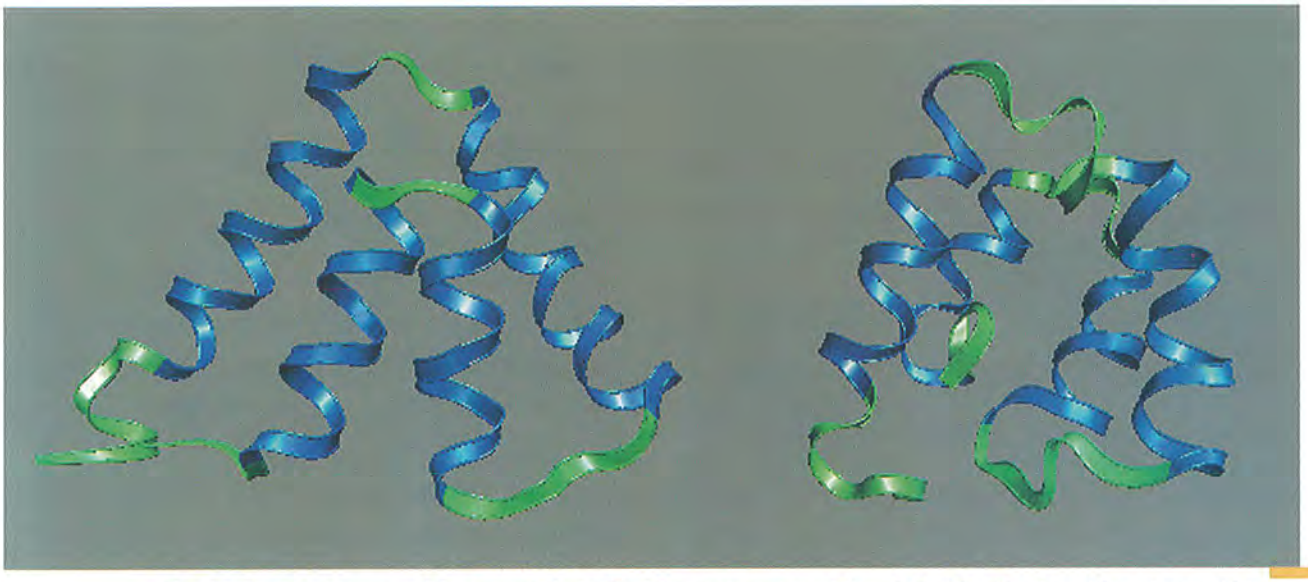
In the past 10 years, as scientists have achieved a better understanding of the Earth's climate, the computer industry has developed ever-more-powerful machines. These two factors are now resulting in increasingly accurate computer modeling tools for studying and predicting climate change. Some important results are coming from the partnership between NERSC and climate modeling experts at the National Center for Atmospheric Research (NCAR) in Colorado.

Collaborating scientists at NCAR, the Naval Postgraduate School, and Los Alamos National Laboratory are able to run their Parallel Climate Model with High Resolution Ocean and Sea Ice (PCM) faster than ever on NERSC's T3E-900. Running PCM on an older model supercomputer, such as a 16-processor Cray C90, would require more than 10 hours to simulate one year, or more than three months of computer time to model a century. Using half of the 512 processors of NERSC's T3E-900, the same model can be run 28 times faster. The entire model could not even be loaded on smaller systems.

"The performance NCAR has acheived is unmatched by other climate codes in the United States," said NERSC Division Director Horst Simon. "The NCAR team has demonstrated that production climate research can be carried out on a parallel processing, distributed memory supercomputer. Not only does NCAR's code run well on our machine, but its design also allows it to be scaled up for creating an even more powerful model in the future."

Warren Washington of NCAR, principal investigator on the project, and his colleagues are investigating the effect of greenhouse gas increases and sulfate aerosols on global warming (see page 83). While increased greenhouse gases cause global warming, sulfate aerosols cause less warming, and in some cases, regional cooling. It is the capability of running the ocean and sea ice components that makes PCM so useful, according to Washington. The higher the resolution for such features as the Gulf Stream or Kurioshio Current, the more accurately their role can be included as transporters of heat and salt.

Just as one year's weather cannot be interpreted as evidence of climate change, one computerized model cannot produce definitive answers. Instead, researchers need to run a series of different modeling experiments to take into account differing possible future climate scenarios. "We need to know if the change is statistically significant in order to confidently answer the questions being asked by policy-makers," Washington says. More powerful computers allow these simulations to be researched at higher resolution.



**The global optimization approach has successfully simulated the protein structure of the α-chain of the 70-amino-acid protein uteroglobin. Shown here are the predictions from crystal structure (left) and sequence (right). (Details on page 75.)**

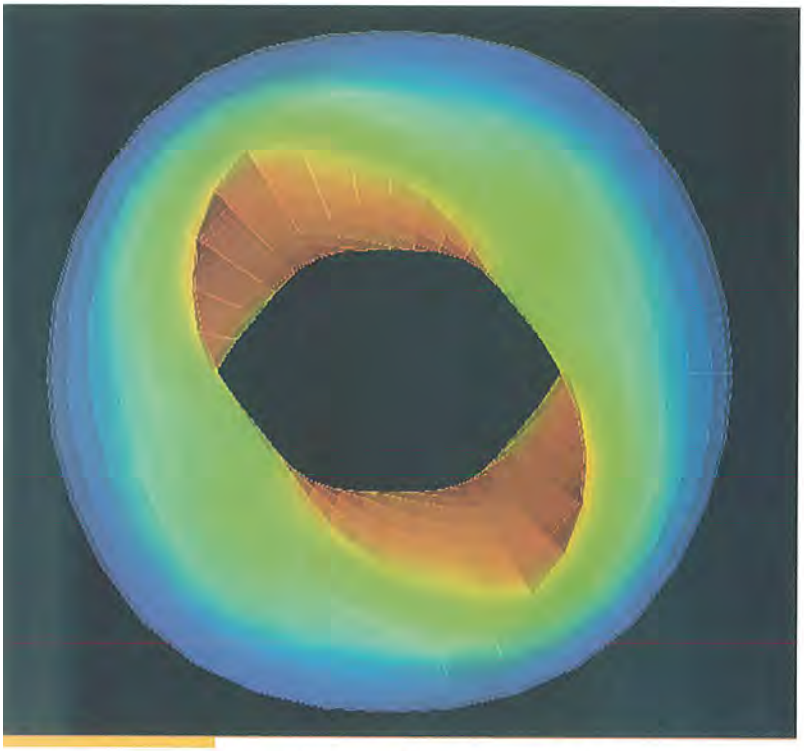
they mean, we must understand how amino acid sequences result in protein structures and functions. Computational biologists are using simulations to predict a protein's three-dimensional atomic structure—that is, how the protein folds. Accurate computational prediction of protein folds, coupled with comparative modeling and *ab initio* predictions, could significantly accelerate the interpretation of genome data.

Several different approaches to protein fold prediction are being tested on NERSC computers. One method, which approaches folding as a taxonometric and statistical problem, uses a neural-network-based expert system to assign proteins to folding classes. As a large-screen filter for predicting gross fold topologies, this method has an advantage over detailed sequence comparison, because sequences belonging to the same folding class can differ significantly at the amino acid level.

A second approach—a global optimization strategy for predicting protein structure—is based on the theory that proteins adopt the structure with the lowest free energy level. Therefore, finding the location of the lowest energy level, or the global minimum, helps identify the fold structure. The global optimization approach has successfully simulated the potential energy surfaces of small homopolymers, homopeptides, and α-helical proteins, including the 70-amino-acid protein uteroglobin.

Even though the process of protein folding occurs in milliseconds, that is too long for the molecular dynamics of the full process to be simulated on the current generation of computers. An ingenious new way around this problem exploits the fact that a small protein fragment can be unfolded at high temperatures in nanoseconds. After simulating the all-atom molecular dynamics of the unfolding process, researchers were able to perform a series of short simulations of protein refolding, starting from the discrete transition states determined by the unfolding simulations. The refolding simulations showed a surprisingly good agreement between high- and low-temperature transition states, as well as experimental results under physiological conditions.

In addition to protein folding, computational biologists are exploring the fundamental dynamics of other biological processes. For example, one team of researchers performed the first molecular dynamics simulation of carcinogen-damaged DNA replicating and mutating in the presence of an enzyme. This 12,000-atom simulation demonstrated the mutagenic effect of benzo[a]pyrene, a common pollutant found in automobile exhaust and tobacco smoke.



**Contours of magnetic field strength on the last closed flux surface of an optimized stellarator configuration, demonstrating good toroidal symmetry. (Details on page 89.)**

## Fusion Energy Sciences

Research sponsored by DOE's Office of Fusion Energy Sciences is steadily bringing the promise of this sustainable and environmentally benign energy source closer to fruition. The broad spectrum of fusion research at NERSC encompasses a variety of magnetic confinement configurations—tokamak, spheromak, and stellarator—as well as inertial confinement.

One of the current objectives of tokamak research is to develop ways to inject cold fuel into the core of the tokamak. Recent experiments indicate that if pellets of cold fuel are injected from the outside of the tokamak, they are expelled without reaching the center, while if the pellets are injected from the inside (i.e., the hole of the donut), the fuel does reach the center. This effect was reproduced this year in a 3D simulation code, which is helping physicists understand the phenomenon.

In other tokamak research, gyrokinetic turbulent transport simulations have been used to analyze and predict experimental results, and a new zero-transport state has been found. Researchers also developed and parallelized the first 3D global-turbulence simulation code in a realistic toroidal x-point geometry.

Simulations are helping physicists develop other fusion configurations as well, including new stellarator configurations that provide improved plasma confinement and stability within a more compact design. Plasma formation and magnetic reconnection in a spheromak were successfully simulated this year. And to help develop an inertial fusion driver, researchers are simulating heavy-ion induction acceleration to study basic beam physics, analyze beam behavior in experiments, and predict beam behavior in future facilities.

## High Energy and Nuclear Physics

Computational nuclear theory is providing the conceptual background to current and future experiments at DOE Office of High Energy and Nuclear Physics facilities. Current studies include the structure of atomic nuclei far from the stability line, and the dynamics of muon-induced nuclear fission, including the viscosity of nuclear matter. In simulations of relativistic heavy-ion collisions in a (3+1) dimensional classical string model, researchers have for the first time added structure functions for the nucleons, as well as mass quantization.

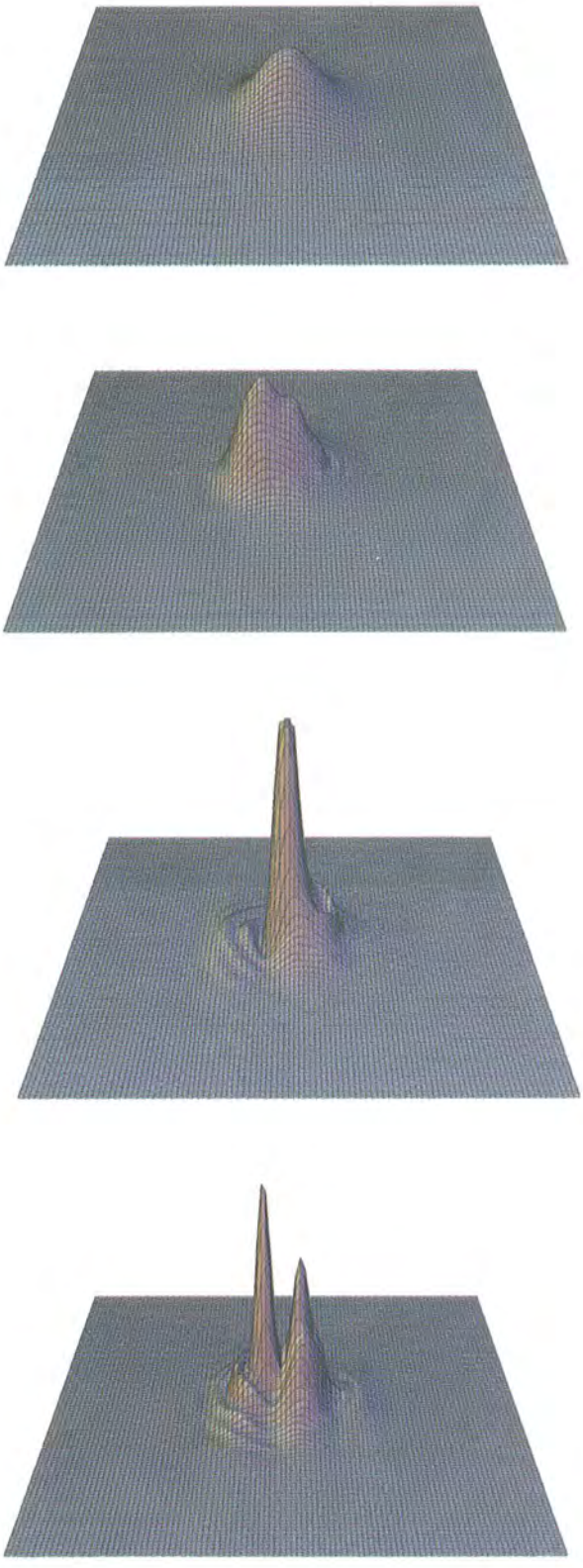
An increasing number of experimental physics applications, from heavy-ion fusion to high-energy colliders, demand higher-intensity beams, which places those beams in the space-charge dominated regime. Computational transport studies of space-charge dominated beams offer a low-cost approach for understanding their complicated physics. The simulations agree very well with the latest experimental observations and even reproduce the transverse density waves seen in experiments.

Nonequilibrium field theory covers a variety of topics such as transport theory of quantum fields, nonequilibrium

phase transitions, the nucleation and transport of topological defects and other nonlinear coherent structures, as well as fundamental issues such as the quantum-classical transition and the coherent control of quantum systems. Computational physicists have recently shown that very high resolution simulations enable new methods for studying the statistical mechanics of field theories. These researchers have demonstrated how the classical limit of certain chaotic systems is obtained from quantum dynamics via decoherence, and have developed a new, accurate method for the characterization of classically chaotic systems.

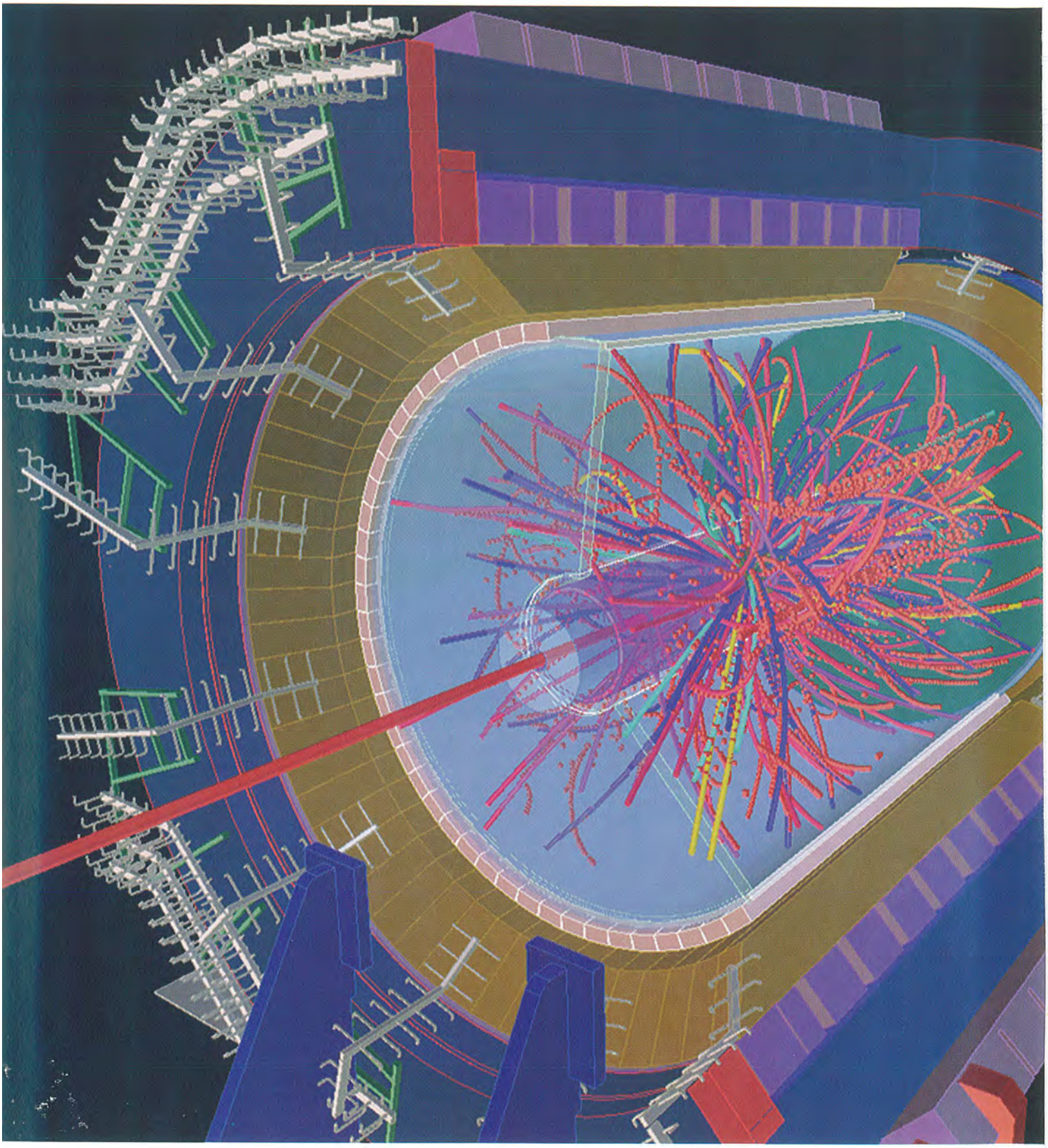
Astrophysicists are developing new methods for analyzing data from cosmic microwave background detectors—the faintest echo of the Big Bang. Computing the maximum likelihood of signal to noise is the critical step in extracting useful information from the data. When all the radiation from astronomical objects is subtracted from what was detected, the cosmic microwave background is what is left over. Tiny perturbations in the background are an imprint of the primordial density fluctuations that seeded the formation of everything from planets to clusters of galaxies. Results of this research will help test the validity of competing cosmological models. Some models see non-topological semilocal strings as a possible source of the primordial density fluctuations. The first three-dimensional simulations of semilocal strings confirmed the possibility of their formation only $10^{-35}$ of a second after the Big Bang.

NERSC's support of high energy and nuclear physics research is discussed below on page 23.



**Simulated snapshots of electron density during a relativistic atomic collision provide information that cannot be accessed in a laboratory.** **(Details on page 43.)**

# Computer Science and Applied Mathematics

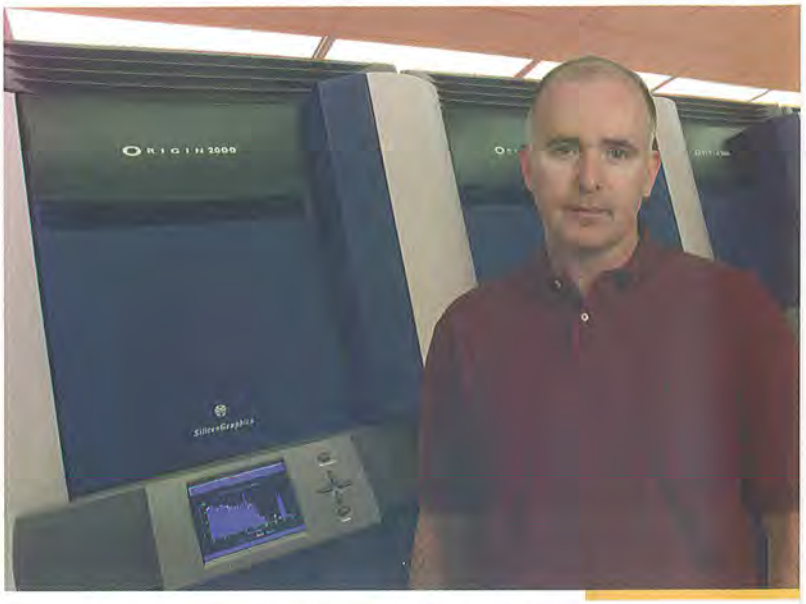


Illustrating the complexity of a typical next-generation experimental physics event, this image shows only 5% of a simulated gold-on-gold nuclear collision at the center of the STAR detector at Brookhaven's Relativistic Heavy Ion Collider. Finding better ways to store, move, access, and analyze huge datasets from experiments like this is one of the goals of NERSC's computer science research efforts. (Details on page 16.)

To better meet our clients' current and future needs, NERSC stays at the forefront of high performance scientific computing by participating in a broad range of computer science and applied mathematics research. We participate in the development and testing of next-generation software and hardware, and many of our research staff members develop advanced numerical algorithms for better solutions to scientific problems.

There were some organizational changes in 1998 to improve the integration of our research efforts. Bob Lucas joined NERSC as head of the High Performance Computing Research Department, and that department welcomed two existing organizations into its ranks: the Center for Computational Sciences and Engineering, headed by John Bell, and the Applied Numerical Algorithms Group, headed by Phil Colella. The Data Intensive Distributed Computing Group, under Brian Tierney, was merged into the Future Technologies/Software Tools Group, led by Bill Saphir. And to focus bioinformatics efforts at Berkeley Lab and support the DOE's Genome Program, staff from NERSC, the Life Sciences Division, and the Information and Computing Sciences Division joined to form the Center for Bioinformatics and Computational Genomics under the joint management of Sylvia Spengler and Manfred Zorn.

NERSC staff research efforts this year included bioinformatics, data-intensive storage access, parallel software libraries, distributed computing, fluid dynamics algorithms for combustion simulations, and cluster architectures. These projects are described below.



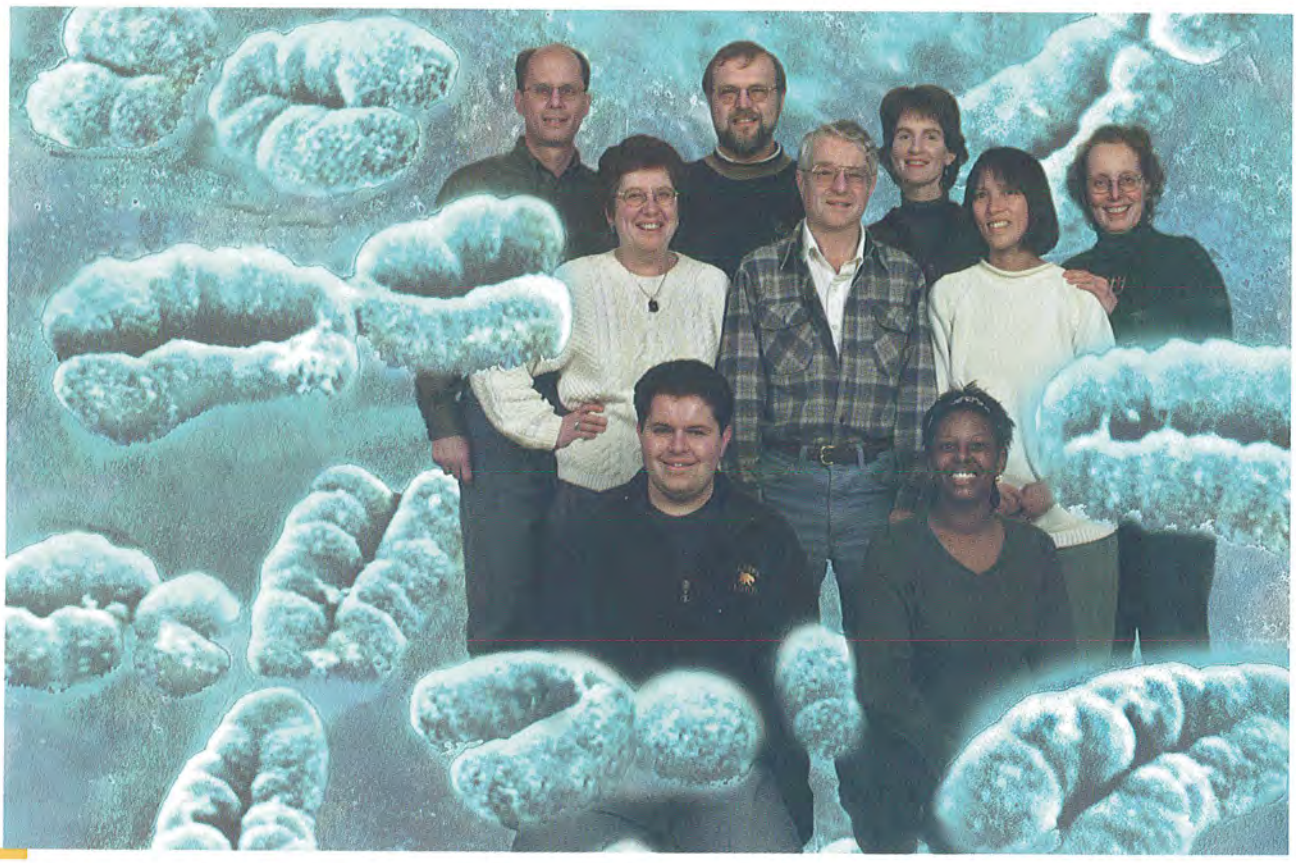

**NERSC's management team was completed by the addition of Bob Lucas as head of research.**

## Center for Bioinformatics and Computational Genomics

The human genome contains about 3 billion base pairs that code for 65,000 to 75,000 genes. Mapping and sequencing the genome is an international effort involving two dozen large centers, including the Department of Energy's Joint Genome Institute. Currently 150 million base pairs are sequenced each year. However, to fully sequence the entire human genome by 2005, the participating centers will need to sequence 2 million per day.

Helping biologists manage and analyze this explosion of data is the goal of NERSC's new Center for Bioinformatics and Computational Genomics (CBCG). Combining the expertise of biologists and computer scientists, CBCG strives to make the tools of both disciplines work together. The Center's work includes creating specialized software modules, designing databases, and developing standardized methods for indexing genomic information.

Providing an accessible format for data stored at two dozen research centers is crucial to making the information useful for scientists worldwide. The web-based Genome Channel provides a prototype graphic interface using standard annotation for all genome sequences completed to date. The interface allows users to zoom in on a particular chromosome and see how much of it has been sequenced, then access each individual sequence and the accompanying annotation. The Genome Channel was developed by scientists at Oak Ridge National Laboratory and Berkeley Lab as part of the Distributed Consortium for High-Throughput Analysis and Annotation of Genomes, a DOE Grand Challenge project.



**NERSC's new Center for Bioinformatics and Computational Genomics combines the expertise of biologists and computer scientists to manage and analyze an explosion of data. Shown here are (from left, standing) David Demirjian, Inna Dubchak, Manfred Zorn, Donn Davy, Denise Wolf, Janice Mann, Sylvia Spengler, (kneeling) Igor Dralyuk, and Mischelle Merritt.**

Other projects at CBCG include:

- the Alternative Splicing Database, which provides information about alternatively spliced genes, their products, and expression patterns
- SubmitData, a user interface that formats data for automated submission to genome databases
- BioPOET, a system for large-scale sequence analysis
- the Resource for Molecular Cytogenetics, a joint project with the Cancer Genetics Program at the University of California, San Francisco
- FoldPred, a program that predicts the protein fold classification for any amino acid sequence
- participation in the University of California Systemwide Life Sciences Informatics Task Force.

By developing partnerships, carrying out research in bioinformatics, and working with the bioinformatics community in areas such as education, training, and standards development, CBCG hopes to become the premier provider of bioinformatics expertise and services both regionally and nationwide.

## Storage Management for Massive Datasets

The next generation of high energy and nuclear physics (HENP) experiments at Brookhaven National Laboratory, Stanford Linear Accelerator Center, Fermilab, and CERN will present computational challenges that are new in scale and nature. For example, about 200 terabytes of data per year are expected from the Relativistic Heavy Ion Collider (RHIC) experiments at Brookhaven beginning in late 1999.

Meeting those challenges requires close collaboration of computer-knowledgeable physicists and physics-knowledgeable computer scientists. NERSC staff are working with collaborators from the experimental facilities and Berkeley Lab to advance the state of the art in physics computing and data-intensive computing in general.

The Grand Challenge Application on HENP Data aims to develop techniques and tools for efficient access to these massive datasets, and NERSC is working on the storage management component of this Grand Challenge. The goals are to achieve efficient access to experimental event data from tertiary storage, to provide multidimensional event indexing for query estimation and execution, and to support simultaneous multiple query execution.

Efficient access requires reorganizing event clusters on tertiary storage according to anticipated access patterns rather than in the order they were generated. Each particle collision event will need to be indexed by 100 properties, such as time, energy, momentum, type and number of particles, etc., so that researchers can make queries and retrieve data on the basis of multiple property ranges.

This year the three components of the Storage Manager system were developed: the Query Estimator, the Query Monitor, and the Cache Manager. The Query Estimator builds indexes of event properties, accepts multiple query requests, estimates the requirements for executing the query, and prepares execute information. The Query Monitor accepts query execute requests, manages the file queue, and schedules file caching. The Cache Manager tracks available cache space, requests caching from HPSS, and purges files when requested by the Query Monitor.

The Storage Manager is designed to work with queries from StAF (Standard Analysis Framework), a modular, customizable, scalable, CORBA-compliant framework for the analysis of physics data, and with Objectivity, a commercial object-oriented database management system. FY99 plans include integrating Storage Manager into the RHIC Computing Facility environment at Brookhaven, performance testing, monitoring, and enhancements.

Major collaborators on the Storage Manager project include Henrik Nordberg, Alex Sim, Luis Bernardo, and Craig Tull from NERSC; Torre Wenaus from RHIC; David Malon from Argonne National Laboratory; and Doug Olson and Jeff Porter from Berkeley Lab's Nuclear Sciences Division.

**The Storage Manager software will give physicists efficient access to massive datasets from experimental facilities now under construction. Key contributors to this project included Henrik Nordberg, Luis Bernardo, and Alex Sim.**

## The China Clipper Project: Data-Intensive Computing in Widely Distributed Environments

Modern science involves multi-site collaborations. Unique instruments and detectors, tape archive systems, high performance computers, and scientists are typically scattered across the country. Organizing, analyzing, visualizing, and moving massive amounts of data depends on many network-based services to aggregate and schedule the required computing and storage components. For example, data must be located and staged; cache and network capacity must be available at the same time as computing capacity; applications being executed must adapt to availability and congestion in

the middleware and infrastructure; and the whole system must respond to human interaction.

The China Clipper Project aims to identify and develop the technological infrastructure that enables scientists to routinely generate, catalogue, and analyze massive volumes of data at high data rates with complete location transparency. Specifically, the project will develop a collection of middleware services that will provide uniform interfaces for distributed resources and will assemble those resources so that they function as a single, integrated system.

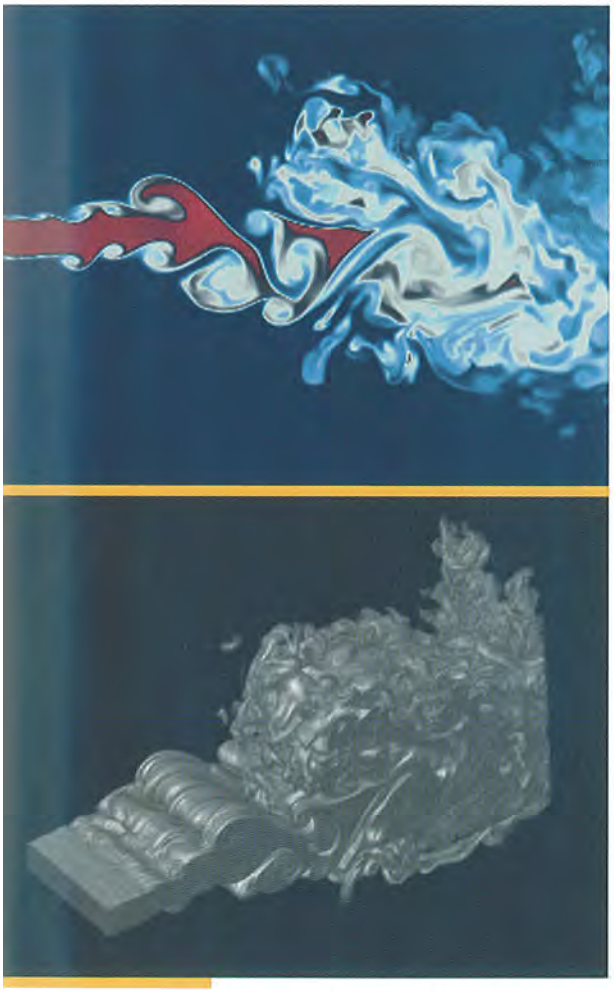
In a May 1998 experiment using DPSS (the Distributed-Parallel Storage System), a team from Berkeley Lab and the Stanford Linear Accelerator Center (SLAC) demonstrated the feasibility of remote analysis of high energy physics data. The team achieved a sustained data transfer rate of 57 MB per second, confirming that high-speed data storage systems could use distributed caches to make data available to computers running analysis codes.

Developers hope that these middleware services will eventually lead to breakthroughs in how science is done. They hope for:

- real-time data analysis so that scientific experiments can be controlled, modified, and validated on the basis of immediate feedback to the scientists
- direct coupling of experimental instruments with the computational simulations of the underlying physics, chemistry, materials science, etc., so that the interplay between experiment, theory, and scientific insight can happen interactively.

Instant comparisons of actual experiments with theoretical and computational models will give researchers better ways to test scientific theories, leading to new insights and faster scientific progress.

Principal collaborators in the China Clipper Project are William Johnston from Berkeley Lab's Information and Computing Sciences Division; Brian Tierney and Craig Tull from NERSC; Jim Leighton from ESnet; Richard Mount and Dave Millsom from SLAC; and Ian Foster from Argonne National Laboratory.



**Successful modeling of combustion processes depends on accurate modeling of turbulence.**

## Combustion Modeling

Combustion research is essential for achieving such goals as improving the gas mileage of automobiles and reducing the harmful emissions of diesels. But computational modeling of combustion processes is enormously complex. For example, many engines are designed to inject fuel and air into the combustion chamber, and mixing of these two streams on the molecular level is necessary for combustion to occur. Near the inflow, the mixing process is dominated by the large-scale structures in the flow; but as the jet develops, the mixing is influenced more by small-scale turbulence. Thus,

successful modeling of combustion depends on accurate modeling of turbulence.

Mathematicians in NERSC's Center for Computational Sciences and Engineering and the Applied Numerical Algorithms Group are helping to develop the algorithms and software needed to resolve the complexities of fluid dynamics in general and combustion modeling in particular. An especially useful tool, adaptive mesh refinement (AMR), is one of our major areas of research. AMR works by dividing a problem into smaller parts, much like putting a mesh over the problem and then looking at each segment. Areas of interest are treated with successively finer meshes to provide more detailed information. The finer the mesh, the higher the accuracy—and the more computing capacity required. AMR allows scientists to make the most effective use of the available computer power by focusing it on the region of the problem where it is most needed. The end result is better answers at a lower cost.

A recent simulation of turbulent flow demonstrated both the capabilities of AMR and the need for faster computing resources to achieve higher resolution. The AMR simulation achieved a resolution equivalent to 8 million data points per time step using only 2 to 3 million data points per time step for 740 time steps. This simulation required 38 wall-clock hours on 32 processors of NERSC's Cray T3E-900, and generated 50 gigabytes of data. But simulating a turbulent jet under the conditions typically studied experimentally would require an estimated 1.3 billion grid points, using 8,160 wall clock hours (340 days) on 512 processors of the T3E, and generating 25 terabytes of data. The algorithms being developed today will achieve their full potential on the next generation of high performance computers.

## Climate Modeling

In October 1997, just as El Niño was getting ready to soak California with one of the wettest winters ever, nearly 150 climate modeling experts from around the world convened at NERSC to discuss advances in computational weather forecasting and climate modeling. At the meeting, scientists demonstrated that their tools for predicting weather are getting more reliable and extending the range of forecasts. Still, the need for higher-resolution modeling tools was also made clear.

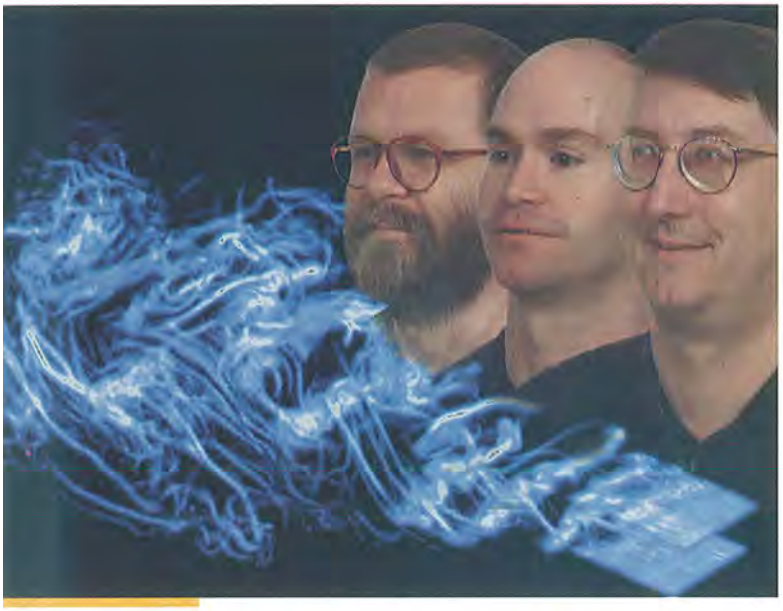
To help meet that need, a joint project between NERSC and the Geophysical Fluid Dynamics Laboratory (GFDL) is developing a massively parallel version of GFDL's Modular Ocean Model code (MOM), which is used by researchers worldwide for climate and ocean modeling. The parallel MOM will be able to run on the world's fastest computers, enabling large-scale, high-resolution, decade- to century-long ocean simulations.

Efficient use of cache-based processor architectures, significantly improved data input/output, and a more convenient user interface will allow MOM to run on both workstations and massively parallel supercomputers. I/O improvements have already enabled part of the code to run 50 times faster on a parallel machine than on a single processor. And integration of the netCDF library into MOM is improving data accessibility and facilitating data sharing. The software tools that are developed in this project are expected to be useful to the entire climate research community. (For more details, see page 72.)

## Parallel Library for Algorithm Development

Vince Beckner, Chuck Rendelman, and Mike Lijewski of NERSC's Center for Computational Sciences and Engineering (CCSE) have performed a valuable service for algorithm developers by designing a parallel version of CCSE's BoxLib software. BoxLib is a library of C++ classes that facilitate the development of block-structured finite difference algorithms such as arise in the solution of systems of partial differential equations. BoxLib is particularly useful for creating AMR algorithms.

Using the Bulk Synchronous Parallelism (BSP) communications package from Oxford University, they were able to



**Mike Lijewski, Vince Beckner, and Chuck Rendelman designed the parallel BoxLib library in such a way that algorithm developers do not have to worry about data distribution.**

hide most details of the parallel code in the C++ libraries on which the algorithms are built. As a result, the algorithm developer does not have to deal with data distribution, communication, etc.—these issues are all handled by the underlying class hierarchies.

The parallel BoxLib is easily portable and has been successfully tested on the Cray T3E and on several SMP systems. It was used to port several atmospheric modeling codes to the T3E. BoxLib contains rich data structures for describing operations which take place on data defined in regions of index space that are unions of non-intersecting rectangles. Because the regions of interest may change in response to an evolving solution, support is provided in BoxLib for efficiently building and destroying the data structures.

## ACTS Toolkit Support

Do general-purpose scientific software libraries make it easier to write parallel code? NERSC's support of the DOE2000 ACTS Toolkit will help answer that question. The Advanced Computational Testing and Simulation (ACTS) program has brought together a set of numerical, infrastructure, and runtime tools for developing parallel programs. Developed as research software at DOE laboratories and universities, the tools are now being tested for general production use and are undergoing further development for interoperability.

The ACTS Toolkit differs from other parallel tools projects in that it focuses primarily on software used inside an application, instead of on software used to develop an application. It includes tools that implement numerical methods, tools that manage the complexity of parallel programming, and tools that support wide-area applications. ACTS tools are mostly libraries (including C, C++, and Fortran libraries). Most are designed specifically for distributed memory parallel computers, using MPI for communication. ACTS tools can make it less cumbersome and costly to develop scalable algorithms and can add functionality that makes applications simpler to use and analyze.

NERSC has established a new information and support center for the ACTS Toolkit (http://acts.nersc.gov). In addition to descriptions of the tools and pointers to documentation, the web site offers independent, unbiased evaluations and advice on what the tools are useful for. The main focus of the support center is on working directly with parallel application programmers, advising and assisting them in the incorporation of ACTS tools into their codes. The goal is to make it easier to develop high performance scientific applications, improving both performance and productivity.

## PC Clusters

Clusters of off-the-shelf PCs have been hailed by enthusiasts as inexpensive alternatives to supercomputers, and clusters have been demonstrated to work well for a number of scientific applications. PC clusters might develop a "mass market" for parallel computing, which today is done almost exclusively at large supercomputer centers. For example, clusters would be ideal for developing and testing parallel codes and for running small to medium-sized parallel applications, freeing up large capability resources at NERSC

and other centers for what they do best.

However, because there is no standardized and comprehensive software package for clusters, building and maintaining a cluster is not easy. Every new cluster project has to reinvent the wheel, and they often wind up with the software equivalent of a system held together with duct tape.

NERSC is working to develop the infrastructure for plug-and-play, high performance PC clusters. The goals of our PC Cluster Project are to develop critical enabling software components, to ensure that there is a uniform HPC software environment on PC clusters and supercomputers, and to perform and collect objective analyses of hardware and software and disseminate that information so that the evaluation does not need to be repeated.

One of our tasks is to develop a Modular Virtual Interface Architecture (M-VIA). NERSC contributed to the development of VIA as part of our COMPS Project (Cluster of MultiProcessor Systems), and Intel, Microsoft, and Compaq have accepted VIA as the standard architecture for communication within clusters (http://www.viarch.org/). NERSC's M-VIA will be the first publicly available full implementation, the first portable high performance implementation, and the first implementation for Linux. We are working with Intel and Argonne National Laboratory to develop more applications, extensions, and implementations of VIA.

NERSC also participates in the Extreme Linux project, a collaboration of the DOE laboratories, NASA, NIST, and several universities and commercial vendors, which aims to improve Linux for high performance clusters.

Our own cluster contains 20 single-processor 400 MHz Pentium II nodes, 2 four-processor Pentium Pro nodes, and 2 dual-processor 233 MHz Pentium II front-end servers.

# Systems and Services


Thanks to the careful planning and preparation of Adrian Wong, Clayton Bagwell, Jonathan Carter, Brent Draney, Mike Welcome, and others, NERSC's T3E-900 was placed into full production service within one week of its installation and acceptance. Their work included software installation, operating system configuration, system tuning and testing, account installation, queue scheduling, and operational support and monitoring.

Like any other commercial venture, high performance computing has its share of exaggerations. In 1998 we heard various vendors make contradictory claims of who built the world's fastest computers and who dominated the market. Experienced users viewed these claims with skepticism, knowing that most of them were based on theoretical peak performance and manipulation of statistics, not real-world results.

At NERSC, we define high performance in practical, not theoretical, terms. High performance to us means providing the most productive and reliable computing, storage, and networking systems, while consistently offering our clients timely services, innovative assistance, and convenient training.

For example, at the beginning of FY98, we promised to deliver to scientists 2.75 million T3E hours and 860,000 normalized CRUs for the PVP systems. (A CRU is a CPU hour × a particular system's performance factor × a variable priority. Normalized CRUs set the priority to 1.) We were proud to deliver more computing time than we promised, as shown in the table to the right. This past year's improvements in our systems and services are described throughout this section.

## Massively Parallel Systems

In January 1998, NERSC's Cray T3E-900, "mcurie," was joined by an 96-processor Cray T3E-600, "pierre," which was installed as a mid-range computing resource primarily for Berkeley Lab researchers. In June, pierre was upgraded to a T3E-900, with 450 MHz processors replacing the 300 MHz units and 48 additional processors installed, along with sixteen 4.5 GB disks and a multi-purpose node.

In October, the two Cray T3E supercomputers were completely rewired to create a unified machine with 640 processors available to clients. This reconfiguration reduced software costs and overall expenses, and allowed larger jobs to be run more frequently. The unified T3E kept the name "mcurie." It provides 512 processors dedicated to batch jobs and another 128 processors dedicated to interactive jobs by day and batch jobs by night, with additional processors for the operating system and serial work.

### FY98 Computing Time

| | Promised | Delivered | % Over |
|---|---|---|---|
| **MPP** | 2,750,000 PE hours | 3,000,000 PE hours | 109% |
| **PVP** | 860,000 NCRUs | 954,449 NCRUs | 111% |

## Parallel Vector Systems

In June a terabyte of new disks were installed on the Cray J90 cluster, and in August the file systems on all the J90s were reconfigured to include these new drives. These changes gave our clients larger temporary work directories, and the work partition is much more fault-tolerant than before—failure of a single disk does not cause any loss of user data. A new file system to store checkpoint files improved users' I/O performance while increasing system reliability.

Two more J90 systems with 64 additional processors were scheduled for installation in January 1999 to replace the Cray C90. In use since September 1992 and the only computer to move with NERSC from Livermore to Berkeley, the C90 was decommissioned on January 1, 1999.

**The HPSS conversion team included (from left) Majdi Baddourah, Jonathon Carter, Steve Lowe, Wayne Hurlbert, Harvard Holmes, Keith Fitzgerald, Jim Daveler, Tom Deboni (front left), and project leader Nancy Meyer.**

## Storage Systems

NERSC increased its mass storage capacity to 600 terabytes and upgraded the storage servers to IBM SP2s. The old storage systems, UniTree and CFS, were replaced with HPSS (High Performance Storage System). Developed by a consortium of industrial, university, and government organizations—including NERSC's Jim Daveler—HPSS is a scalable parallel software system designed to move very large data objects between high performance computers, workstation clusters, and storage libraries at speeds many times faster than is possible with previous software systems.

The HPSS storage control system uses "data movers"—specialized software modules—to send large data streams, such as complex images and visualization objects, directly to the requesting computers without passing them through the HPSS storage server itself. HPSS takes itself out of the loop so that the only limiting factors are the maximum speed of the network and the devices themselves.

## HENP Support

NERSC's support to the high energy and nuclear physics community includes consulting, software development, and operation of a specialized data-intensive computing facility, the PDSF (Parallel Distributed Systems Facility). The PDSF is a networked distributed computing environment—a cluster of clusters—used by six large-scale HENP investigations for detector simulation, data analysis, and software development.

The PDSF underwent a major hardware upgrade this year. We retired 32 Hewlett-Packard HP 735/9000 workstations and 24 Sun Sparc 10 workstations. The new configuration consists of four clusters—with a total of 68 Pentium II processors and a quad-CPU Sun E450 fileserver—plus eight disk vaults, each containing 66 GB of shared storage. The PDSF hardware supports multiple operating systems—Linux, Solaris, and Windows 95, 98, and NT—for maximum flexibility. We are integrating the PDSF with high-bandwidth networking, disk cache, and the HPSS storage system as an advanced prototype of the architecture necessary for future HENP data analysis.

A milestone in physics software development was reached when a NERSC-led collaboration with Brookhaven National Laboratory and the Pittsburgh Supercomputing Center ported the CERNLIB collection of codes to a parallel architecture—a large and complex task that had been attempted several times before but never completed. Born at CERN (the European Organization for Nuclear Research), CERNLIB has been developed and supplemented by HENP researchers around the world. The codes for mathematics, physics simulations, statistical analysis, user interfaces, graphics, memory management, data I/O, etc., are centrally maintained and codified by CERN in Geneva, Switzerland, and are used by probably every university physics department and HENP research center.

While simulation codes have already been running on parallel machines, porting of CERNLIB to NERSC's T3E paves the way for analysis of actual data from facilities such as Brookhaven's STAR detector, which is scheduled to start data acquisition in late 1999. Finding the scientific significance

in the huge quantities of data from these experiments will require the power of massively parallel processing.

## Specialized Servers

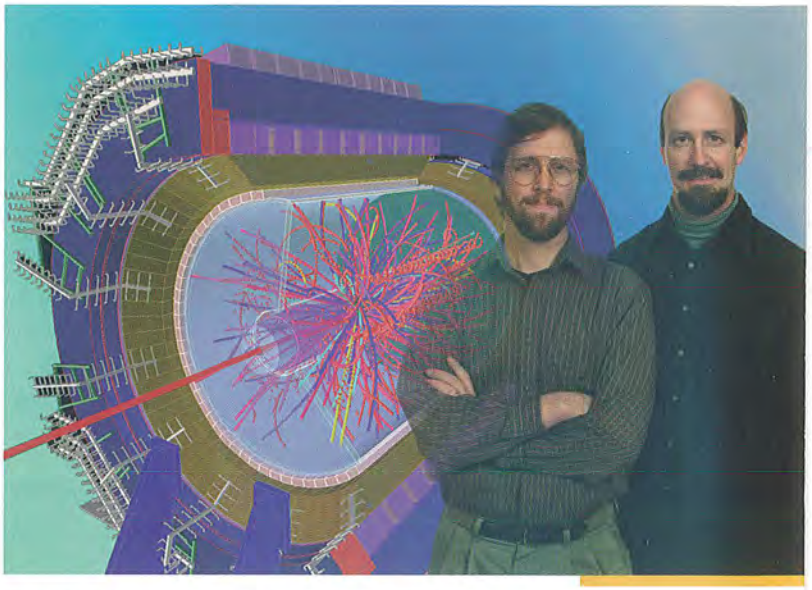
This year NERSC installed two platforms for users with specialized processing needs: a remote visualization server and a symbolic manipulation server.

The visualization server, named "escher," allows NERSC users to perform visualizations from remote locations and develop new techniques in large data visualization and collaboration. It is a Silicon Graphics Onyx 2 system with six 195 MHz R10000 processors, 3 GB of memory, two InfiniteReality graphics pipes, ATM, HIPPI, 100 BT network connectivity, and a 100 GB disk array. Its dual graphics pipes allow for two simultaneous graphics displays to be driven by the system, for a minimum of two simultaneous video streams. The server supports nearly 20 visualization, graphics, and data formatting packages.

In one major application, escher was used in conjunction with an ImmersaDesk to display medical data showing a human spine. The data was volume-rendered in 3D so the viewer could move around and inside the vertebrae. The path of the spinal cord was shown as a 3D curve along with 2D slices through the data perpendicular to this curve.

Escher has also been used as the visualization platform for an architectural lighting simulation system known as RADIANCE. This project involved using the massively parallel architecture of the Cray T3E to perform calculations while using escher to visualize the results. In the future, the techniques developed with this project will allow NERSC researchers to visualize their simulations in real time from remote locations.

The NERSC symbolic manipulation server, named "newton," allows users to perform symbolic and numerical mathematical and statistical operations. This system complements NERSC's high performance systems by providing a dedicated platform for non-floating-point-intensive calculations.



**Principal collaborators in porting the CERNLIB physics library to the T3E were Craig Tull and Mark Durst of NERSC (shown here), as well as Jeff Porter of the Berkeley Lab Nuclear Science Division and Pavel Nevski from Brookhaven. Enabling the codes to run on parallel machines makes it possible to analyze massive datasets from the next generation of experiments.**

**By reusing pixels, NERSC's Visualization Group is working to speed up computation in the RADIANCE lighting simulation software so that viewers will be able to explore a virtual building in real time.**

The Sun server has a single 248 MHz UltraSPARC-II CPU, 512 MB of memory, and 26 GB of user disk space. Installed applications include MATLAB, Mathematica, Maple, SAS, and S-Plus.

## NERSC-3 Procurement

A request for proposals for NERSC's next generation high performance computer system was issued on July 15, 1998. Proposals were accepted until October 1, when confidential evaluation of the competing systems began. Deciding which technology to pursue is critical to NERSC's future, and a task force under the direction of Bill Kramer is weighing the options carefully. "With this procurement, NERSC will continue on its innovative path in production-level high performance computing," Kramer said.

Delivery of the initial system is expected by mid-1999.

**Bill Kramer, head of high performance computing, led the NERSC-3 procurement task force.**

## Advanced Systems Group

A new Advanced Systems Group, headed by Tammy Welcome, was formed to assess and implement new computing technologies. While the NERSC-3 procurement is the group's highest priority, they will also have responsibility for the Sun Wildfire cluster and the SGI Origin 2000.

As part of our research into alternative computer architectures, NERSC is participating in a collaborative research program with Sun Microsystems involving a prototype shared-memory multiprocessor system code-named WildFire. Sun is using WildFire to explore possible architectures for highly-scalable NUMA-based (non-uniform memory access) servers. A goal of WildFire is to evaluate the effectiveness of leveraging large SMPs in the construction of even larger systems. The WildFire installed at NERSC connects four Sun Ultra Enterprise E4000s to form a system with 32 167 MHz UltraSPARC 2 processors, 6144 MB of memory, and a 150 GB disk. NERSC staff are testing and evaluating this prototype system and providing feedback to Sun. Areas of particular interest are system design (scheduling, memory management, resource allocation), system administration, benchmarking, algorithm development, and system scalability.

The Advanced Systems Group is also testing the SGI Origin 2000 to evaluate its performance in production scientific computing.

## User Survey Results

NERSC conducted a user survey this year to provide feedback about every aspect of our operation, help us judge the quality of our services, point out areas that need improvement, and show how we compare to similar facilities. We intend to repeat the survey yearly to monitor our progress.

Our clients rated NERSC in the areas of computational and file storage resources, account and allocations support, consulting services, documentation, and training. Software support was not included explicitly in the survey, but users commented on this area as well.

There were 138 respondents. About 56 percent said they used the C90; another 54 percent used the T3E and 46 percent the J90s. There was less representation for the archival systems: 32 percent said they used CFS and 26 percent HPSS.

The three areas rated most important were network access, the center overall, and consulting services. The three areas that received the highest ratings were consulting services, network access, and account support services.

Overall, our clients say we provide a high level of service. On a scale of 7 (very satisfied) to 1 (very unsatisfied), our scores ranged from 5.8 for consulting services, C90 uptime, and CFS reliability to 4.4 for C90 and T3E turnaround time. Many users pointed out that NERSC is an excellent high-end production center, with a good user focus. Comments included:

> *"Gives us access to high-end, high-capacity and capability machines without too many limitations on the way codes can be run. There is a good mix of machines, serial and parallel, and a good mix of running modes, interactive and batch."*

> *"Supplies reliable cycles to a broad user base. Excellent user support, probably the best in the world for high-end computing."*

> *"As a service center, NERSC does a great job keeping the T3Es up and providing easily accessible information relating to hardware and software. Moreover, the intellectual quality of NERSC support and research staff is excellent and they are easy to communicate with."*

> *"Over the years, NERSC has been the most reliable source of production computing for scientific research and development, by concentrating on scientific computing ahead of computer science."*

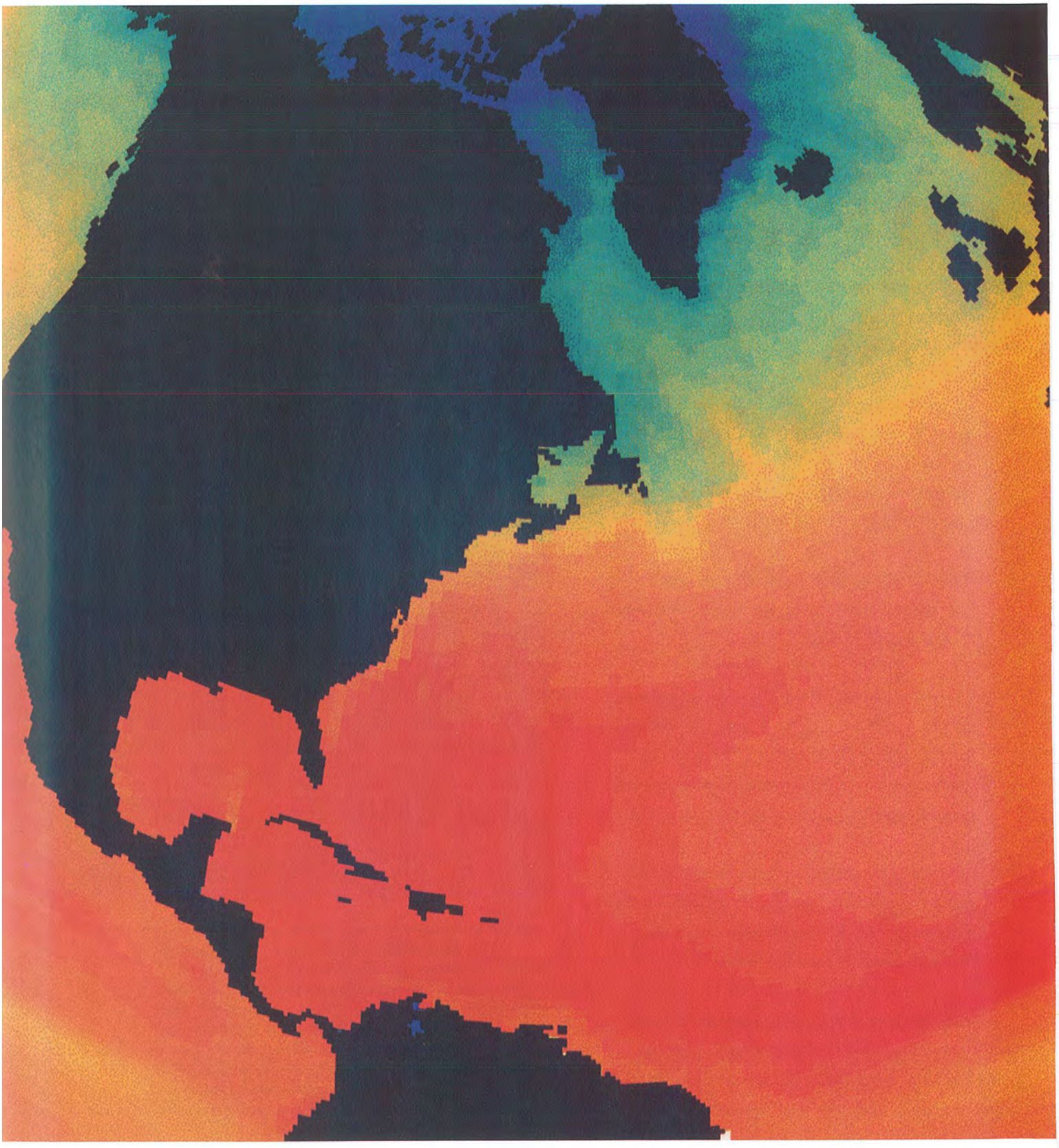
When asked what they wanted more of, most users said "more cycles." Specific software requests were also popular, as were longer T3E queues and additional batch queues in general. Areas that need improvement include:

- *Turnaround time:* We are addressing the need for more cycles with the NERSC-3 procurement process under way.
- *Queue structures:* A new T3E queue structure with more 4-hour queues and a new 12-hour queue was implemented in December. The J90 queues were unified under NQE in October. Further improvements will be considered in early 1999.
- *Web site:* A reorganized NERSC web site with improved contents will be implemented in early 1999.
- *More direct communications with users:* As a result of this survey, we have been using email more often to communicate system changes to users.
- *Training process:* We are now conducting teleconference classes in order to reach all users more effectively.

Complete survey results are available at http://www.nersc.gov/whatsnew/survey/

**Our high level of service is made possible by many NERSC and ESnet staff members working behind the scenes, including (back row) Brent Draney, Cheri Lawrence, Clint Wadsworth, Mark Heer, James Lee, (front row) Jackie Scoggins, and Suzanne Smith. Brent, Mark, Jackie, and Suzanne installed and configured NERSC's new email hub systems in a five-day process that was transparent to NERSC clients. Cheri prepared financial data for several successful audits and reviews. Clint coordinated network connections for the Berkeley Lab/NERSC booth at the SC98 conference. And James improved staff productivity by introducing the Psion palmtop computer and providing training.**

# Science Highlights



This image depicts the sea surface temperature from a coupled simulation with the DOE Parallel Climate Model (details on page 83). Note the Gulf Stream meander pattern and the cooler tropical Atlantic surface temperatures caused by upwelling of cold water. Also depicted is the cold water under the Arctic and East Greenland sea ice. (Graphic by Gary Strand, NCAR.)

# Protein Dynamics and Biocatalysis

*P. A. Bash, Northwestern University Medical School*
*M. Karplus, Harvard University*

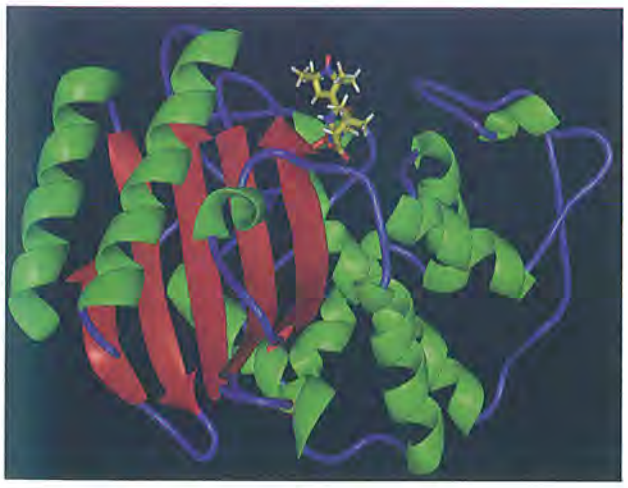
## Research Objectives

A guiding principle of molecular biology is that the structure of a biomolecule defines its function. This principle is especially true in the case of the protein molecules known as enzymes, which serve as highly specific and extraordinarily efficient catalysts of biochemical reactions. Despite the growing availability of the atomic structures of enzymes, details of the chemical mechanisms employed by enzymes to achieve their catalytic prowess remain elusive.

The goal of this project is to develop a greater understanding of the mechanisms involved in enzyme catalysis. We are studying two different enzymes, one a protein, the other a nucleic acid. The protein enzyme that we are investigating is beta-lactamase, which is responsible for the efficient hydrolysis of antibiotic agents such as penicillin and cephalosporin. The nucleic acid enzyme we are investigating is the hammerhead ribozyme, which is a self-cleaving ribozyme suggested as a model for the primordial enzyme before proteins came into existence.

## Computational Approach

The methods we use are based on the physical and chemical principles of statistical mechanics and quantum mechanics, and they are implemented in computational form using techniques from computational chemistry. To carry out our calculations, we used both the T3E and the J90 machines at NERSC. The molecular dynamics and quantum mechanical calculations were done on the T3E and J90 machines, respectively.



**A model of the Michaelis complex for the TEM-1/penicillin system from molecular dynamics simulations.**

## Accomplishments

We have developed a model of the Michaelis complex for the TEM-1/penicillin system from molecular dynamics simulations (see figure). We have also developed a model quantum and molecular mechanics (QM/MM) Hamiltonian for the beta-lactamase system, calibrating the Hamiltonian parameters against high level *ab initio* calculations.

The catalytic mechanism of the hammerhead ribozyme is being investigated using a number of techniques that have been developed in our laboratories. An important goal is to determine the conformational flexibility of the active site of the ribozyme and the role that this may play in the catalytic mechanism. The new nucleic acid molecular mechanics force field in the CHARMM program will help us perform a classical molecular dynamics study of the hammerhead ribozyme.

## Significance

The dynamic properties of proteins and nucleic acids are difficult to investigate experimentally, but they are essential for an understanding of their function. Computer simulations can provide the necessary insights, at an atomic level of detail, for a complete understanding of the relationship between biomolecular dynamics/structure and function. For example, while the class of enzymes known as beta-lactamases are largely responsible for the increasing resistance of bacteria to antibiotics, the precise chemical resistance mechanism used by this enzyme is still unknown. Simulations are critical for further study of this mechanism. Similarly, RNA was recently discovered to catalyze its own cleavage or that of other RNA molecules. The dual capacity of RNA to act as an information transfer molecule and an enzyme has led to speculation on the role of RNA in primordial life. Simulations involving the hammerhead ribozyme, the smallest of the catalytic RNAs, will be very useful in further investigations of RNA.

## Publications

M. A. Cunningham and P. A. Bash, "Systematic procedure for the development of accurate QM/MM model Hamiltonians," in *Computer Simulations in Biomolecular Systems*, edited by W. F. Van Gunsteren, P. K. Weiner, and A. J. Wilkinson (Kluwer, Dordrecht, Neth., 1997), pp. 177–95.

M. A. Cunningham, R. E. Gillilan, and P. A. Bash, "Computational enzymology," Can. Chem. News **49**, 9 (1997).

M. A. Cunningham and P. A. Bash, "Computational enzymology," Biochimie. **79**, 687–9 (1997).

http://www.pharm.nwu.edu/facultypages1/bash2.html

# Numerical Tokamak Turbulence Project

*B. I. Cohen, Lawrence Livermore National Laboratory*
*J. M. Dawson, University of California, Los Angeles*
*J. V. W. Reynders, Los Alamos National Laboratory*
*V. K. Decyk, University of California, Los Angeles*
*W. D. Dorland, University of Maryland*
*G. W. Hammett, Princeton Plasma Physics Laboratory*
*G. D. Kerbel, Lawrence Livermore National Laboratory*
*J.-N. Leboeuf, Oak Ridge National Laboratory*
*W. W. Lee, Princeton Plasma Physics Laboratory*
*S. E. Parker, University of Colorado, Boulder*
*R. E. Waltz, General Atomics*
*A. M. Dimits, D. E. Shumaker, and W. M. Nevins, Lawrence Livermore National Laboratory*
*M. Beer and Z. Lin, Princeton Plasma Physics Laboratory*
*R. Sydora, University of California, Los Angeles, and University of Alberta*
*V. Lynch, Oak Ridge National Laboratory*
*S. Smith and T. Williams, Los Alamos National Laboratory*

## Research Objectives

The primary research objective of 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

Two classes of three-dimensional initial-value simulation algorithms, gyrokinetic (GK) and gyro-Landau-fluid (GLF), are being applied to the simulation of tokamak turbulent core transport. The GK simulations are based on particle-in-cell (PIC) methods for the self-consistent solution of Poisson's equation (reduced to a quasi-neutrality relation) and plasma equations of motion, and domain decomposition methods to run efficiently in parallel on the T3E and other parallel computers. The GLF algorithm is based on an alternative solution of the fundamental GK and quasi-neutrality equations, in which fluid moment equations are solved instead of particle equations. The GLF simulations have been performed on both massively parallel and parallel vector computers, particularly the T3E and C90 at NERSC. Both flux-tube, i.e., toroidal annulus, and global toroidal GK and GLF simulations are being performed to study tokamak turbulence.

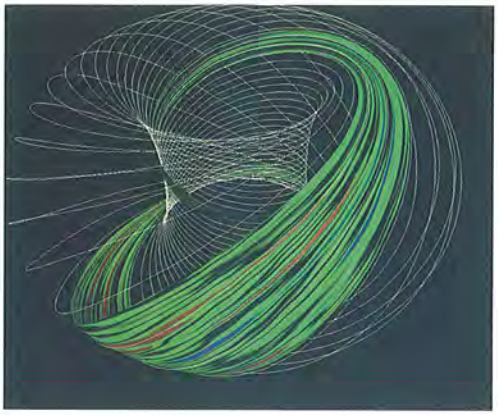
## Accomplishments

We continue to conduct detailed parameter studies with our GK and GLF simulations, addressing discharge #81499 in the General Atomics DIII-D tokamak as a base case because of its relevance to the International Thermonuclear Experimental Reactor (ITER). Careful comparisons have been made between the results of the GLF and GK simulations of shot 81499 and variants to determine parametric dependences and points of agreement between the simulation algorithms (as part of the Cyclone Project, the purpose of which was to study the physics basis and reliability of the various transport models used for ITER projections).

We have compared flux-tube and global gyrokinetic code results. Previous simulations have shown that global codes have significantly lower flux (as much as 20 times lower). In addition, global codes show a global structure to the radial $E \times B$ shear flow mode, whereas the flux-tube simulations show a shorter scale radial mode structure. We have implemented profile variation and bounded radial boundary conditions in a flux-tube code. This allows more direct comparisons of the two types of domain representations. We have found that flux-tube simulations including profile variation now agree well with small global simulations, both in terms of heat flux and radial mode structure. We have also found that large global simulations with weak profile variation have a heat flux only 30% lower than similar flux-tube simulations. In addition, these simulations show a broken-up radial mode structure with wavelengths on the order of 20 ion Larmor radii, qualitatively similar to flux-tube simulations.

Much of our effort during this past year has been in comparing the gyrokinetic, gyrofluid, IFS-PPPL and multi-mode models for core transport in tokamaks (e.g., the Cyclone Project). Cyclone Project results indicate that the IFS-PPPL and gyrofluid models predict heat diffusivities that are high compared to gyrokinetic simulations. These differences are significant enough to impact previous ITER projections made by the IFS-PPPL model. Discussion of the Cyclone Project work has recently appeared in *Science* and *Nature*.

The NTTP simulations have demonstrated the importance of flow shear and negative central magnetic shear in reducing drift-wave turbulence in tokamaks as observed in experiments. In particular, the simulations demonstrated that equilibrium scale $E \times B$ shear flows are important when the linear-mode growth rates are comparable to the $E \times B$ shear rates. This criterion has become a standard part of routine experimental transport analysis and incorporated in reduced models. The dynamics of turbulence-driven $E \times B$ zonal flows have been systematically studied in fully three-dimensional gyrofluid flux-tube codes and gyrokinetic simulations of microturbulence in magnetically confined toroidal plasmas using massively parallel computers, including the NERSC T3E. Linear-flow damping simulations with both flux-tube and global gyrokinetic codes exhibit an asymptotic residual flow, in agreement with recent analytic calculations. Nonlinear simulations of turbulence, driven by the toroidal ion temperature gradient (ITG) instability with both global and flux-tube codes, provide key first-principles results supporting the physics picture that turbulence-driven fluctuating $E \times B$ zonal flows



**These images show the results for the perturbed plasma density from a Gryffin gyrofluid ion-temperature-gradient (ITG) instability simulation viewed in noncircular magnetic geometry. The visualization technique used hardware-accelerated 3D volume texture rendering on a graphics server (SGI Onyx 2) and displayed to a remote GLX capable workstation. Equivalent resolution using (standard) shaded polygon rendering would require 30 to 100 times as much computation. The ITG perturbations are shown on a bundle of magnetic flux lines in the second image.**

can significantly reduce turbulent transport. A key discovery is the existence of states with zero thermal transport for linearly unstable values of the ion temperature gradient in the limit of no collisions. These simulations have been carried out using global, annular, and flux-tube geometries, with a variety of boundary conditions, to resolve the differences in previous simulation results between global and local codes.

A new electromagnetic fluid model has been developed and has been incorporated into a toroidal gyrofluid code. These fully nonlinear electromagnetic simulations are computationally more demanding (typically by 5×) than previous electrostatic simulations, since they resolve the faster shear-Alfven time scale, and will be able to make great use of NERSC resources. New schemes for treating nonadiabatic and adiabatic responses for the passing and trapped electrons in tokamaks have been developed. One is based on a careful treatment of the electron weights in different parts of phase space, and another is a new bounce-averaged delta-f scheme. These new schemes will enable us to remove the parallel CFL restriction while retaining the correct linear and nonlinear wave-particle interactions for the electrons, and will also have significant statistical advantages relative to previous particle-based drift-kinetic electron algorithms.

Nonlinear gyrokinetic particle simulations, including electromagnetic effects, are being used to investigate anomalous electron thermal transport from small-scale drift magnetic islands. The regimes where the islands interact radially or remain isolated from each other are considered. The growth and nonlinear formation of gyroradius scale islands with real frequency above the electron diamagnetic drift frequency are observed. The growth and saturation dynamics are sensitive to the electron temperature gradient relative to the density gradient.

Work is in progress to evaluate the anomalous radial heat flux and its scaling with plasma parameters.

## Significance

The NTTP simulations are being used to produce linear and nonlinear calculations of drift-type instabilities in realistic tokamak equlibria, which are leading to a deeper understanding of anomalous transport in current experiments and to improving their performance. This simulation work is providing a basis for reduced transport models that fit current experimental databases and from which it is hoped that performance in future experiments can be reliably predicted and optimized. As controlling the energy transport has significant leverage on the performance, size, and cost of fusion experiments, reliable NTTP simulations can lead to significant cost savings and improved performance in future experiments.

## Publications

L. Garcia, B. A. Carreras, V. E. Lynch, J.-N. Leboeuf, and D. E. Newman, "Resistive pressure gradient driven turbulence at stellarator plasma edge," Phys. Plasmas **4**, 3282–3292 (1997).

Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang, and R. B. White, "Turbulent transport reduction by zonal flows: Massively parallel simulations," Science **281**, 1835 (1998).

R. E. Waltz, R. L. Dewar, and X. Garbet, "Theory and simulation of rotational shear stabilization of turbulence," Phys. Plasmas **5**, 1784 (1998).

http://www.acl.lanl.gov/GrandChal/Tok/tokamak.html
http://www.er.doe.gov/production/cyclone/

# Computational Chemistry for Nuclear Waste Characterization and Processing: Relativistic Quantum Chemistry of Actinides

*R. J. Harrison, J. A. Nichols, R. A. Kendall, D. A. Dixon, T. H. Dunning, Jr., J. Nieplocha, and G. I. Fann, Pacific Northwest National Laboratory*
*R. Shepard, A. F. Wagner, W. Ermler, R. Stevens, J. L. Tilson, and M. Minkoff, Argonne National Laboratory*
*C. W. McCurdy and A. T. Wong, Lawrence Berkeley National Laboratory*
*R. M. Pitzer, The Ohio State University*
*D. E. Bernholdt, Syracuse University*
*K. G. Dyall, Eloret, NASA Ames Research Center*

## Research Objectives

We aim to develop and apply the methods of relativistic quantum chemistry to assist in the understanding and prediction of the chemistry of actinide and lanthanide compounds.

## Computational Approach

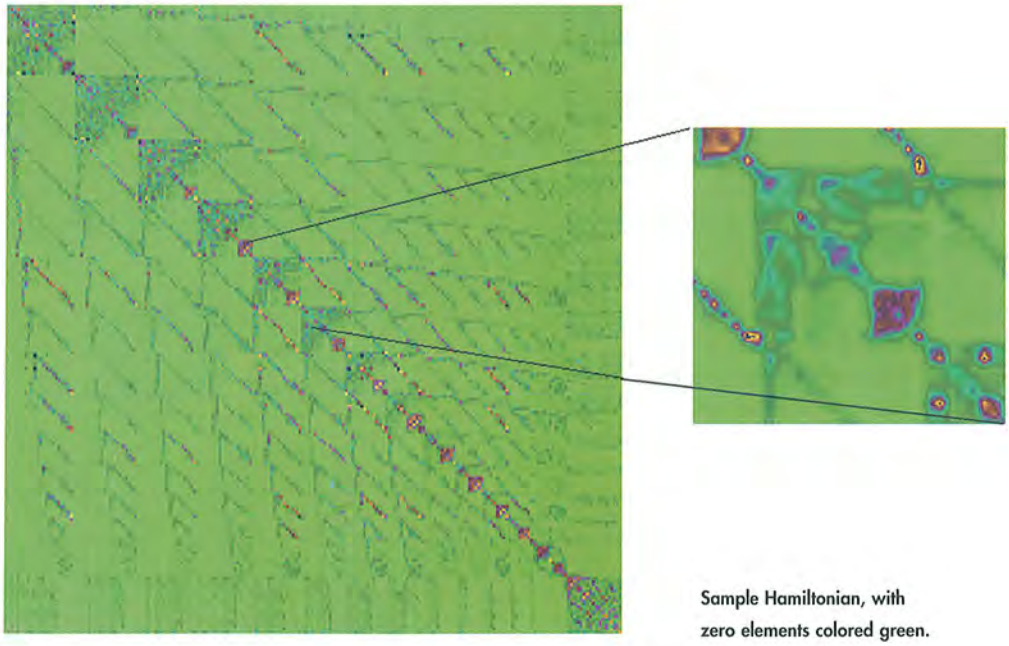
The work involves determination of the electronic structure of molecules, including relativistic effects necessary for heavy elements. Most calculations are very challenging and well suited to the Cray T3E. There are four major categories of activities:

*Benchmarking of methods:* Detailed and systematic comparison of various theoretical approaches with each other and with experiment. Few such studies are available for rigorous relativistic methods and still fewer for systems containing actinides. This work uses the J90s and the T3E.

*Application work:* Among many topics, we are studying the speciation of aqueous uranium (VI) carbonates and the electronic spectra of several systems including $AmCl^{2+}$. A detailed understanding of the actinide-carbonate-water system is essential to modeling the fate and transport of actinides in the environment. This work uses the T3E.

*Method and computer program development:* Existing programs are being parallelized for the T3E and extended to enable calculations on larger molecules at higher levels of accuracy.

*Computer science:* Extensions of Global Arrays, parallel I/O, new linear algebra, metacomputing, and prototyping of new parallel programming tools for the T3E and other parallel computers.



Sample Hamiltonian, with zero elements colored green.

## Accomplishments

This is the second year of this project. For benchmark purposes, the very rigorous relativistic models continue to be used to provide data for small uranium carbonates and also to design basis sets. This work has been performed on the J90s and the T3E. In order to determine even qualitatively correct electronic spectra for heavy metals, especially for actinides, the effects of both electron correlation and the spin-orbit interaction must be taken into account. A large component of the work on the T3E has been spin-orbit configuration interaction (SO-CI) calculations on various actinide ions. Experimental results indicate that aqueous lanthanides and actinides may be physically separated under conditions of high concentration of the soft donor chloride ion. A fundamental understanding of this process would assist in suggesting better choices and design of soft donor ligands for more selective and faster separation of these classes of elements. We are beginning to acquire pertinent information on this process by generating large spin-orbit electronic structure models of the $AmCl^{2+}$ and $EuCl^{2+}$ molecules and are looking into the differences in bonding characteristics.

The new parallel SO-CI code is now scaling very well and is functioning on the NERSC Cray T3E as well as the IBM SP machines at ANL and PNNL. The improved performance is due to numerous optimizations and use of the Global Array and ChemIO tools. A spin-orbit CI calculation comprises several steps. The input is the molecular orbital integrals arising from a self-consistent field calculation. Then the CI space must be defined. This step can require some skill in order to provide a balanced and accurate description of the electronic states of interest in a computationally tractable expansion. Work on this project has extended the size of viable expansions by over an order of magnitude. Next the Hamiltonian matrix must be generated and stored on disk. The structure and sparsity of this matrix is illustrated in the figure, and must be accounted for in efficient implementations. Finally, Davidson's method is used to determine iteratively the eigenvalues of interest, usually about the lowest dozen states.

## Significance

Most radioactive waste involves actinides, and their large atomic number implies that relativistic effects have important chemical consequences. Our implementation and application of relativistic quantum chemical methods on massively parallel computers will provide capabilities for modeling heavy-element compounds similar to those currently available for light-element compounds. The theoretical and computational methodology so developed will supplement current, very expensive experimental studies of the actinides and lanthanides. This will allow limited experimental data to be extrapolated to many other regimes of interest.

## Publications

http://www.emsl.pnl.gov/pub/proj/tms/hpcc_actinides

# Simulating Ultra-Relativistic Heavy-Ion Collisions for the STAR Experiment at RHIC

*P. Jacobs, D. Olson, I. Sakrejda, R. Snellings, F. Wang, D. Zimmerman, M. Durst, and C. Tull, Lawrence Berkeley National Laboratory*
*Y. Fisyak, P. Nevski, and T. Wenaus, Brookhaven National Laboratory*
*D. Russ and M. Kaplan, Carnegie Mellon University*
*M. Madrid, M. Mathis, N. Nystrom, R. Reddy, and S. Sanielivici, Pittsburgh Supercomputer Center*

## Research Objective

The Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory will begin operation in fall 1999, colliding beams of gold nuclei at a total center of mass energy of 39 TeV. RHIC will open a new era in the study of strongly interacting matter under extreme conditions of high temperature and pressure, hopefully leading to the discovery and study of the deconfined state of strongly interacting matter known as the quark-gluon plasma. The complexity of these heavy-ion collisions will be unprecedented in accelerator-based experimentation, with over 10,000 secondary particles generated in the most violent central interactions. The Solenoidal Tracker at RHIC (STAR) is one of two major experimental facilities being constructed to observe these collisions. STAR will generate over 300 TB of data per year.

The massive data handling needs of the STAR experiment are typical of the next generation of large high-energy and nuclear physics (HENP) experiments nearing completion in the U.S. and around the world. Numerous data intensive computing issues must be addressed for STAR and other experiments to meet their scientific goals. These include storage issues resulting from the total volume of data, efficiency issues related to moving data from tertiary storage to program memory, and access pattern issues resulting from the scientific algorithms and content of the data being analyzed. Simulating and analyzing large volumes of realistic data at NERSC is helping physicists clarify and resolve these issues.

STAR is carrying out two "Mock Data Challenges" (MDCs) prior to the start of the experiment in order to gain experience in the handling and analysis of huge datasets. The generation of simulated data on the Cray T3Es at NERSC (part of the HENP Grand Challenge on Data Access) is targeted primarily at supplying realistic input data for use in the MDCs. But more generally, the data will serve the STAR collaboration as an important resource for understanding the experimental environment and preparing for real data analysis.

## Computational Approach

Generation of realistic simulated data for heavy ion collisions requires two components: (1) an event generator, which simulates the dynamics of the collision on the nuclear scale within a particular theoretical framework, and whose output consists of 4-vectors of the particles produced in the collision, and (2) a model of the response of the detector to these particles.

From the variety of event generators for heavy ion collisions, we have chosen to focus on the Hijing event generator (X. N. Wang and M. Gyulassy), which contains physics of special interest to the STAR collaboration.

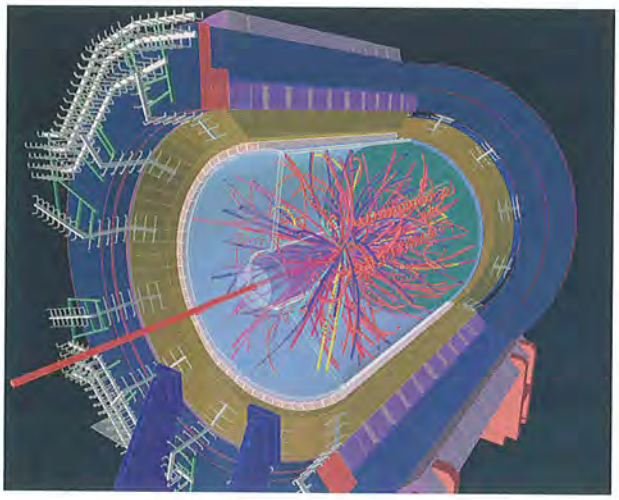
Modeling the response of the detectors in HENP experiments is done with the GEANT detector description and simulation tool, which was developed principally at CERN in Geneva over the last two decades and represents the research community's accumulated knowledge of the interaction of particles with matter. Using GEANT to generate data is extremely compute-intensive. Depending on the run configuration, generation of a single event (~20 MB data volume) can consume up to 2 PE-hours on a 450 MHz T3E processor.

In order to take full advantage of the Hijing and GEANT simulation codes, which were designed for serial machines, processing occurred in an "embarrassingly parallel" fashion, with separate events generated and processed independently on each processor. The output of each processor run was a file that contained the physics information corresponding to some number of events, typically ten events per file. These output files were archived in the NERSC HPSS system for subsequent analysis and processing.

Subsequent stages of the STAR simulations are performed at Brookhaven's RHIC Computing Facility (RCF). The data files were transferred from the NERSC HPSS to the RCF using the DPSS tool developed at Berkeley Lab.

## Accomplishments

All of the code needed for this project was developed on non-T3E architectures. Porting the GEANT code and associated software (called CERNLIB) to the T3E was a large and complex task which had never before been successfully completed, though there had been several attempts. We successfully ported GEANT (in its STAR-specific manifestation, called GSTAR) and the event generators Hijing and RQMD.



Illustrating the complexity of a typical STAR event, this image shows 5% of a simulated gold-on-gold nuclear collision at the center of the STAR detector. (Image by Craig Tull, Doug Fritz, and James Osborn of Berkeley Lab, and Herb Ward of the University of Texas, Austin)

The simulated event production was managed using a set of PERL scripts based on the SimProd package for the BABAR experiment. This package set up the input and output files for the parallel jobs and maintained a database of information about the experimental conditions and physics assumptions used for each simulation run.

Following development and debugging of the code and management scripts, Hijing/GSTAR was run intensively over a period of six weeks during August and September, using about 90k PE-hours on NERSC's T3E and generating over 1 TB of simulated data (~50k events). The cross-country data transfer to the RCF at Brookhaven achieved transfer rates of 800–900 kB/sec over brief periods and an average 200 kB/sec sustained over days.

## Significance

Handling and accessing huge quantities of data is the critical computing problem to be overcome in order to achieve the scientific goals of the new large-scale HENP experiments. Developing these capabilities is an essential component of the STAR collaboration's (and RHIC's) preparations for real data acquisition. The simulated data serve as the testbed for developing data analysis tools and algorithms. Use of the Cray T3Es for this purpose was essential: there is no other computing resource available to STAR that can supply the processing power needed for this large project.

## Publications

http://www-rnc.lbl.gov/GC/
http://www.rhic.bnl.gov/STAR/star.html

# Particle Physics Phenomenology from Lattice QCD

*Gregory Kilcup, The Ohio State University*
*Rajan Gupta, Los Alamos National Laboratory*
*Stephen Sharpe, University of Washington*
*Phillipe de Forcrand, Federal Institute of Technology (ETH), Zürich*

## Research Objectives

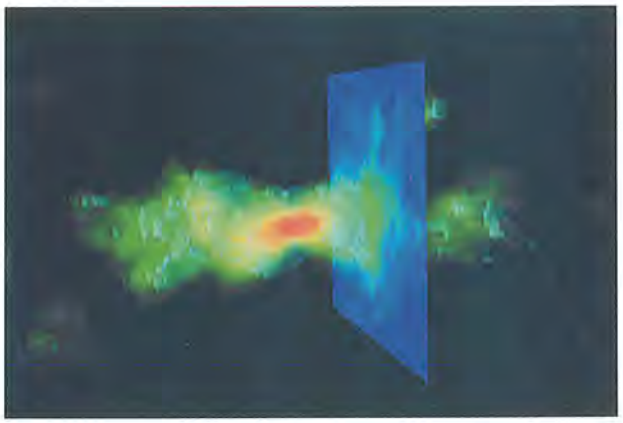
To compute the theoretical rates for certain weak interaction decay modes of elementary particles, thereby helping constrain our knowledge of the Standard Model of particle physics.

## Computational Approach

We use lattice gauge theory, a technique which discretizes space and time and models the quantum fluctuations in the vacuum by Monte Carlo. The propagation of quarks in random background fields is computed by solving discretized partial differential equations with conjugate gradients. These algorithms fit very naturally on parallel machines such as NERSC's T3E.

## Accomplishments

Our primary focus continues to be on the weak decays of hadrons. One long-standing puzzle in the decay of kaons is the so-called "delta I=1/2 rule," which is the experimental observation that two seemingly similar decay processes actually proceed at vastly different rates. For the first time, we have been able to compute the relevant decay amplitudes and successfully reproduce the observed effect. We have also computed the matrix elements needed to interpret experiments on direct CP violation currently under way at Fermilab.



**A visualization of the "quark propagator" in one typical random background chromoelectric field. A quark is created at the center of the image, and the color intensities show the probability of finding it elsewhere. Red indicates a high probability; blue is the lowest. By studying spatial and temporal correlations in the patterns of fluctuations, researchers can discern properties of the strongly interacting particles.**

In a related project, we have also performed a non-perturbative determination of the light quark masses. One of the major sources of uncertainty in many lattice QCD calculations is the use of the "quenched" approximation, in which one neglects the effects of virtual quark pairs which polarize the vacuum. Including these effects is feasible, but quite computationally intensive. We have made two steps to help alleviate this problem. First, we are developing a promising new algorithm which speeds up calculations that include virtual quarks. Second, we have established a publicly available archive for gauge configurations at NERSC. This "Gauge Connection" archive allows the sharing and re-use of the valuable unquenched configurations generated at NERSC and elsewhere.

## Significance

Together with results from particle physics experiments currently under way at labs in the U.S. and Europe, these calculations allow direct and detailed tests of the Standard Model of particle physics. At a minimum they will help determine some of the fundamental constants of nature. Eventually such tests may find small gaps in our current understanding of particle interactions, thereby giving us clues to the new physics which lies beyond.

## Publications

G. Kilcup, R. Gupta, and S. Sharpe, "Staggered fermion matrix elements using smeared operators," Physical Review D **57**, 1654 (1998).

D. Pekurovsky and G. Kilcup, "Weak matrix elements: On the way to the delta I=1/2 rule and epsilon-prime/epsilon with staggered fermions," Nuclear Physics B (Proc. Supp.) **63**, 293 (1998).
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# High-Throughput Analysis Engine for Large-Scale Genome Annotation

*E. Uberbacher and R. Mural, Oak Ridge National Laboratory*
*M. Zorn and S. Spengler, Lawrence Berkeley National Laboratory*

## Research Objectives

Interpretation of the human genome represents the next grand challenge at the interface of computing and biology. Many genome sequencing projects are producing sequence data at a rate that exceeds current analysis capabilities. New methods and infrastructure need to be implemented for effective analysis and management of this data. Our overall objective is to design and implement a distributed computational framework for the genome community that will provide users with services, tools, and infrastructure for high quality analysis and annotation of large amounts of genomic sequence data.

The main components of the Analysis and Annotation Engine consist of a number of services, a broker that oversees task distribution, and a data warehouse, with services implemented through distributed object technology. We will use state-of-the-art computational technologies, algorithms, and data management techniques to provide biologists with as much information about a sequence as is feasible at any given time and to provide mechanisms for updating descriptions of genomic regions over time. This framework will make maximal use of existing tools and database systems and integrate services across many resources. It will address issues of software sharing and reuse, generic interfaces to analysis tools, and methods for analysis system interoperation. These issues have not been addressed adequately in informatics developments.

## Computational Approach

In a phased development over the course of the project, we will construct a framework for an Analysis and Annotation Engine that deals with the design and construction of a genome analysis environment using distributed object technology and issues of interoperability. Data collection agents visit web sites of various genome centers and retrieve new sequence data for processing by the analysis services. The analysis includes high-performance implementations of a number of commonly used sequence analysis programs and development of specific new algorithms and software to provide a most complete annotation. Data mining services deal with collecting links and relevant information from outside databases and web sites. A series of data marts serve as data management and storage facilities.

## Accomplishments

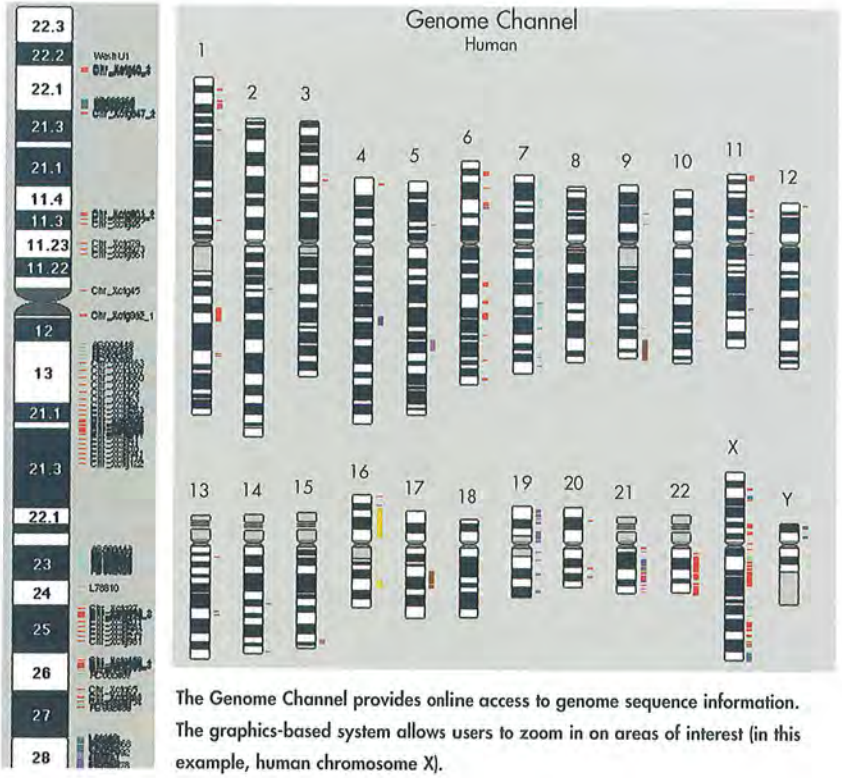
The team developed a prototype web-based framework, The Genome Channel, that shows the current progress of the international sequencing effort and allows navigation through the data down to individual sequences and gene annotations. The team at NERSC is working on the following tasks: (1) developing a CORBA-based analysis framework to facilitate automation of the genome annotation process; (2) preparing to utilize the NERSC T3E for production analysis; (3) developing specialized software and databases, such as a protein fold predictor to gauge possible structural folds for a predicted gene, an alternative splicing database to sharpen the prediction of alternatively spliced genes, and a motif processor to identify possible functional motifs in the sequence.

## Significance

The direct significance of this work is to enhance biological knowledge by providing comprehensive annotation of the human and other genomes. The Genome Channel overview also shows the current progress of the international human genome sequencing efforts.

## Publications

http://compbio.ornl.gov/gac/
http://cbcg.lbl.gov/




**The Genome Channel provides online access to genome sequence information. The graphics-based system allows users to zoom in on areas of interest (in this example, human chromosome X).**

# Computational Accelerator Physics: Advanced Modeling for Next-Generation Accelerator Applications

*R. Ryne, S. Habib, and J. Qiang, Los Alamos National Laboratory*
*K. Ko, Z. Li, B. McCandless, W. Mi, C. Ng, M. Saparov, V. Srinivas, Y. Sun, M. Wolf, and X. Zhan, Stanford Linear Accelerator Center*
*V. Decyk, University of California, Los Angeles*
*G. Golub, Stanford University*

## Research Objectives

Particle accelerators are playing an increasingly important role in basic and applied science, and are enabling new accelerator-driven technologies. But the design of next-generation accelerators, such as linear colliders and high intensity linacs, will require a major advance in numerical modeling capability due to extremely stringent beam control and beam loss requirements and highly complex three-dimensional accelerator components. The primary goal of the Grand Challenge in Computational Accelerator Physics is to develop a parallel modeling capability that will enable high-performance, large-scale simulations for the design, optimization, and numerical validation of next-generation accelerators.

## Computational Approach

The Grand Challenge is focusing on two areas: electromagnetics and beam dynamics.

The new set of tools being developed for high-resolution electromagnetics incorporates:

- unstructured grids to better treat geometries
- new algorithms to improve accuracy and convergence
- refinement techniques to optimize computing resources
- parallel processing to simulate large problems.

Presently, there are two types of solvers in the tool set. The first type includes a 3D eigensolver using linear and quadratic elements; the MPI version, Omega3P, currently runs on the Cray T3E at NERSC. The second type includes a 3D time-domain solver, Tau3P, based on the modified Yee algorithm; this code is also being ported to the T3E via MPI. Tau3P models power transmission components, whereas Omega3P simulates rf cavities. Both are designed to handle large, complex geometry meshes generated from solid models provided by popular CAD tools such as AutoCAD and ProEngineer.

Many systems involving intense charged-particle beams can be described by the Vlasov/Poisson equations. The IMPACT (Integrated-Map and Particle Accelerator Tracking) code suite now under development as part of the Grand Challenge is based on particle simulation methods for solving the Vlasov/Poisson equations as applied to accelerators. This code suite uses modern split-operator methods to combine the best features of particle simulation techniques with map-based, magnetic optics tools for simulating beam transport in accelerators. Three parallel versions have been developed using HPF, F90/MPI, and the POOMA framework based on C++. All codes now run on the T3E. The charge resolution of these codes will very soon become "real-world," i.e., the number of particles in the simulation will be approximately the same as the actual number of particles in a bunch.

## Accomplishments

The past year has seen significant achievements, especially in the successful parallelization of electromagnetics codes and in further development of the parallel beam dynamics capability.

Omega3P has been used to design the Damped Detuned Structure (DDS) for the Next Linear Collider (NLC) to within 0.01% accuracy in frequency (Figure 1). This is accomplished on the T3E by employing 128 to 256 PEs to process several million elements in one octant of the DDS geometry. A similar high-resolution calculation has been performed on the radio frequency quadrupole (RFQ) for the Spallation Neutron Source (SNS), in which an agreement with measurement to less than a MHz in the cavity frequencies has been achieved.

In the area of beam dynamics, we have performed the largest simulations to date for the Accelerator Production of Tritium (APT) project, using a parallel version of the code LINAC running on the T3E. These simulations are essential for validating designs and, in particular, for making beam loss predictions. Using the IMPACT suite of codes, we are now performing simulations of superconducting linacs, using a new algorithm that is more accurate than traditional methods in regard to the treatment of rf accelerating cavities. An example output is shown in Figure 2, which is a snapshot of a beam that is improperly matched and has developed a pronounced beam halo. We have also developed a parallel version of the Lie algebraic beam dynamics code MaryLie, and using split-operator methods, turned that code into a parallel particle-in-cell (PIC) code that combines a high-order magnetic optics capability with a capability to model intense beams. Finally, we have included the effects of external noise and collisions in the particle equations of motion using Langevin techniques.

Figure 1a. The mesh for the Next Linear Collider Damped Detuned Structure cell.

Figure 1b. The domain decomposition of the mesh on the T3E.

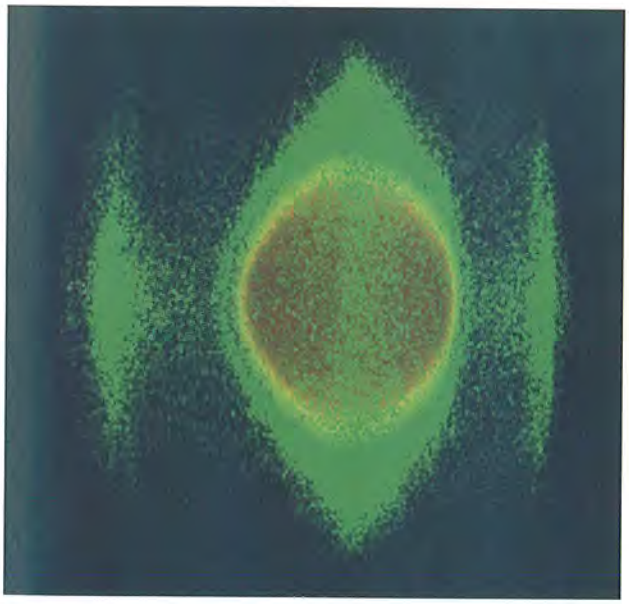


Figure 2. Three-dimensional visualization of the output from the LINAC3D code showing the particle density in a mismatched beam in the presence of nonlinear accelerating fields. The beam is moving from left to right, and the left-right asymmetry is due to the nonlinearities. The diffuse region far from the central core constitutes the beam halo. Understanding and predicting beam halo is a major issue in next-generation high-current linear accelerators.

## Significance

The advanced modeling tools developed through this Grand Challenge will allow future particle accelerators to be designed with reduced cost and risk as well as improved reliability and efficiency. The projects that this effort supports will have significant societal, economic, and scientific impacts, including impacts on DOE missions in the offices of Energy Research, Defense Programs, and Environmental Management.

## Publications

R. Ryne, S. Habib, J. Qiang, K. Ko, Z. Li, B. McCandless, W. Mi, C. Ng, M. Saparov, V. Srinivas, Y. Sun, X. Zhan, V. Decyk, and G. Golub, "The US DOE Grand Challenge in computational accelerator physics," *Proceedings LINAC98* (1998).

B. McCandless, Z. Li, V. Srinivas, Y. Sun, and K. Ko, "Omega3P: A parallel eigensolver for modeling large, complex cavities," *Proceedings ICAP98* (1998).

C.-K. Ng, B. McCandless, V. Srinivas, M. Wolf, and K. Ko, "Tau3P: A parallel time domain solver to simulate large rf structures," *Proceedings ICAP98* (1998).

http://gita.lanl.gov/people/salman/capgca

# Materials, Methods, Microstructure, and Magnetism

*G. Malcolm Stocks, Oak Ridge National Laboratory*
*Bruce N. Harmon, Ames Laboratory/Iowa State University*
*Michael Weinert, Brookhaven National Laboratory*

## Research Objectives

To develop first-principles quantum mechanical methods for addressing materials problems microscopically, especially the relationship between technical magnetic properties and microstructure. Towards this goal are major problems involving microstructure (independent of magnetism), magnetism (independent of microstructure), giant magneto-resistance, and thermal properties.

## Computational Approach

A number of different first-principles techniques, including tight-binding molecular dynamics (TBMD), an iterative pseudopotential (IP) method, and the locally self-consistent multiple scattering (LSMS) method, are used to perform fundamental studies of the atomistic, electronic, and magnetic structure of microstructural defects in metals and semiconductors that involve the interactions between large numbers of atoms (TBMD 20,000 atoms, IP > 200, LSMS 250 to 3000 atoms). In addition, we are developing spin dynamics based on both model Hamilitonians and (local) spin density calculations as a fundamental theory of the magnetic properties of metals and alloys.

## Accomplishments

A new constrained local moment (CLM) theory of non-equilibrium states in metallic magnets has been developed that places a recent proposal of our co-workers at Ames Laboratory for first-principles spin dynamics (SD) on firm theoretical foundations. In SD, non-equilibrium "local moments" (for example, in magnets above the Curie temperature, or in the presence of an external field) evolve from one time step to the next according to a classical equation of motion. As originally formulated, the instantaneous magnetization states that are being evolved were not properly defined within density functional theory. The CLM theory properly formulates SD within constrained density functional theory. Local constraining fields are introduced, the purpose of which is to force the local moments to point in directions required at a particular time step of SD. A general algorithm for finding the constraining fields has been developed.

The existence of CLM states has been demonstrated by performing calculations for large (up to 1458 atom) unit cell disordered local moment (DLM) models of bcc Fe above its Curie temperature. This DLM model can be considered prototypical of the state of magnetic order at a particular step in a finite temperature SD simulation of paramagnetic Fe. Figure 1 illustrates the calculated magnetic moments (arrows in the left frame) and constraining fields (spikes in the right frame) corresponding to a 512-atom DLM model of paramagnetic bcc Fe. Magnitudes of magnetic moments and constraining fields are color coded. These calculations represent significant progress towards the goal of full implementation of SD and a first-principles theory of the finite temperature and non-equilibrium properties of magnetic materials.

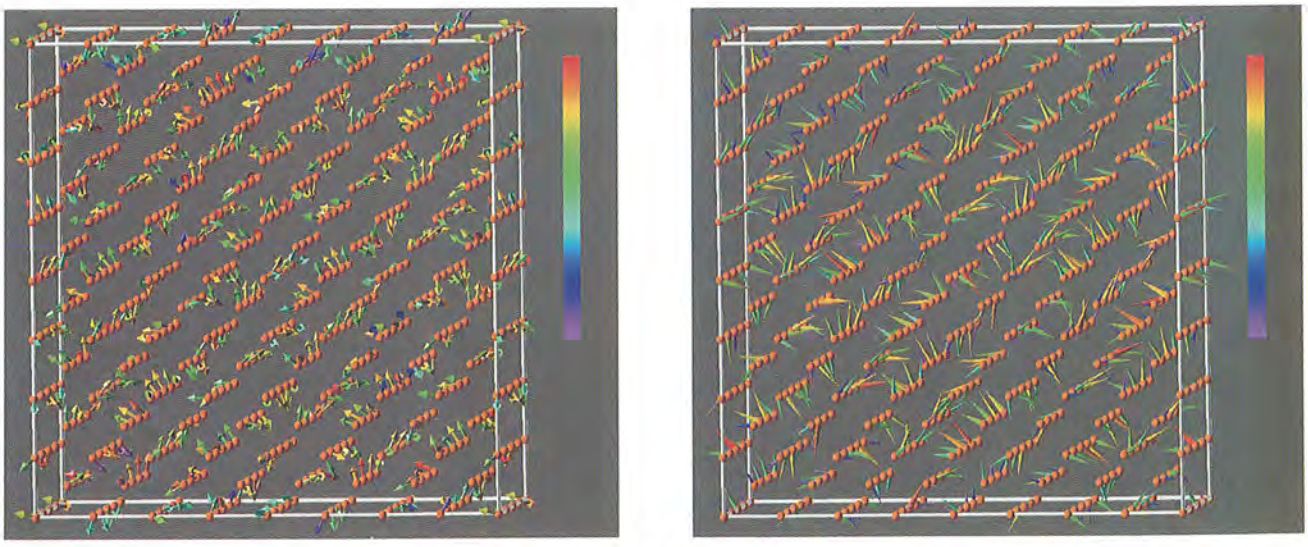


**Figure 1. 512-atom base-centered cubic iron system. The left frame shows the self-consistent field magnetic moments for the atoms, while the right frame shows the corresponding constraining fields. Atom positions are denoted by spheres, magnetic moments by arrows, and constraining fields by cones.**

The record-setting computational performance we obtained during our work demonstrating the existence of CLM states for large unit cell models (up to 1024 atoms) resulted in our receiving the 1998 Gordon Bell Award for parallel processing applications. The calculations that resulted in our nomination were performed using the LSMS method extended to treat CLM states. The basic LSMS method is an O(N) local density approximation (LDA) method that was specifically designed for implementation on MPPs and for treating the quantum mechanical interactions between large numbers of atoms. The constrained non-collinear LSMS code showed near linear scale-up for system sizes from 2 to 1024 atoms per unit cell, utilizing 2 to 1024 processing elements (PEs). We obtained a performance of 657 gigaflops on a Cray T3E-1200 LC1024/512 at a U.S. government site, and 276 and 329 Gflops on T3E-900 and T3E-1200 LC512 machines at NERSC and Cray Research, respectively. After our award nomination, we obtained a performance of 1.02 teraflops during a CLM calculation of a 1458 atom/unit cell CLM state of paramagnetic Fe (a 9×9×9 repeat of the underlying bcc unit cell). The calculations were performed on a 1,480-processor Cray T3E at the manufacturer's facility in Minnesota.

The 7×7 reconstruction of the Si(111) surface is one of the most fascinating surface structures. The presence of adatoms is a unique feature of the 7×7 reconstruction as compared to other reconstructed structures on the semiconductor surface. Using the recently developed environment-dependent silicon tight-binding potential, we have studied the structures, energies, and electronic properties of the adatom vacancies on the Si(111)-7×7 surface. The results show that adatom vacancies on the edge of the 7×7 unit cell have formation energies lower than those on the corner of the unit cell by about 0.1 eV. These results are in good agreement with experimental observations. We also observed a sharp defect state located at 0.5 eV below Fermi energy level which arises from the new bonding state of a pair of backbone atoms around the vacancy. Simulation of STM images shows that this localized vacancy state gives a pair of bright spots in the STM picture located at the two backbone atoms associated with the vacancy. Figure 2 shows the calculated STM images of the adatom vacancy on the Si(111)-(7×7) surface in the energy window of 0.6 to 0.1 eV below the Fermi energy level.

## Significance

The availability of powerful and accurate first-principles techniques permits the study of quantum interatomic interactions on a length scale not previously accessible, opening up the possibility of relating these fundamental interatomic interactions to the strength, ductility, transport and magnetic properties of materials. Applied to magnetic materials, these techniques should help establish the foundations for understanding the relationship between the technical magnetic properties (permeability, coercivity, remenance) of magnets and microstructure.

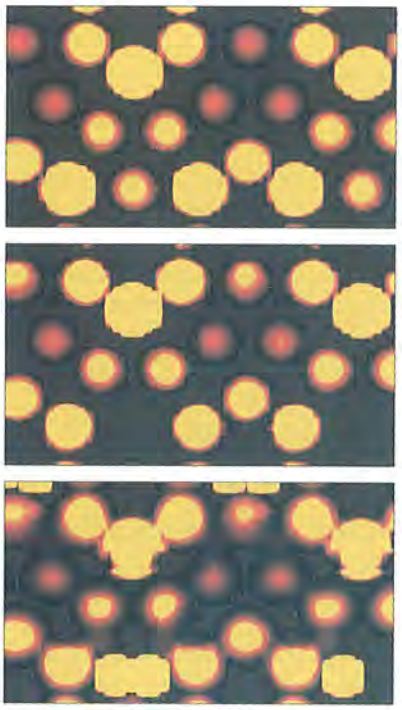


**Figure 2. Calculated STM images of the adatom vacancy on the Si(111)-(7×7) surface in the energy window of 0.6 to 0.1 eV below the Fermi energy level. Top: STM image of the perfect (7×7) reconstruction at a constant height of 4.5 Angstrom. Middle: 7×7 reconstruction with an adatom vacancy at a constant height of 4.5 Angstrom. Bottom: Image of the same vacancy at a lower height of 4.0 Angstrom.**

## Publications


B. Ujfalussy, Xindong Wang, Xiaoguang Zhang, D. M. C. Nicholson, W. A. Shelton, G. M. Stocks, A. Canning, and B. L. Gyorffy, "High performance first principles method for complex magnetic properties," in *Proceedings of the ACM/IEEE SC98 Conference, Orlando, Florida, November 7–13* (IEEE Computer Society, Los Alamitos, CA 90720–1264), CD-ROM (1998).

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http://oldpc.ms.ornl.gov/~gms/M4home.html

# Density Functional Theory Calculations of Ion Pair Association in Aprotic Electrolytes

*Perla B. Balbuena, University of South Carolina*

## Research Objectives

This project is part of a comprehensive study for first-principles prediction of materials for electrolytes and electrodes used in batteries and fuel cells. We are investigating the pair interactions of lithium perchlorate in an organic solvent, ethylene carbonate (EC), and the formation of ion pairs for different solvent conditions. The assessment of ion pairing in these systems is important because of its effect on the ionic conductivity. We are also studying the possible paths of decomposition of the solvent in the presence of an electron donor.

## Computational Approach

We are using density functional theory as implemented in the program GAUSSIAN 94 to investigate ion-ion and ion-solvent pair interactions, and charge distributions for effective force fields to be used in molecular dynamics simulations. Solvent effects are calculated using a polarizable continuum model. Reaction paths for the solvent decomposition are proposed, via formation of a transition state, which is calculated by *ab initio* techniques. The calculations are being done on the Cray C90.

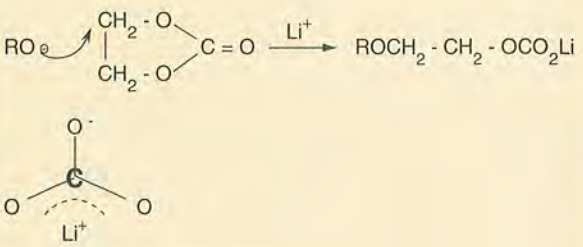
## Accomplishments

Solvation structures and selective solvation effects are analyzed and used to interpret experimental results. Interactions between lithium and perchlorate ions, and the solvent effect on these interactions, have been investigated. Among the monodentate, bidentate, and tridentate complexes for $LiClO_4$, bidentate is the most stable one in gas phase and under solvent. Vacuum and solvent ion-pair potential-energy surfaces are examined. In solution, the minimum corresponding to the ion-pair association is shifted toward larger values of the ion-ion separation. Yet a second minimum is found in the potential energy surface in solution that may be attributed to a solvent-separated ion pair complex. A mechanism for the decomposition of EC has been proposed. It is a ring opening reaction taking place in two steps, each one with the formation of an intermediate transition state. All transition states and activation energies have been calculated, and transition state theory has been used to calculate the rate of reaction.

## Significance

Aprotic electrolyte systems are being used in many current lithium-ion batteries. However, most of the design is still based on expensive trial-and-error experimentation. These studies provide data (ionic conductivity, heats of reaction) to macroscopic models to predict battery performance and help in the interpretation of experimental data obtained at the Center for Electrochemical Engineering at the University of South Carolina.

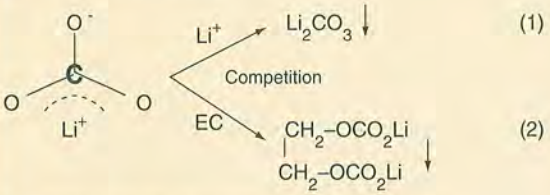
1: First nucleophilic attack:




2: Second nucleophilic attack:


Active nucleophilic $CO_3^{2-}$ is generated after two-electron transfers.

3: Competition studies:




Different products are produced according to the concentration of the solvent.

***Ab initio* calculations were performed to study the surface chemistry taking place on graphite/lithium electrode surfaces in an organic solvent, such as ethylene carbonate (EC) and propylene carbonate (PC). The calculated reaction paths, transition state structures, and activation energies were used to establish the feasibility of the proposed reactions at the operation conditions. The proposed ethylene carbonate (EC) reduction mechanism is shown.**

## Publications

T. Li and P. B. Balbuena, "Density functional theory studies of ion-ion and ion-molecule interactions of lithium perchlorate and organic solvents," J. Phys. Chem B (submitted, 1998).

A. Marquez, A. Vargas, and P. B. Balbuena, "Computational studies of lithium intercalation in model graphite in the presence of tetrahydrofuran," J. Electrochem. Soc. **145**, 3328–3334 (1998).

http://www.che.sc.edu/faculty/balbuena

# Numerical Treatment of Lepton Pair Production in Relativistic Heavy Ion Collisions

*A. Belkacem and D. Ionescu,*
*Lawrence Berkeley National Laboratory*

## Research Objectives

Electron-positron pair production will play a major role in colliders such as the Relativistic Heavy Ion Collider (RHIC) or the Large Hadron Collider (LHC). In particular, a copious amount of electron-positron pairs is expected to be produced at each of the interaction regions at RHIC. A good understanding and accounting of this process is very critical from the standpoint of background in these machines.

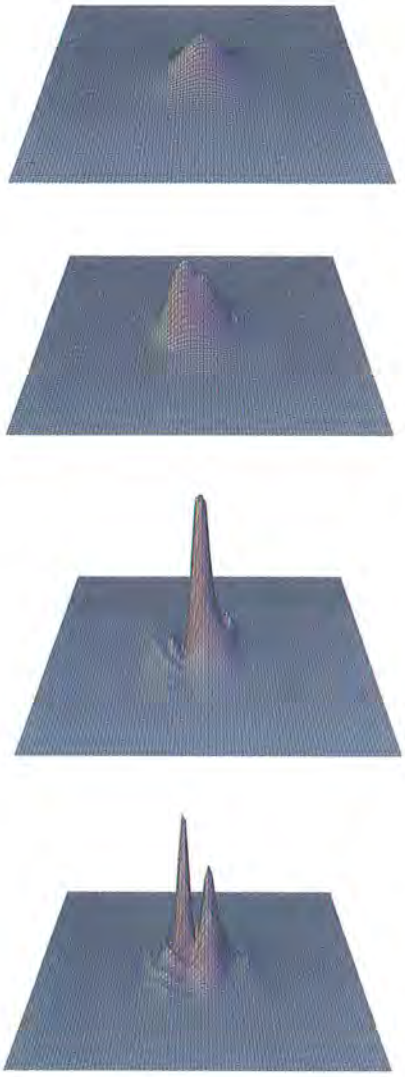
The purpose of this project is to use the T3E to solve numerically the time-dependent Dirac equation that describes the production of electron-positron pairs in relativistic heavy ion collisions. The solution on a grid will give a direct visualization of the pair-creation process as the collision between the ions evolves in time, providing a powerful nonperturbative treatment for an inherently difficult problem.

## Computational Approach

Our code uses standard PVM for message passing, and the programming language is Fortran 90. The current version uses fairly standard numerical techniques to solve the integro-differential equation. The wave function itself is represented within a finite volume by defining a global three-dimensional interpolating function on a grid. This interpolating function is constructed from cubic splines. The integration over the momentum space showing as a right-hand side of the integro-differential equation is performed cell by cell, using three-dimensional Gaussian quadrature technique.

## Accomplishments

After constructing analytically continuum wave packets representing electrons and positrons, we started a first set of intensive production runs on the T3E in January 1998. In these production runs, we limited the energy of the collision to up to 10 GeV/n, where we have the best handle on the level of precision and time integration of the computer code. The comparison of the dynamic of the collision for different initial conditions constructed from the negative and positive energy continuum states, respectively, shows a very striking behavior of the quantum electrodynamics vacuum. We use the output at each time-step to generate a movie that shows the evolution of the electronic wave function as the collision unfolds with time. As an example, we show in the figure some snapshots of the electron density at various times for the collision of a fully stripped uranium ion with a hydrogen-like gold. These snapshots are extracted from an animation that dramatically shows how the wave function grows, flows, recedes, and grows again throughout the period of the collision.



**Snapshots of the electron density at various times for the collision of a fully-stripped uranium ion with a hydrogen-like gold.**

## Significance

The animation of the collision allows a unique and direct look at the complexity and richness of what happens in the time domain in an atomic encounter. This unique information, which cannot be accessed in a laboratory, changes how we view relativistic atomic collisions.

## Publications

D. Ionescu, A. Belkacem, and A. Sorensen, "Momentum-space imaging of electronic excitations in fast ion-ion collisions using parallel processing," Contributed paper to the 1998 Annual Meeting of the Division of Atomic, Molecular, and Optical Physics, Santa Fe, NM, **43** (1998), p. 1347.

# Electronic Structure of a Polar Ceramic/Metal Interface: {222} MgO/Cu

*R. Benedek and D. N. Seidman, Northwestern University*
*L. H. Yang, Lawrence Livermore National Laboratory*
*A. Alavi, The Queen's University of Belfast*

## Research Objectives

This project is part of an effort to characterize on an atomic scale the structure and physical properties of ceramic-metal interfaces. When such interfaces are formed internally within a specimen, for example by internal oxidation, nitridation, or carburization, polar orientations typically occur, i.e., the ceramic facets at precipitate interfaces with the metal matrix are exclusively either anion or cation. Although such polar interfaces are more strongly bonded than neutral ceramic-metal interfaces, they have received much less attention theoretically. This research intends to elucidate the electronic structure and the chemical bonding at a model polar ceramic-metal interface on which considerable experimental information exists, {222} MgO/Cu.

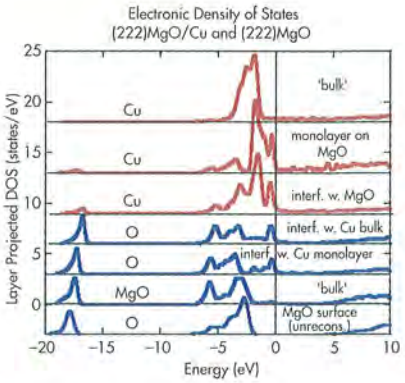
## Computational Approach

Local density functional theory (LDFT) is a first-principles computational framework that gives a physically accurate description of atomic and electronic structure of condensed matter. A convenient and numerically efficient inplementation of LDFT is the planewave pseudopotential representation. A sequential planewave pseudopotential code (developed by L. H. Yang) based on a preconditioned conjugate gradient optimization algorithm is used on the Cray J90; and a parallel planewave code (developed by A. Alavi et al.), based on the Lanczos algorithm, is employed on the Cray T3E.

## Accomplishments

Calculations are performed for a {222} MgO/Cu interface to elucidate the electronic structure in the vicinity and show how the electronic states at the interface differ from those in bulk MgO and bulk Cu. The results are analyzed to determine the layer-projected electronic density of states in the vicinity of the interface or free surface (see figure). The densities of states for the layers other than the CuO bilayer at the interface are relatively bulklike, which indicates that the interface perturbation is essentially confined to the interface bilayer. The panels labeled "bulk" represent layers two layers removed from the interface.

A noteworthy feature of the densities of states of the interface bilayer (second through fifth panels from the top of the figure) is the appearance of a peak a few tenths of an eV below the Fermi level, within the bulk MgO gap. This peak is absent from the surface O-layer spectrum at an MgO free surface (bottom panel), and results from antibonding hybrid states that mix Cu 3*d* and O 2*p* character. These are metal-induced gap states, which decay exponentially with distance from the interface. The presence of such high-lying antibonding states of d-character (as well as corresponding low-lying bonding states) is typical of




**Calculated layer-projected densities of states for unreconstructed {222} MgO free surface (bottom panel), oxygen-terminated MgO/Cu interface (second, fourth, fifth, and seventh panels), and Cu monolayer on oxygen-terminated MgO substrate (third and sixth panels).**

copper-oxide bonding, and is found, for example, in crystalline $Cu_2O$ and O adsorbed onto Cu {100} substrates. Some characteristics of the bonding of these three systems are qualitatively similar, in spite of the differences in their detailed geometries.

The theoretical effort is complemented by experimental investigations by atom-probe-field-ion microscopy, high-resolution and scanning-electronic microscopy, and electron energy loss (EELS) spectroscopy. The electronic density of states in the oxygen layer above the Fermi energy is found to agree closely with the EELS O-K edge spectrum.

## Significance

Ceramic-metal interfaces are prominent in many advanced materials, including high-temperature alloys, sensors, electronic components, and medical prostheses. It is of both practical and scientific interest to characterize the structure and properties of such interfaces.

## Publications

D. A. Muller, D. A. Shashkov, R. Benedek, L. H. Yang, D. N. Seidman, and J. Silcox, "Chemistry and bonding at {222} MgO/Cu heterophase interfaces," in *Proc. Microscopy Society of America, August 1997*, edited by G. W. Bailey et al. (Springer, New York, 1997), 647.

R. Benedek, D. A. Shashkov, D. N. Seidman, D. A. Muller, J. Silcox, M. F. Chisholm, and L. H. Yang, "Atomic structure of a polar ceramic/metal interface: {222} MgO/Cu," Materials Research Society Symposium Proceedings **492**, 103 (1998).

D. A. Muller, D. A. Shashkov, R. Benedek, L. H. Yang, J. Silcox, and D. N. Seidman, "Atomic scale observations of metal-induced gap states at {222} MgO/Cu interfaces," Phys. Rev. Lett. **80**, 4741–4744 (1998).

# Determining Macroscopic Mechanical Properties from Microscopic Calculations

*X. Blase, Centre National de la Recherche Scientifique, Lyon, France*
*K. Lin, A. Canning, S. G. Louie, and D. C. Chrzan, University of California, Berkeley, and Lawrence Berkeley National Laboratory*

## Research Objectives

The goal of this research is to apply *ab initio* electronic structure techniques to calculate the minimum stress required to move a dislocation in C in the diamond cubic phase. This value is important to engineering hard materials, as it provides a benchmark for materials performance. In addition, successful completion of this research will allow us to identify the aspects of electronic structure and bonding relevant to the motion of dislocations. This knowledge can then be used to develop an improved physical intuition concerning the strength of materials.

## Computational Approach

Calculations to date have been performed using a parallel implementation of the plane-wave *ab initio* pseudopotential technique. The calculations were run on the T3E. Supercells employed included up to 192 C atoms.

## Accomplishments

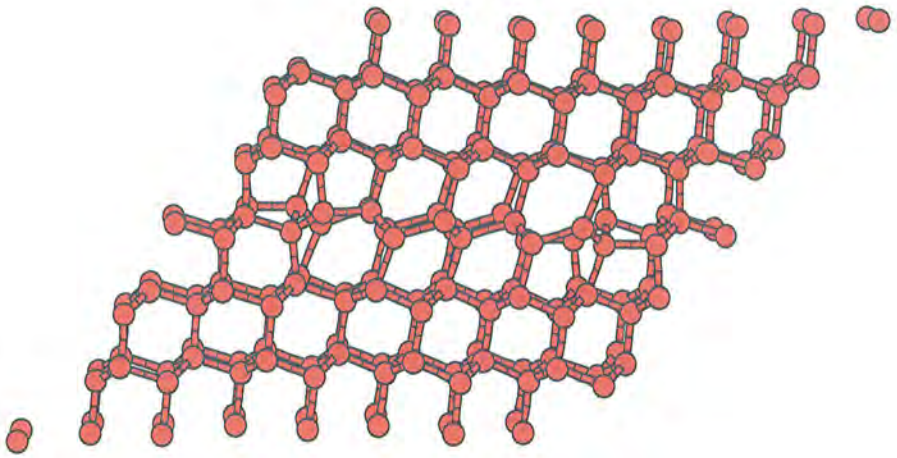
To date, we have established that the 90° partial dislocation in diamond cubic C is most stable in the period doubled reconstructed in both a dipolar and quadrupolar arrangement. We have run a number of unit cells with differing distances between the dipoles, and have begun to analyze the results within simple elasticity theory to assess if we can use the current calculations to estimate the dislocation core radius, $r_c$, which enters into classical elasticity theory descriptions of the dislocations.

## Significance

The calculation of the minimal stress required to move a dislocation places a lower limit on the strength of a material. At a minimum, the stress required to observe plastic deformation must be above the limits we will calculate. This information establishes an important benchmark that could be used to gauge the properties of materials engineered to be ultrahard, and will accelerate the search for hard materials that can be used as protective coatings.

## Publications

http://surfers-paradise.berkeley.edu/Daryl/ERCAP99.html



**The unit cell used in the calculations. The 90° partial dislocations are clearly visible as the highly distorted regions. The period doubled structure along the core is also clearly visible. The center of the cell reveals the stacking fault separating the two partial dislocations.**

# PRISM—Piece-Wise Reusable Implementation of Solution Mapping

*N. J. Brown and S. R. Tonse, Lawrence Berkeley National Laboratory*
*N. W. Moriarty and M. Frenklach, University of California, Berkeley*

## Research Objectives

The study of combustion through numerical simulations involves computational fluid dynamics and computational chemical kinetics. The responsibility of the chemistry is to calculate the heat production and the change in concentration of each chemical species as time progresses. This is done by solving a system of ordinary differential equations (ODE) but is often computationally expensive, as the number of chemical species can reach into the hundreds. We have developed a procedure (PRISM) by which the solution of the ODE is parametrized by a set of algebraic polynomial equations in chemical composition space (an artificial space in which the concentration of each chemical species is plotted along each axis). As a reaction proceeds, it traces a trajectory through this space.

Additionally, over the duration of a flame simulation, it is likely that a particular set of concentrations and temperatures will occur repeatedly at different times and positions. Hence, it is tempting for economic reasons to store the outcome of a calculation and retrieve the result when required. Therefore, we have designed an approach in which we store the information in a data structure until needed again.

## Computational Approach

We partition chemical composition space into hypercubes, each adjacent to one another. As the reaction trajectory proceeds through composition space, we calculate the polynomials for a hypercube when it is entered for the first time. Given a virgin input point, we determine the hypercube in which it lies and proceed to determine the polynomial expressions. The hypercube can be quite large, 0.25 to 0.5 of an order of magnitude in concentration per side. To parametrize the response of the ODE solver, the solver itself needs to be called repeatedly to provide the final solution at various data points within the hypercube. The optimal placement of these points is determined by the use of a factorial design method known as Response Surface Theory, by which the number of points is kept relatively low. Using these few data points, we form a set of polynomials from which we can obtain the time evolution of any input point within the hypercube. We now place the hypercube and polynomial information into a data structure (a combination of binary tree and double-linked list) for future re-use. As we proceed with our chemistry calculation, we merely have to evaluate an algebraic polynomial instead of solving a system of differential equations.

## Accomplishment

We have tested our PRISM method on three diverse combustion simulations, a zero-dimensional burn, a 1D laminar flame, and a 2D turbulent jet. These are time-evolving initial value problems. The accuracy of the method is excellent, and there is good agreement with the ODE solution even after 200 ms.

## Significance

We have shown that it is possible to do a turbulent jet simulation using a parametrized substitute for the ODE solver, in a fraction (one-tenth) of the previous CPU time.

# Electronic Structure Studies of Pyrolytic Reactions of Hydrocarbons

*J. Cioslowski, M. Schimeczek, P. Piskorz, and D. Moncrieff, Florida State University*

## Research Objectives

The main objective of this project is the theoretical investigation of the possible reaction mechanisms involved in the pyrolytic formation of cyclopentafused polycyclic aromatic hydrocarbons (cp-PAHs) from ethynylsubstituted PAHs. Five main pathways were examined:

1. A direct insertion of the terminal C atom of the ethynyl substituent into an aromatic C-H bond of the neighboring ring, followed by a 1,2-hydrogen shift in the resulting carbene.
2. An acetylene-vinylidene rearrangement in the ethynyl substituent, followed by insertion of the resulting carbene into an aromatic C-H bond of the neighboring ring.
3. A homolytic fission of the terminal C-H bond of the ethynyl substituent, followed by an insertion of the resulting radical into an aromatic bond of the neighboring ring, and a final recombination with an H radical.
4. A homolytic fission of an aromatic C-H bond, followed by insertion of the resulting radical into the terminal C-H bond of the ethynyl substituent, and a final recombination with an H radical.
5. The addition of an H radical to the nonterminal C atom of the ethynyl substituent, followed by insertion of the resulting radical into an aromatic C-H bond of the neighboring ring, and final abstraction of an H radical.

## Computational Approach

The density functional approach within the *ab initio* electronic structure model was used to evaluate the electronic wavefunctions. A BLYP functional in conjunction with a 6-311G** Gaussian basis set were used in all calculations. Using the GAUSSIAN94 suite of programs, optimization and vibrational-frequency analysis were calculated for all the minima and transition states possibly involved in the reactions of ethynylsubstituted naphthalene, acenaphthylene, fluoranthene, and pyrene (1- and 4-substituted), yielding the corresponding cyclopentafused systems acenaphthylene, pyracylene, cyclopenta[c,d]fluoranthene, and cyclopenta[c,d]pyrene. The NERSC J-90 cluster was used in performing these calculations.

## Accomplishments

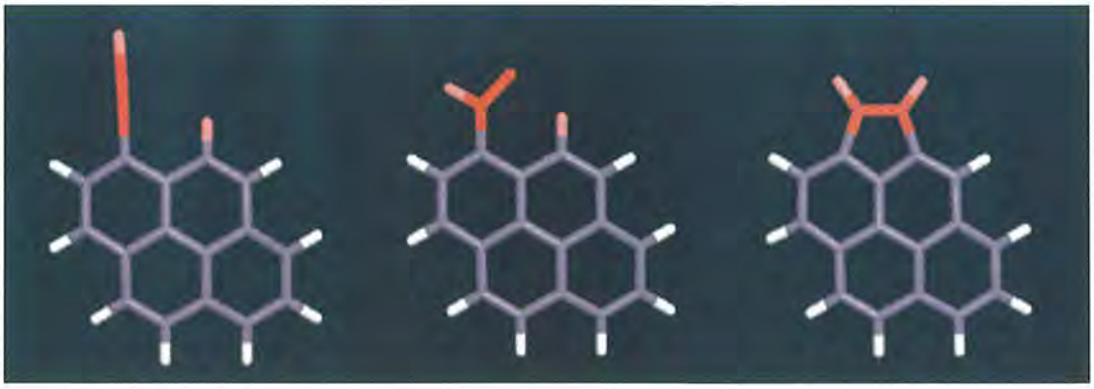
Except for three transition states in Pathway 5, all relevant stationary points on the energy hypersurfaces of the above-mentioned reactions were successfully localized and characterized as minima or transition states. Pathway 2 was identified as the most important reaction channel for the pyrolytic buildup of the cp-PAHs under investigation. Changing the aromatic systems did not affect the overall picture of the energetic relation between different pathways. However, a general energetic upshift was observed for all cyclizations of acenaphthylene and fluoranthene compounds, due to an increased strain in these cyclopentafused systems.

## Significance

In general, cp-PAHs are potent carcinogens and mutagens. They are formed during incomplete combustion of fossil fuels and other hydrocarbon material. Our identification of the exact mechanism that determines the formation of these compounds can help to effectively suppress or avoid their unwanted buildup.

## Publications

J. Cioslowski, M. Schimeczek, P. Piskorz, and D. Moncrieff, "Thermally induced rearrangement of ethynylarenes to cyclopentafused polycyclic aromatic hydrocarbons: An electronic structure study," J. Am. Chem. Soc. (submitted, 1998).



The three energetic minima in the most favorable reaction path of the cyclization of 1-ethynylpyrene.

# Molecular-Based Simulation of Complex Fluids

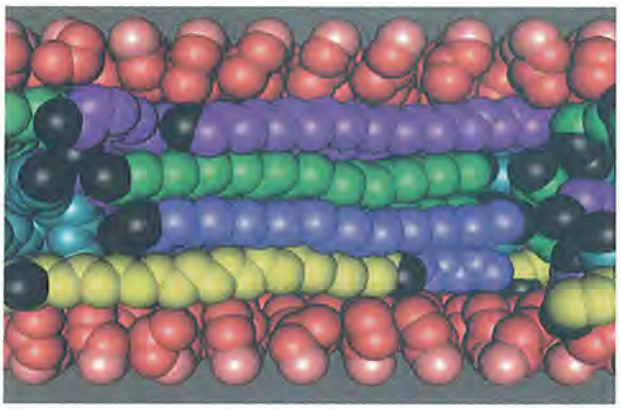
*P. T. Cummings, University of Tennessee*

## Research Objectives

Our research is aimed at elucidating the molecular basis for the properties of complex materials and liquid systems, such as lubricants, self-assembling micellar systems, polymers, and high-temperature aqueous solutions. A common thread in all of our research is to develop and use the most accurate and realistic models for the interactions between molecules, and to predict properties that can be compared directly with experiment, or to guide the development of new experiments.

## Computational Approach

We use parallel molecular dynamics codes, developed within our group, running on the NERSC T3E. We use a variety of parallelization strategies, including domain decomposition and data parallel (or replicated data). We have developed our own visualization tool, MDVIZ, which is PVM-based and can be used for remote visualization and steering of ongoing simulations.



**The image shows tetracosane, $C_{24}H_{50}$, confined between two walls 3.9 nm apart, undergoing a high degree of shearing (i.e., top wall moving to the right and bottom wall moving to the left) as is experienced in critical lubrication applications. The temperature and density of the tetracosane are at typical values for lubrication applications. The walls have butane molecules ($C_4H_{10}$) tethered to them. Only the carbon atoms in each molecule are shown. The tethered butanes are colored in red, with the attached carbon shown in pink. The tetracosane molecules are in various colors (such as yellow, blue, green, and purple) so that they can be easily distinguished. All end groups, however, are colored black. Note that the molecules have formed an ordered structure, with molecules lying in layers parallel and perpendicular to the plane of the image. The ordered nature of the tetracosane in this situation gives rise to a very large effective viscosity, in agreement with experiments on alkane liquids confined to nanoscale gaps.**

## Accomplishments

One of our key accomplishments was the first molecular-simulation-based prediction of the viscosity index—a key measure of lubricant performance—of typical lubricant base-stocks (in this case, alkane liquids in which each molecule contains 30 carbons). We have examined the impact of molecular architecture (linear vs branched) on the viscosity index and rheology of these lubricants.

Another key accomplishment is the development of intermolecular potentials for perfluoralkane systems that can be used in our study of reversed micelles in supercritical carbon dioxide.

## Significance

This research will lead to better understanding of such issues as what makes one automotive lubricant better than another. This will lead to improved lubricants in automobile engines, which will, in turn, result in better energy efficiency. Our research also is aimed at finding new candidates for replacing organic solvents in chemical processes with more environmentally benign alternatives.

## Publications

J. D. Moore, S. T. Cui, P. T. Cummings, and H. D. Cochran, "Lubricant characterization by molecular simulation," A.I.Ch.E. Journal **43**, 3260–3263 (1997).

S. T. Cui, P. T. Cummings, H. D. Cochran, J. D. Moore, and S. A. Gupta, "Nonequilibrium molecular dynamics simulation of rheology of linear and branched alkanes," Int. J. Thermophys. **19**, 449–459 (1998).

S. T. Cui, H. D. Cochran, and P. T. Cummings, "Vapor-liquid phase coexistence of alkane-$CO_2$ and perfluoroalkane-$CO_2$ mixtures," J. Phys. Chem. (submitted, 1998).

http://flory.engr.utk.edu

# Modeling of Thin-Film Diamond Growth

*L. A. Curtiss, D. Gruen, D. Horner, and P. Redfern,*
*Argonne National Laboratory*

## Research Objectives

This project involves a fundamental theoretical study of diamond thin-film growth from fullerene precursors to understand why nano-crystalline diamond results from growth in plasmas containing little hydrogen. At Argonne National Laboratory, we have grown extremely smooth nano-crystalline diamond films, with crystallite sizes in the range 3–10 nm, in experiments involving chemical vapor deposition following fragmentation of fullerene in a microwave discharge.

## Computational Approach

*Ab initio* molecular orbital and density functional theory is being used to investigate reaction mechanisms involved in thin-film growth on (110) and (100) diamond surfaces, with the carbon dimer as the growth species. The diamond surface is modeled using clusters of carbon atoms. The reaction energies and barriers are calculated at various levels of theory. At the highest level is G2 theory, which is used for model molecule reactions. Density functional theory is used for the large cluster models.

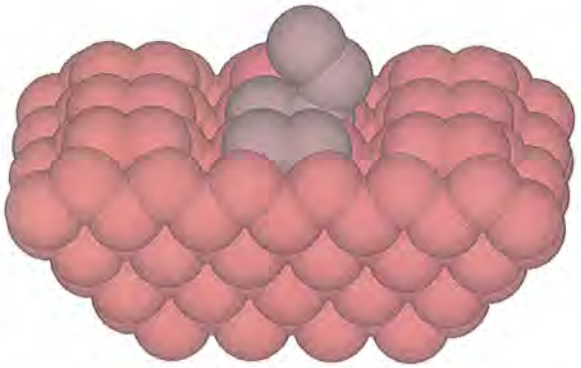


**Figure showing insertion of $C_2$ into a bare (100) diamond surface that leads to a nucleation site for a new diamond crystallite.**

## Accomplishments

Density functional calculations of growth on the (110) diamond surface using carbon dimer $C_2$ as the growth species found that the various steps were energetically very favorable, without requiring the participation of atomic hydrogen and with small activation barriers. The $C_2$ is found to insert into the CH bonds in this mechanism. Similar calculations on the (100) surface have used clusters that model the unhydrided and monohydride surfaces, respectively. The results indicate that on the monohydride surface, the $C_2$ inserts into the CH bond and growth is similar to that for the (100) surface. In contrast, for the bare (100) surface, the $C_2$ insertion is found to occur into the CC double bonds with no barrier. This has important implications for diamond growth.

## Significance

The results of these reaction-mechanism studies indicate that lack of hydrogen on the surface can lead to insertion into a CC double bond and a possible new nucleation site. The disparate nucleation rates of diamond crystallites grown in hydrogen-rich vs. hydrogen-poor microwave plasmas (leading to nano-crystalline diamond in the latter case) are accounted for qualitatively by these results.

## Publications

D. A. Horner, L. A. Curtiss, and D. M. Gruen, "A theoretical study of the energetics of insertion of dicarbon ($C_2$) and vinylidene into methane C-H bonds," Chemical Physics Letters **233**, 243 (1995).

P. Redfern, D. A. Horner, L. A. Curtiss, and D. M. Gruen, "Theoretical studies of growth of diamond (110) from dicarbon," Journal of Physical Chemistry **100**, 11654 (1996).

D. M. Gruen, L. A. Curtiss, P. C. Redfern, and L. C. Lin, "Nucleation of nanocrystalline diamond by fragmentation of fullerene precursors," *Proceedings of the Symposium on Fullerenes: Chemistry, Physics, and New Directions XI: 193rd Meeting of the Electrochemical Society* (in press, 1998).

http://chemistry.anl.gov/compmat/diamond.htm

# Fundamental Studies of Metastable Liquids

*P. G. Debenedetti, Princeton University*

## Research Objectives

The broad theme of my research project addresses fundamental problems in metastable liquids and glasses. Metastable liquids are ubiquitous in nature (clouds, living systems surviving under sub-freezing conditions, fluid transport in plants) and in technology (cavitation erosion; vapor explosions; cryopreservation of cells, seeds, and labile biochemicals in supercooled emulsions; pharmaceutical formulations). However, the connection of metastable liquids to the rigorous molecular theory of matter remains incomplete. My research aims at enriching fundamental understanding of metastability.

## Computational Approach

In our work we use computational methods we have previously developed for simulating fluids under constraints (restricted ensemble), which we then use to explore the relationship between fluid properties and the severity of the applied constraint. Additionally, we have examined the topology of the multi-body potential energy surface in supercooled liquids via the corresponding inherent structures or local potential energy minima. This requires large-scale minimizations for systems having on the order of $10^3$ degrees of freedom.

## Accomplishments

A representative example of the progress we have made during the past year is that by the approach described above, we have been able to demonstrate that the onset of nonexponential relaxation and of non-Arrhenius dependence of the structural relaxation time correspond to a well-defined temperature, below which the depth of the potential energy minima explored by the liquid decreases with temperature, and above which it does not. We have also found that the energy landscape approach provides valuable insight into the mechanical stability of liquids and its possible relevance to the process of vitrification.

## Significance

Our findings suggest a general way of describing supercooled liquids. A long-term application would be to use this approach to predict for any fluid the temperature dependence of its low-temperature properties, based only on the microscopic interactions between the molecules. Additionally, many of the techniques we employ and develop have applications that are not restricted to metastable states. Hence, our research has broad implications for the understanding of the liquid state of matter in general.

## Publications

P. G. Debenedetti, D. S. Corti, S. Sastry, and F. H. Stillinger, "Constraints, metastability, and inherent structures in liquids," Phys. Rev. E **55**, 5522 (1997).

P. G. Debenedetti, S. Sastry, and F. H. Stillinger, "Statistical geometry of particle packings: II. Weak spots in liquids," Phys. Rev. E **56**, 5533 (1997).

———, "Signatures of distinct dynamical regimes in the energy landscape of a glass-forming liquid," Nature **393**, 554 (1998).

http://www.princeton.edu/~pdebene

# Theoretical Studies of Atomic Transitions

*C. Froese Fischer, Vanderbilt University*

## Research Objectives

Accurate computational procedures are being developed for atomic structure calculations that can predict properties such as energy levels, binding energies, transition probabilities, lifetimes, hyperfine structure, isotope shifts, and photoionization cross sections.

## Computational Approach

Our approach is a variational one, starting either from nonrelativistic theory and adding the low-order relativistic corrections, or from a fully relativistic Dirac-Fock theory including Breit and quantum electrodynamics corrections. These are referred to as MCHF (multiconfiguration Hartree-Fock) and MCDF (multiconfiguration Dirac-Fock) methods, respectively. Rule-based schemes are being devised for expanding the wavefunction, describing the electronic charge distribution in terms of a basis of configuration states, a basis which is then optimized. An important part of the calculation is the matrix eigenvalue problem for which we use the Davidson algorithm for finding a few selected eigenvalues of the sparse symmetric interaction matrix. Since this algorithm relies primarily on matrix-vector multiplication, a parallel version on the T3E could readily be implemented, and cases as large as 100,000 × 100,000 have been considered.

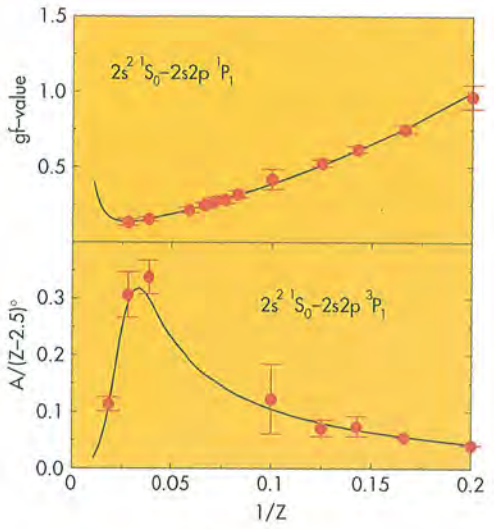
## Accomplishments

The MCHF codes had been parallelized previously using MPI. This year the MCDF matrix eigenvalue problem was also converted. These codes were used on the T3E in two important applications:

*1. Spectrum calculations for the lithium-like sequence for nuclear charges, Z=3-10, for decay from 2p, 3s, 3p, and 3d levels.* This allows for the calculation of not only the individual transition rates, but also the lifetime of the excited levels, which often is the measured experimental quantity. Only in Li are experimental lifetimes available. Our computed results appear to be more accurate than experiment.

*2. Forbidden E2 and M1 transitions in $Fe^{+3}$ $3d^5$.* For the former, the MCHF method was most efficient, but for the latter, where there are many closely spaced levels, both methodologies were tested. Currently, the MCHF calculations are better able to account for many-body effects, though MCDF provides a better description of relativistic effects.

The accuracy that can be achieved by MCDF studies for both light and heavy elements of the Be-like sequence was investigated without the use of the T3E, but comparison with experiment provides a benchmark study of the reliability of our methods.




**A comparison of computationally predicted atomic transition data with experiment for four electron ions of nuclear charge Z, plotted against 1/Z. For the top graph, relativistic effects are small for Z < 20, but they are crucial for all Z in the bottom graph.**

The figure shows that for some four-electron systems, atomic properties can be computed to experimental accuracy.

## Significance

Atomic data are needed in many scientific endeavors, for example, in plasma diagnostics and astrophysical applications. Of particular interest has been the prediction of lifetimes of excited states that decay through the emission of a photon. Such data for the rare earths are currently of interest in the lighting industry. Iron is produced predominantly in supernovae, with measurements of the Fe abundance providing fundamental information on nucleosynthesis and galactic chemical evolution. Data for Fe at several stages of ionization are needed in modeling studies.

## Publications

C. Froese Fischer and R. H. Rubin, "Transition rates for some forbidden lines in Fe~IV," J. Phys. B **31**, 1657 (1998).

C. Froese Fischer, M. Saparov, G. Gaigalas, and M. Godefroid, "Breit-Pauli energies, transition probabilities, and lifetimes for 2s,2p,3s,3p,3d,4s $^2$L levels of the lithium sequence, Z=3-8," Atomic Data and Nuclear Data Tables **70**, 1 (1998).

P. Jonsson, C. Froese Fischer, and E. Trabert, "MCDF calculations of transition probabilities in the Be isoelectronic sequence," J. Phys. B **31**, 3497 (1998).

http://www.vuse.vanderbilt.edu/~cff/mchf.html

# Nonequilibrium Processing of Materials Using Beams of Particles and Clusters

*M. Ghaly, K. Nordlund, H. Zhu and R. S. Averback,*
*University of Illinois at Urbana-Champaign*

## Research Objectives

This research aims at clarifying how the properties of materials are changed during ion irradiation or cluster bombardment. This kind of non-equilibrium processing enables synthesis of materials which in many cases are difficult or impossible to produce by more conventional means. Using computer simulations in combination with experiments, we aim to obtain fundamental knowledge that enables production of new kinds of materials and improvements in the properties of existing materials.

## Computational Approach

Phenomena of interest include sintering of nanoparticles, interactions of nanoparticles with surfaces, damage produced by shallow implants in semiconductors, electron-phonon coupling, and the role of surfaces on damage production in solids. We primarily use classical molecular dynamics simulations to study these phenomena on an atomistic level. The NERSC T3E enables direct simulation of experiments involving millions of atoms, corresponding to system sizes of tens of nanometers. This scale is sufficient to simulate collision cascades produced by irradiation in most materials.

## Accomplishments

- We simulated the dynamics of energetic impacts of clusters on surfaces where the collision energy is negligible (see figure).
- We employed two types of computer simulations to provide a clearer picture of defect production in irradiated Si.
- We developed a combined experimental-simulation method to solve the problem of electron-phonon coupling. The results showed that in Ni, Pd and Pt, where coupling has traditionally been believed to be the strongest, it is in fact negligible, roughly an order of magnitude weaker than the most widely used models predict.
- We examined collision cascades between 30 and 100 keV in a variety of materials, including both metals and semiconductors, and looked at events where energetic recoils are initiated in the bulk and by ion implantation. The results showed that a variety of special damage mechanisms are possible in the presence of a surface.

## Significance

Understanding the damage structures in silicon clarifies the mechanisms leading to amorphization of silicon during semiconductor processing. This knowledge may enable better control of implant processing in the industry. Understanding the large effect played by surfaces in metal irradiation may lead to new methods of modifying the properties of metal surfaces and thin films. Comprehending the nanocluster interactions of surfaces may enable the manufacture of nanocrystalline materials and surface coatings out of exotic combinations of materials such as normally immiscible metals.

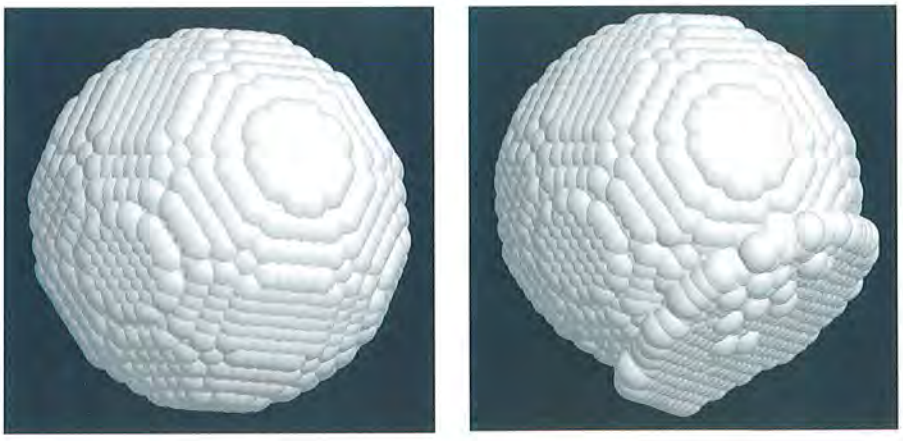
## Publications

K. Nordlund, M. Ghaly, R. S. Averback, M. Caturla, T. Diaz de la Rubia, and J. Tarus, "Defect production in collision cascades in elemental semiconductors and FCC metals," Phys. Rev. B **57**, 7556 (1998).

K. Nordlund, L. Wei, Y. Zhong, and R. S. Averback, "Role of electron-phonon coupling on collision cascade development in Ni, Pd and Pt," Phys. Rev. B (Rapid comm.) **57**, 13965 (1998).

M. Ghaly, K. Nordlund, and R. S. Averback, "Molecular dynamics investigations of surface damage produced by keV ion bombardment of solids," Phil. Mag. A **1998**, in press.

http://www.mrl.uiuc.edu/~nordlund/nersc/report.html



This figure illustrates how a Cu cluster reorganizes as it hits a Cu surface. Before impact, the cluster is a perfect sphere; after the impact, the lower interface has reorganized to minimize the surface and interface energy. Note that the lowest surface has an almost perfect crystal structure, corresponding to the structure of the substrate.

# Photonic Band Gap Structures

*B. Harmon, K.-M. Ho, M. Sigalas, R. Biswas, C. Soukoulis, G. Tuttle, K. Constant, D. Turner, and B. Vasiliu, Ames Laboratory/Iowa State University*

## Research Objective

Electromagnetic (EM) waves propagating through structures of periodically modulated dielectric constants are organized into photonic bands that are analogous to the electronic band structures in crystals. These photonic band gap (PBG) structures can be designed to affect EM waves in a variety of ways. Applying the power of massively parallel computers such as the Cray T3E at NERSC allows us to design and study a broad range of optical devices made from dielectric and metallic photonic crystals.

## Computational Approach

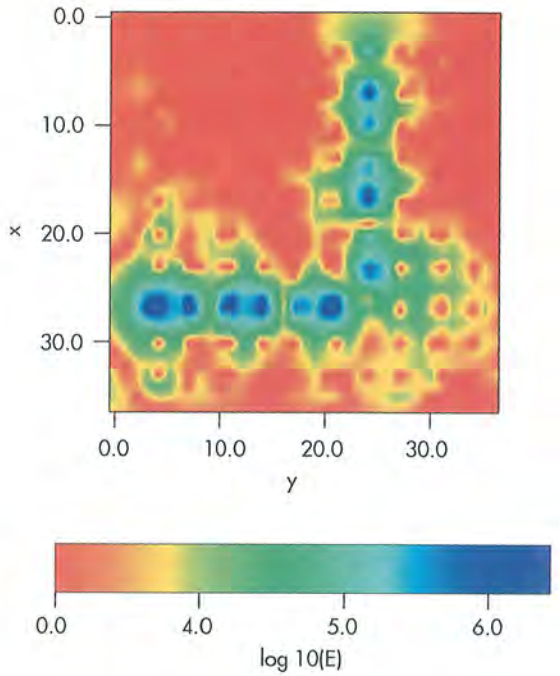
We use two main methods to investigate PBG structures. With the Transfer Matrix Method (TMM), we can calculate the transmission and reflection coefficients of a plane wave incident on a PBG structure consisting of metals and/or dielectrics. With the Finite Difference Time Domain (FDTD) method, we can investigate the time-dependent effects of EM wave propagation through finite size systems. The power of the Cray T3E allows us to attack much larger problems involving a higher degree of disorder for both of these methods.

## Accomplishments

The TMM code has been instrumental in allowing us to study defects in PBG materials and to investigate the effects of disordered states. With the FDTD code, we have simulated the transmission of light around a sharp corner made from defects in the PBG material, as pictured in the waveguide. We have also calculated the radiation patterns from dipole antennas on 3D photonic crystals, where the dielectric crystal acts as a perfectly reflecting substrate.

## Significance

This work is allowing us to develop a more fundamental understanding of PBG structures, including the effects of defects and disordered states that are computationally very demanding. This understanding and the ability to simulate photonic structures on the Cray T3E at NERSC are allowing us to design and study a variety of optical devices, which we can then build and investigate experimentally.




**Transmission of light around a sharp corner in a 3D PBG waveguide.**

## Publications

M. M. Sigalas, R. Biswas, K. M. Ho, W. Leung, G. Tuttle, and D. Crouch, "Applications of photonic band gap materials," *Proceedings of the 13th Annual Review of Progress in Applied Computational Electromagnetics* (1997), p. 412.

M. M. Sigalas, R. Biswas, K. M. Ho, C. M. Soukoulis, and D. D. Crouch, "Waveguides in photonic band gap materials," *Proceedings of the 14th Annual Review of Progress in Applied Computational Electromagnetics* (1998), p. 144.

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http://www.public.iastate.edu/~cmpexp/groups/ho/pbg.html
http://cmp.ameslab.gov/cmp/cmp.html

# Direct Numerical Simulation of Liquid-Solid Flow

*D. Joseph and Y. Saad, University of Minnesota*
*R. Glowinski, University of Houston*
*H. Hu, University of Pennsylvania*
*A. Sameh, Purdue University*

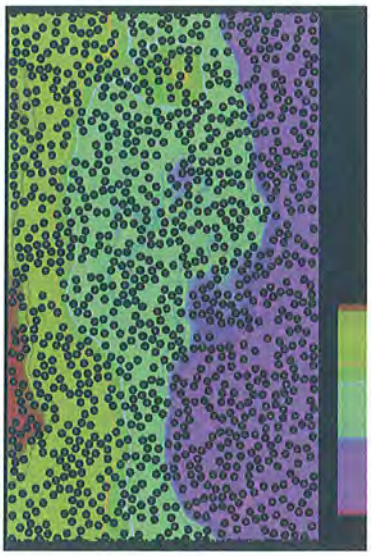
## Research Objectives

Sponsored by a National Science Foundation Grand Challenge high performance computing grant, the DOE Office of Basic Energy Sciences, and several industrial partners (Dowell-Schlumberger, Schlumberger, Shell, Stimlab, and Intevep, S.A.), we seek to develop state-of-the-art software packages that solve initial-value problems for dispersion of thousands of particles on parallel computers. To achieve this, a marriage between computational fluid dynamics (CFD) and computer science (CS) is created to produce the most efficient parallel preconditioners and iterative schemes. These are needed to handle the large, time-consuming nonlinear and linear algebraic equations that arise in this investigation.

## Computational Approach

In this project, particles are moved by Newton's laws under the action of hydrodynamic forces computed from the numerical solution of the fluid equations. Solutions of the initial value problem for dispersion of solid particles in fluidized beds and slurries, sand placement in fracture oil reservoirs, cleaning of drill cuttings from oil wells, and other applications are solved without approximations beyond those inherent in simulations.

The two parallel software packages developed in this project use a new, combined weak formation. In this formation, the fluid and particle equations of motion are combined into a single, weak equation of motion from which hydrodynamic forces and torques on the particles have been eliminated. These and other results achieved in this Grand Challenge project have opened new and promising lines for investigation.



**1,109 particles flowing in a Newtonian fluid in a channel. The mixture is pumped upwards against gravity. The color shows the stream function.**

## Accomplishments

The collaboration of CFD and CS communities, which traditionally speak different languages, has given rise to an interdisciplinary group that communicates with ease across disciplinary boundaries. This interdisciplinary research effort has already resulted in two state-of-the-art parallel software packages. The first, which uses a moving unstructured body-fitted grid, is the only numerical package anywhere that can move solid particles in a viscoelastic fluid in direct simulation. The second is an elegant package that uses a fixed grid in which particles are represented by a field of Lagrange multipliers associated with the constraint of rigid body motion. The fixed-structured grid offers opportunities for using rapid solvers that are ideally suited for parallel implementation.

## Significance

Performance results obtained on two parallel computational platforms, an SGI Origin 2000 and a Cray T3E, indicate that routine fine-tuning of various kernels results in efficient utilization of the parallelism offered by these architectures. A future aim is to produce industrial-strength counterparts of the codes that are portable across a variety of parallel architectures.

## Publications

P. Y. Huang, J. Feng, H. H. Hu, and D. D. Joseph, "Direct simulation of the motion of solid particles in Couette and Poiseuille flows of viscoelastic fluids," Journal of Fluid Mechanics **343**, 73–94 (1997).

P. Y. Huang, H. H. Hu, and D. D. Joseph, "Direct simulation of the sedimentation of elliptic particles in Oldroyd-B fluids," Journal of Fluid Mechanics **362**, 297–325 (1998).

http://www.aem.umn.edu/Solid-Liquid_Flows


**Interactions shown between two spheres mixing in a channel. The color shows the stream function.**

# Modeling of Microstructural Pattern Formation in Directional Solidification

*A. Karma and M. Plapp, Northeastern University*

## Research Objectives

Our research aims at understanding the complicated spontaneous pattern formation processes occuring during the growth of solids. Examples for such phenomena are the dendritic or eutectic microstructures formed when an alloy is directionally solidified, or the growth spirals observed during epitaxial thin-film growth. The particular difficulty common to all these diffusion-limited processes is the presence of moving phase boundaries of complex and changing shape. We use the phase-field method to investigate these notoriously difficult free-boundary problems.

## Computational Approach

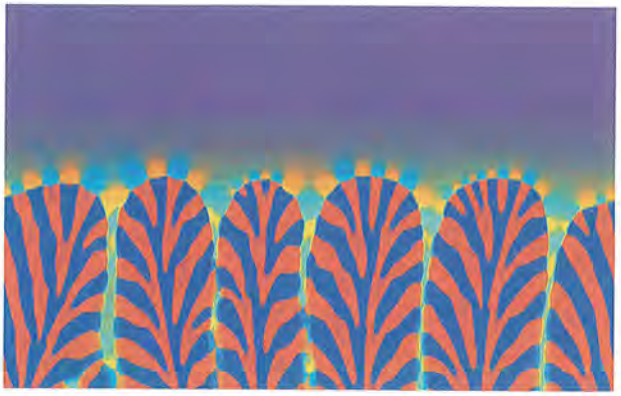
The traditional formulation of free-boundary problems in terms of mathematically sharp interfaces between different thermodynamic phases is difficult to implement because of front tracking. The phase-field method introduces indicator fields (or phase fields) and allows for a finite interface thickness. The equations of motion become nonlinear partial differential equations that can be solved using standard methods. In this setting, the problem can be very easily parallelized. We simulated systems of considerable complexity on the NERSC T3E.

## Accomplishments

We have investigated the influence of the surface tension anisotropy on the dynamics of pattern selection during the directional solidification of a binary alloy. Whereas the importance of this anisotropy is well documented for free dendritic growth, its role in directional solidification was recognized only recently. The possibility of simulating large arrays of solidification cells allowed us to monitor the complete dynamics of spacing selection, starting from a slightly perturbed interface (as is usually the case in experiments). In particular, it was shown that recently discovered multiple cells can be dynamically selected if the initial perturbation has a fixed periodicity. These results are in excellent agreement with recent experiments where a perturbation of fixed wavelength is imposed at the beginning of the solidification process, using a modulated laser beam.

We have also developed a phase-field model for the directional solidification of eutectic alloys with an additional ternary impurity. Simulations show the development of large two-phase eutectic cells, in agreement with experiments. The dynamics of eutectic cell ("colony") formation are at present ill understood and can be further investigated with our model.

As an extension of our main project, we have recently adapted the phase-field method to model step-flow growth on faceted crystal surfaces. The step dynamics in epitaxial thin-film growth are governed by the interplay of the flux of deposited atoms, the surface diffusion, and the desorption from the surface. In particular, we have investigated the dynamics of spiral ridges around screw dislocations. Whereas these spirals are well understood in the regime where desorption is dominant, our method enables us to investigate the opposite case, relevant for molecular beam epitaxy, where surface diffusion is dominant.



**Eutectic two-phase cells, or colonies, form during the directional solidification of a binary eutectic alloy with a ternary impurity. The growth direction is from bottom to top; the two solid phases are shown in red and blue. The dynamics of the interface are determined by the diffusion through the liquid (violet). The concentration of the ternary impurities in the liquid is shown as intensity levels in green. Yellow and light blue regions in the liquid indicate a strong concentration of "red" or "blue" atoms.**

## Significance

Both directional solidification and epitaxial growth are important industrial methods for advanced materials fabrication. Many properties of the final material are largely influenced by the microstructure of the material, which in turn is determined by the dynamics of the growth front. Understanding the influence of various control parameters on the growth dynamics is therefore of great practical importance.

## Publications

A. Karma and W.-J. Rappel, "Quantitative phase-field modeling of dendritic growth in two and three dimensions," Phys. Rev. E **57**, 4323–4349 (1998).

G. W. Losert, D. A. Stillman, H. Z. Cummins, P. Kopczynski, W.-J. Rappel, and A. Karma, "Selection of doublet cellular patterns in directional solidification through spatially periodic perturbations," Phys. Rev. E (in press, 1998).

A. Karma and M. Plapp, "Spiral surface growth without desorption," Phys. Rev. Lett. (in press, 1998).

http://www.circs.neu.edu

# Parallel Quantum Monte Carlo for Molecules

*W. A. Lester, Jr., Lawrence Berkeley National Laboratory and University of California, Berkeley*

## Research Objectives

Accurate computation of energies, reaction pathways, and other properties of high combustion systems.

## Computational Approach

The quantum Monte Carlo method is used in both the variational Monte Carlo and diffusion Monte Carlo forms. The method as implemented in this project uses trial functions constructed using basis-set *ab initio* techniques to define the nodes of the many-body system.

## Accomplishments

The reaction pathway for ground-state oxygen atom, $O(^3P)$, reacting with cyclopentadiene, $C_5H_6$, to form 2- and 3-cyclopentenone was determined. These calculations included the accurate determination of molecular species at each of the critical points along the reaction pathway: reactants, diradical intermediates, transition states, and products.

Our calculations show that the reaction for the formation of 2-cyclopentenone and 3-cyclopentenone arising from the electrophilic addition of $O(^3P)$ to a double bond of cyclopentadiene proceeds through an initially formed triplet diradical, undergoes triplet-singlet intersystem crossing to an open-shell diradical singlet, and progresses along the singlet manifold through transition states to the appropriate products.

As $O(^3P)$ approaches $C_5H_6$, two stable triplet-diradical states can be formed, depending on which carbon atom of the double bond the oxygen atom attaches. The O attachment site determines the remainder of the reaction path (and therefore the final product). The illustration shows these two configurations, labeled D-2CP for the triplet diradical precursor of 2-cyclopentenone, and D-3CP for the triplet diradical precursor of 3-cyclopentenone.

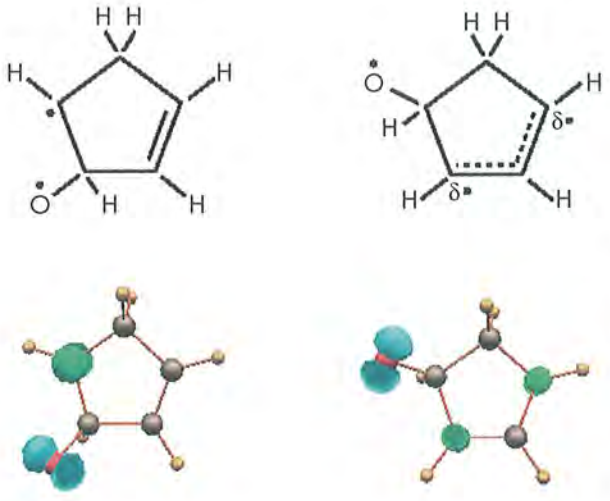
## Significance

Cyclopentadiene is a constituent of diesel fuel. The present reaction provides a substantive example to demonstrate the capability of the diffusion Monte Carlo method to yield results for a mid-size system of comparable high accuracy to that obtained earlier for small systems. It is essential to be able to compute combustion energetics of sufficient accuracy to resolve ambiguities in complicated combustion mechanisms that may be dominated by selected elementary steps.

## Publications

J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Cyclopentadiene stability: Quantum Monte Carlo, coupled cluster, and density function theory determinations," Mol. Phys (in press, 1998).

J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Quantum Monte Carlo and density functional theory characterization of 2-cyclopentenone and 3-cyclopentenone formation from $O(_3P)$ + cyclopentadiene," J. Am. Chem. Soc. (submitted, 1998).




**The triplet diradical precursor of 2-cyclopentenone (D-2CP) and the triplet diradical precursor of 3-cyclopentenone (D-3CP). In addition to atom positions, the orbitals of the triplet electrons are shown. In each case, one of these electrons is clearly localized on the O atom. For D-2CP, the molecular orbital for the second electron is localized on the carbon atom of the double bond that was broken. In the case of D-3CP, the second electron is partially delocalized across the three carbon atoms indicated, with more charge on the outer atoms than the center one.**

# Finite-Element Ray-Tracing Tomography

*J. Li and G. Xie, Lawrence Berkeley National Laboratory*

## Research Objectives

To implement and develop a new ray-tracing method that provides a useful tool to analyze surface-to-surface, surface-to-borehole, and crosshole data. To develop next-generation wave propagation and hydrodynamics codes for computational geophysics.

## Computational Approach

A graphic topology method is developed to generate a finite element mesh that not only eliminates the complications posed by complex, unstructured computational grids, but also enhances the efficiency of the ray-tracing method. The rays are accurately traced using the known velocity expression in the current element instead of in-layered or stratified medium. Critical conditions for total refraction and total internal reflection have been developed and applied. Instead of only tracing for one kind of reflection or refraction ray, the method traces the ray according to the critical conditions. Therefore, we obtain not only the first arrival ray, but also the last arrival ray. Obviously, the last arrival ray brings us more information about the deeper subsurface. These calculations are ideally suited to take advantage of developments in parallel computing on the T3E.

## Accomplishments

We have tested the ray-tracing method using the SEG/EAGE salt model (in the Gulf of Mexico). The numerical experiment was conducted for the velocity distribution in two dimensions, in which ray tracings with 109 sources and 22 initial angles for each source were used. In the figure, we plotted only the farthest rays that returned to the surface, with the highest velocity representing the salt dome. The difficulties in ray tracing come from both the geometry and the velocity distribution of the model. The interfaces are complex; some parts are linear, some parts are curved, and some parts are fuzzy; and there are many corners that could result in a singularity when a ray passes them. Velocity distribution is complex with a large contrast (3.16 times), while some parts change continuously.

## Significance

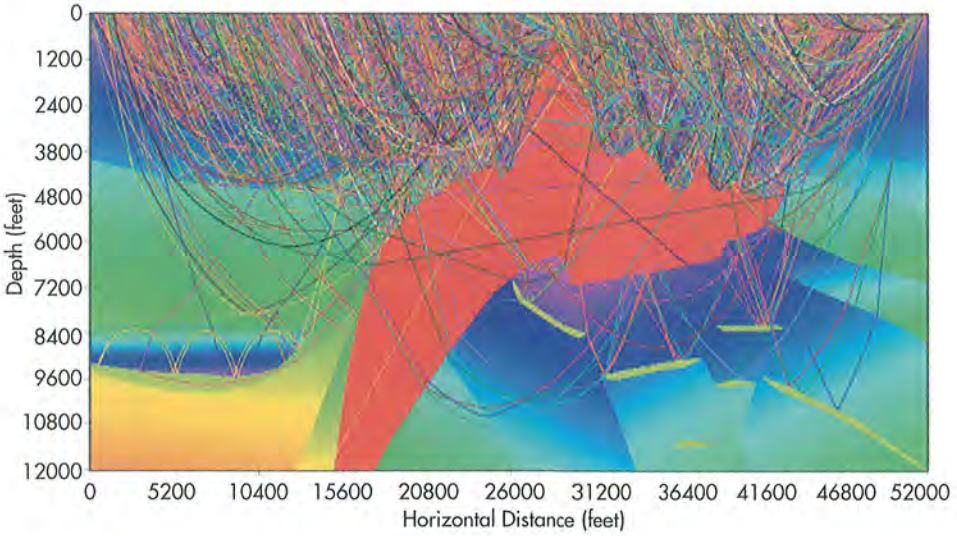
The method is applicable regardless of how heterogeneous the medium is, as long as the geological parameters (shape and size) and physical parameters (velocity of propagation and gravity) are known analytically or numerically. The method has been implemented for a two-dimensional case, and it can be easily extended to a three-dimensional case.

## Publications

J. Li and R. P. Srivastav, "Computing the singular behavior of solutions of Cauchy singular integral equations with variable coefficients," Appl. Math. Lett. **10**, N3, 57–62 (1997).

J. Li and G. Xie, "A new cubic-hole element and its application in resistivity imaging," *Proceedings of the International Symposium on Three-Dimensional Electromagnetics* (1995), pp. 415–419.

J. Li, K. H. Lee, I. Javandel, and G. Xie, "Nonlinear three-dimensional inverse imaging for direct current data," *SEG 65th Annual International Meeting and Exposition, Expanded Abstracts* (1995), pp. 250–253.




**Finite-element ray-tracing tomography of a salt dome in the Gulf of Mexico.**

# Kinetics of Elementary Processes Relevant to Incipient Soot Formation

*M. C. Lin, Emory University*

## Research Objectives

Rate constants for key elementary reactions relevant to incipient soot formation (e.g., reactions of $C_2H_3$, $C_3H_3$, and $C_6H_5$ with alkanes, alkenes, and alkynes), measured with multiple experimental methods, are elucidated and quantitatively extrapolated to the combustion regime with high-level *ab initio* MO and statistical theory calculations.

## Computational Approach

For reactions containing seven or fewer heavy atoms (e.g., $C_6H_5 + CH_4 \rightarrow C_6H_5 + CH_3$) we employed the modified Gaussian 2 method (G2M) to obtain the energies and molecular parameters of reactants, transition states, and products. For systems greater than seven heavy atoms, the hybrid density functional theory with the 6-31G(d,p) basis set (such as B3LYP/6-31G(d,p)) was used. Rate-constant calculations were carried out with the conventional and/or canonical variational transition-state theory (TST or RRKM).

## Accomplishments

Rate constants for several reactions involving $C_6H_5$ (phenyl radical) have been calculated, e.g.:

(a) $C_6H_5 + CH_4 \rightarrow C_6H_6 + CH_4$

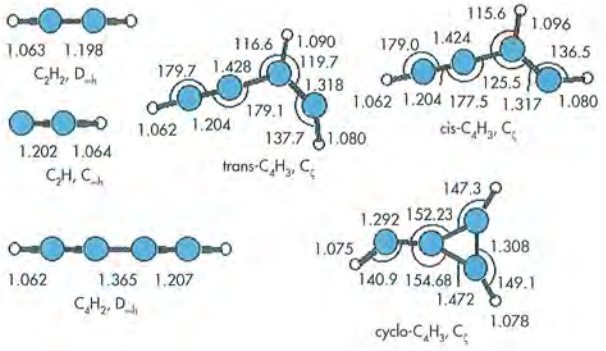
(b) $C_6H_5 + C_6H_6 \rightarrow C_{12}H_{11} \rightarrow C_{12}H_{10} + H$

(c) $C_6H_5 + C_6H_5CH_3 \rightarrow C_6H_6 + C_6H_5CH_2$

Reaction (a) is a direct abstraction process; this open-shell system contains seven heavy atoms. We have carried out the *ab initio* MO/TST calculation up to G2M (rcc, MP2)//B3LYP/6-31G(d,p). The predicted rate constant with tunneling corrections agrees closely with our measured value. The barrier for the reaction was predicted to be 10±1 kcal/mole.

Both reactions (b) and (c) were studied at the B3LYP/6 31G(d,p) level of theory because of the large molecular size. Reaction (b) takes place by a long-lived $C_{12}H_{11}$ adduct involving the addition and decomposition transition states. RRKM calculations for the forward and reverse addition ($H+C_{12}H_{10}$) processes correlate the measured rate constants for the two processes very well.

Reaction (c) is dominated by the direct H-abstraction process, whose barrier was predicted to be 1.4 kcal/mole at the B3LYP/6-31G(d,p) level of theory, agreeing nicely with the experimental value of 1.8 kcal/mole. The results of these three systems are being prepared for publication.




**Optimized geometries of various species involved in the reaction of the $C_3H_3$ radical with acetylene.**

## Significance

Both experimental measurements for these phenyl-radical reactions and *ab initio* MO calculations for reactions such as $C_6H_5 + CH_4$ have been carried out nearly to the limits of our current technology. The $C_6H_5 + CH_4$ reaction, calculated at the G2M//B3LYP/6-31G(d,p) level of theory to approximate the restricted open-shell RCCSD(T)/6-311+G(3f,2d) method, requires more than 2000 hrs of NERSC CPU time.

The results of these calculations not only help elucidate the mechanisms of large combustion-reaction systems, but also help extend low-temperature kinetic data reliably to the combustion regime.

## Publications

I. V. Tokmakov, J. Park, S. Gheyas and M. C. Lin, "Experimental and theoretical studies of the reaction of phenyl radical with methane," J. Phys. Chem. (submitted, 1998).

L. V. Moskaleva and M. C. Lin, "Theoretical investigation of the unimolecular decomposition of $C_5H_5$ and $C_5H_6$ and their reverse processes" (in preparation, 1998).

http://www.chem.emory.edu/~faculty/Lin/mclin.html

# Computation of Materials Properties from First Principles

*S. G. Louie and M. L. Cohen, University of California, Berkeley, and Lawrence Berkeley National Laboratory*

## Research Objectives

Determination and prediction of the structure of materials using quantum theories.

## Computational Approach

Materials properties are computed using (1) the density functional formalism by solving a set of self-consistent Schrödinger-like equations and (2) many-body perturbation theory by solving the one- and two-particle Green's functions. Computations involve extensive determination and manipulation of the eigenvalues and eigenvectors of large matrices with dimensions up to several hundred thousand on the Cray C90 and T3E.

## Accomplishments

First-principles calculations have been performed on a number of materials systems. The $C_{36}$ fullerene was predicted to have several interesting electronic properties, some of which have now been observed experimentally. Nuclear magnetic resonance (NMR) chemical shift calculations of several materials have been performed. A new theory was developed and applied to the *ab initio* study of the optical properties for solids and clusters. Studies have been performed pertaining to the periodic trends of hard materials.

## Significance

$C_{36}$ is a smaller cousin of the famous $C_{60}$ "buckyball." We predicted that $C_{36}$ could be synthesized, and that it should be very interesting. Notably, it has a larger electron-phonon interaction than $C_{60}$ does, which suggests that it may be a higher-temperature superconductor. If this is the case, $C_{36}$ could have a wide range of practical applications. Experimentalists with whom we are collaborating have since synthesized and purified $C_{36}$ and are in the process of characterizing it.

Calculating the optical properties of solids from first principles has been a long-sought goal of physicists. For the first time, our method enables such calculations for insulators and semiconductors. This approach not only provides quantitative understanding, but also the means of predicting the optical responses of new materials.

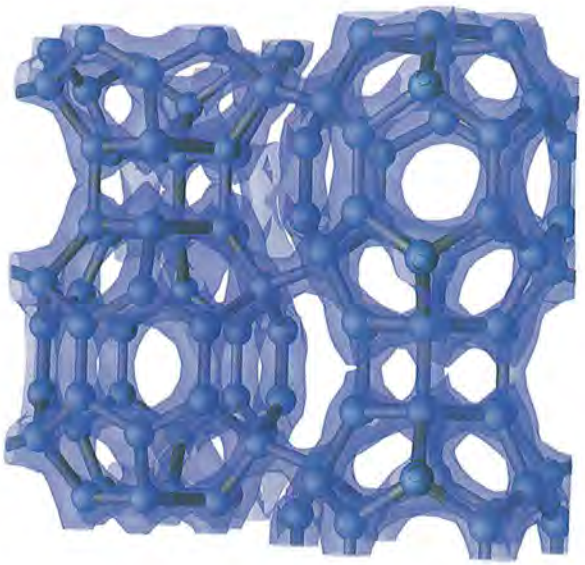
## Publications

M. Rohlfing and S. G. Louie, "Electron-hole excitations in semiconductors and insulators," Physical Review Letters **81** (11), 2312–2315 (1998).

M. Cote, J. C. Grossman, M. L. Cohen, and S. G. Louie, "Electron-phonon interactions in solid $C_{36}$," Physical Review Letters **81** (3), 697–700 (1998).

Y.-G. Yoon, B. G. Pfrommer, F. Mauri, and S. G. Louie, "NMR chemical shifts in hard carbon nitride compounds," Physical Review Letters **80** (15), 3388–91 (1998).

http://tiger.berkeley.edu



**A proposed crystal structure for $C_{36}$ solid. The shaded region corresponds to electron density, indicating strong covalent bonds between $C_{36}$ molecules.**

# Experimental and Theoretical Studies of Electron Transfer Dynamics at Semiconductor-Liquid Interfaces

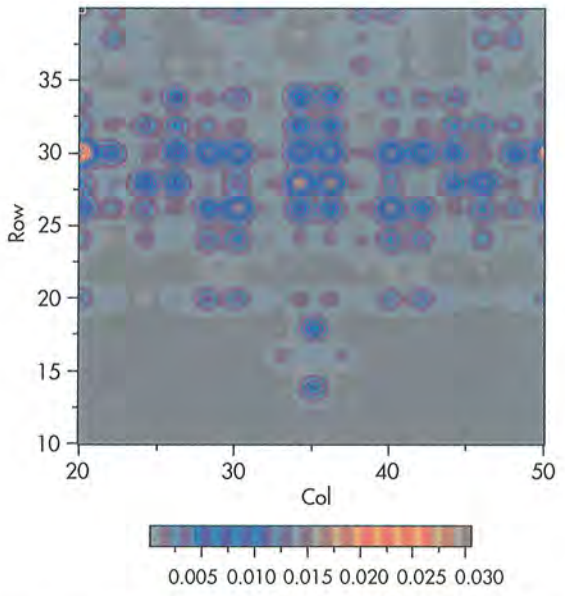
*A. Nozik, National Renewable Energy Laboratory*

## Research Objectives

Our ER/Chemical Sciences Solar Photochemistry Program involves a coupled experimental and theoretical study of photoinduced and dark electron transfer (ET) between a semiconductor and a molecular species solvated in a liquid next to the semiconductor. The experimental program for study of this semiconductor-liquid interface (SLI) ET involves measurements of its dynamics, using femtosecond and picosecond time-resolved spectroscopy. To interpret the experimental data, and to discover new experimental research directions, we use computationally intensive theoretical methodologies.

## Computational Approach

Our computational methods include first-principles molecular-dynamics (FPMD) simulations of the SLI. We have also developed new computational methods of wave packet propagation to study the ET scattering event at the SLI, and new model Hamiltonian approaches for these systems. A second class of methodologies use the semiclassical Monte Carlo, drift-diffusion, and balance-equation approaches to model very-large-scale systems.




**Electron density trapped in a redox species (solvated) next to a semiconductor-liquid interface. The redox species density appears at the bottom of the picture (four atoms have significant electron density). The rest of the electron wave packet is localized around semiconductor atoms (top two-thirds of the picture). This is a snapshot of a dynamic electron transfer simulation, and is a cross section through the 3D system.**

## Accomplishments

In past years we have developed a number of new theoretical methodologies to address SLI ET. In our FPMD, both electron and nuclear dynamics are realistically described, allowing the full dynamical quantum mechanical structure to be explored. Our new computational methods of wave-packet propagation allow detailed study of the ET scattering event at the SLI. New model Hamiltonian approaches for these systems allow physically transparent interpretation of the simulations. Our FPMD simulations represent among the first applications of FPMD to solid-liquid interface ET.

Key outcomes of these studies are a detailed description of how electrons become relocalized from the redox species to the semiconductor and vice versa; trends in overall electron transfer rate constants (as a function of electric fields, temperature, crystal face, and solvent and redox species); vibrational spectra of molecules at surfaces before and after electron transfer; a large catalogue of local densities of states that is (in principle) explorable by scanning tunneling microscopy (STM); and detailed studies of the time-scale and configurational dependencies of SLI electron transfer.

## Significance

Our FPMD simulations have opened up a new window for the understanding of SLI systems, which up to now have been primarily addressed by archaic analytical models. Pronounced shortcomings of conventional models have been revealed, which call into question even their qualitative foundations. These results have led to qualitatively new insights and suggest new experiments to be performed, leading to greater understanding of alternative energy sources, and possibly new or improved alternative energy devices. The benefits of our studies are central to the fundamental mission of our institute, and are important for the future of our planet.

## Publications

B. B. Smith and A. J. Nozik, "Study of electron transfer at semiconductor-liquid interfaces addressing the full system electronic structure," Chem. Phys. **205**, 47–72 (1996).

B. B. Smith and A. J. Nozik, "Theoretical studies of electron transfer and electron localization at the semiconductor-liquid interface," J. Phys. Chem. B **101**, 2459–2475 (1997).

A. Meier, D. C. Selmarten, B. B. Smith, and A. J. Nozik, "Ultrafast electron transfer across semiconductor-molecule interfaces: GaAs/Co(Cp)2+/0," J. Phys. Chem. B (in press, 1998).

# Molecular Simulations of Clay Mineral Surface Geochemistry

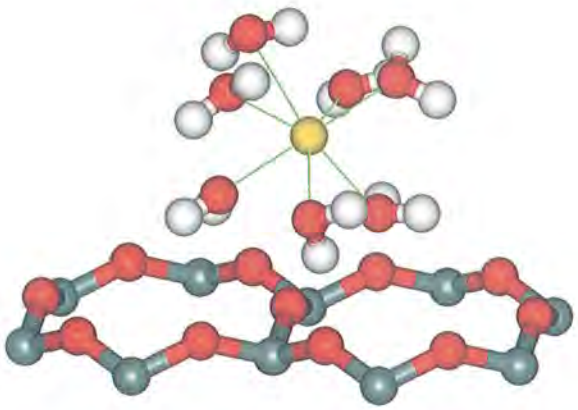
*G. Sposito, S.-H. Park, and R. Sutton,*
*Lawrence Berkeley National Laboratory*

## Research Objectives

This project involves basic research directed toward an accurate model of molecular structure at the surface of hydrated 2:1 clay minerals (smectites). These minerals are of great importance in petroleum production, nuclear waste containment, and contaminant attenuation by designed clay liners. The specific objective addressed was Monte Carlo (MC) simulations of molecular structure on smectite minerals adsorbing water and either $Na^+$ or $K^+$ cations. The results obtained were compared to recent neutron diffraction data for these systems, based on H/D isotopic-difference techniques.

## Computational Approach

Computational algorithms for the MC simulations, based on the code MONTE developed by our collaborators N. T. Skipper (University College London) and K. Refson (Oxford University), were optimized and run on Cray C90 supercomputers at NERSC.



**Visualization of adsorbed $Na^+$ bound in an outer-sphere surface complex to an octahedral charge site of the clay mineral montmorillonite. The MC output indicated individual Na-$H_2O$ separations varying from 2.2 to 2.5 Å, with a most-probable Na-$H_2O$ distance of 2.3 Å and a solvation shell confined to within 3.2 Å. The water molecules form a distorted octahedron in agreement with Na-$H_2O$ distances and coordination numbers determined for concentrated NaCl solutions.**

## Accomplishments

Monte Carlo simulations based on tested intermolecular potential functions were used to calculate radial distribution functions for O-O, O-H, and H-H spatial correlations in the interlayer region of two-layer hydrates of Na- and K-montmorillonite (see figure). The simulated radial distribution functions then were used to compute the total radial distribution function for interlayer water $G_h(r)$, a physical quantity that can be determined experimentally by H/D isotopic-difference neutron diffraction. The simulated total radial distribution functions were compared to that for bulk liquid water and to a total radial distribution function recently determined experimentally for the two-layer hydrate of Na-montmorillonite. The shape of the simulated $G_h(r)$ for either montmorillonite hydrate was similar to that of $G_h(r)$ measured by neutron diffraction. For example, a well-defined peak in the simulated $G_h(r)$ was predicted near $r \approx 1.9$ Å, reflecting O-H spatial correlations, and this peak appeared as well in the measured $G_h(r)$, as did a peak predicted to arise near $r \approx 3.3$ Å. Our simulation results suggest that water molecules in the two-layer hydrates of montmorillonite have nearest-neighbor configurations, which differ significantly from the tetrahedral ordering of nearest neighbors that characterizes bulk liquid water.

## Significance

The results obtained in this project support the essential correctness of our MC simulation model as a predictor of clay-mineral hydration behavior. A fundamental understanding of this behavior is critical to the effective use of clay minerals in designed containment scenarios at DOE waste sites, as well as to improved control of waste plume attenuation in natural porous formations.

## Publications

F.-R. C. Chang, N. T. Skipper, and G. Sposito, "Monte Carlo and molecular dynamics simulations of electrical double-layer structure in potassium-montmorillonite hydrates," Langmuir **14**, 1201 (1998).

G. Sposito, S.-H. Park, and R. Sutton, "Monte Carlo simulation of the total radial distribution function for interlayer water in sodium and potassium montmorillonites," Clays and Clay Minerals (in press, 1998).

http://ccs.lbl.gov/sposito/

# Equation of State and Activity Coefficient Models for Improved Engineering Practice

*Amadeu K. Sum and Stanley I. Sandler,*
*University of Delaware*

## Research Objectives

This project investigates the application of *ab initio* molecular orbital theory to determine parameters often encountered in applied thermodynamics models, such as equations of state and activity coefficient models used in phase equilibria predictions.

## Computational Approach

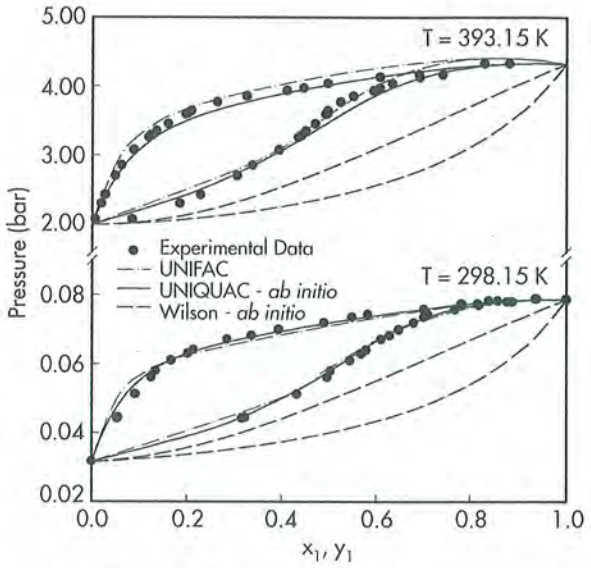
Energy minimizations of molecule clusters were used to determine the interaction energies between pairs of molecules computed using *ab initio* methods, in particular Hartree-Fock theory. Calculations were performed with the Gaussian 94 computational chemistry program. Most of the calculations were done on the Cray J90 machines.

## Accomplishments

A collection of binary aqueous systems was studied to determine the interaction energy between pairs of molecules. At first, clusters of as large as eight molecules were optimized by minimizing the energy of the system, using Hartree-Fock theory. Interaction energies were then calculated for the like and unlike pairs of molecules (also using Hartree-Fock theory) which subsequently were used as parameters in the widely used Wilson and UNIQUAC activity coefficient models for phase equilibria calculations. This method resulted in excellent phase behavior predictions using the UNIQUAC model.

## Significance

Our current research focuses on using microscopic information available from computational chemistry to determine parameters in engineering models predicting the phase behavior of fluids and their mixtures. We have successfully applied this approach to two engineering equations of state, and are now expanding the scope of our project to include liquid solution (activity coefficient) models. By being able to determine these parameters in engineering models from first-principle calculations, we are developing a new generation of predictive models—the tools engineers need for making predictions about thermodynamic properties and phase behavior.




**Vapor-liquid equilibria for ethanol (1) + water (2) using parameters determined from *ab initio* methods.**

## Publications

A. K. Sum and S. I. Sandler, "Use of *ab initio* methods to make phase equilibria predictions using activity coefficient models," in *Proceedings of Eighth International Conference on Properties and Phase Equilibria for Product and Process Design* (Netherlands, in press, 1998).

A. K. Sum and S. I. Sandler, "A novel approach to phase equilibria predictions using *ab initio* methods," presented at the AIChE Annual Meeting, Miami Beach, FL, November 15–20, 1998.

# Numerical Modeling of Turbulent Combustion

*L. Talbot, R. K. Cheng, and I. G. Shepherd,*
*Lawrence Berkeley National Laboratory*
*C. K. Chan, Hong Kong Polytechnic University*

## Research Objectives

The objectives of this research are threefold:

1. To model numerically the dynamics of premixed flame surfaces in the reaction sheet regime.
2. To determine the modification to flow turbulence produced by such flames.
3. To determine the effect of turbulence on flame shape, speed, and thickness.

## Computational Approach

The random vortex method is combined with the level-set formulation for the tracking of propagating surfaces under curvature to model the dynamical behavior of turbulent premixed flames, including baroclinic vorticity generation.

## Accomplishments

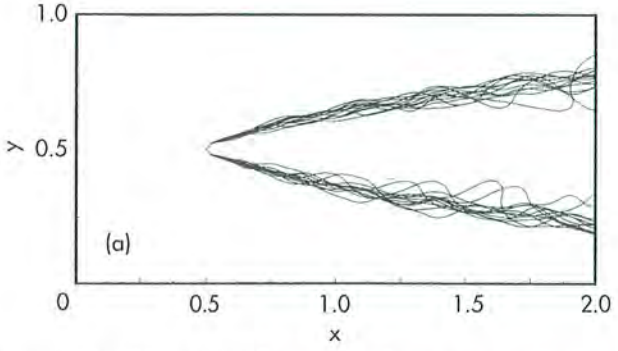
Significant improvements to our earlier work on dynamical behavior of a premixed open V-flame were achieved in the form of better simulation of the inflow-outflow boundary conditions and better statistical resolution of the dynamical properties of the flame, including turbulence generation, Reynolds stresses, and flame motion, with good agreement with experiment. These results, including comparisons with experimental data obtained by us at Berkeley Lab, will be reported in a forthcoming publication.

## Significance

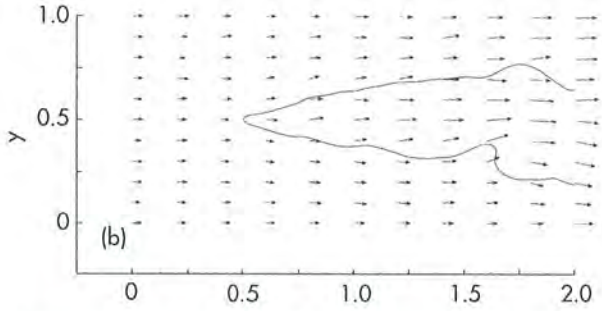
A major technological combustion problem is the design of more energy-efficient, low-emission industrial and home-heating turbulent-flame gas burners. In the design of such burners, a primary objective is to achieve stable combustion under the most fuel-lean conditions possible, since the leaner the flame, the lower the maximum temperature and the lower the amount of $NO_x$ produced. The limit of stable lean flame operation is directly related to the effective turbulent-burning velocity. Thus, it would be of great benefit to designers of premixed turbulent-flame burners to have at their disposal a numerical model that reliably predicts turbulent-burning speed, flame configuration, and other related quantities as a function of reactant turbulence intensity and effective heat release.

## Publications

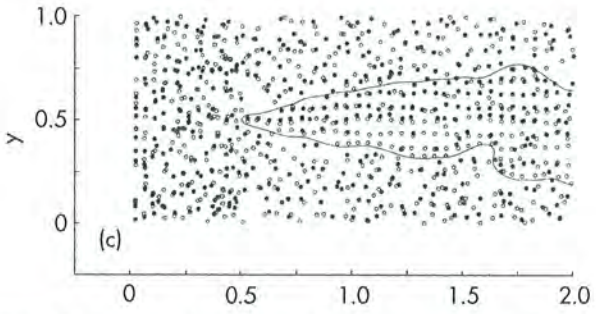
C. W. Rhee, L. Talbot, and J. A. Sethian, "Dynamical behavior of a premixed open V-flame," J. Fluid Mech. **300**, 87–115 (1995).




**Superposition of instantaneous flame configurations at successive time steps.**




**An instantaneous flame configuration for the conditions of figure (a).**




**Vortex distribution: filled symbols, positive circulation; open symbols, negative circulation.**

# Correlated Motion in Atomic Many-Body Systems

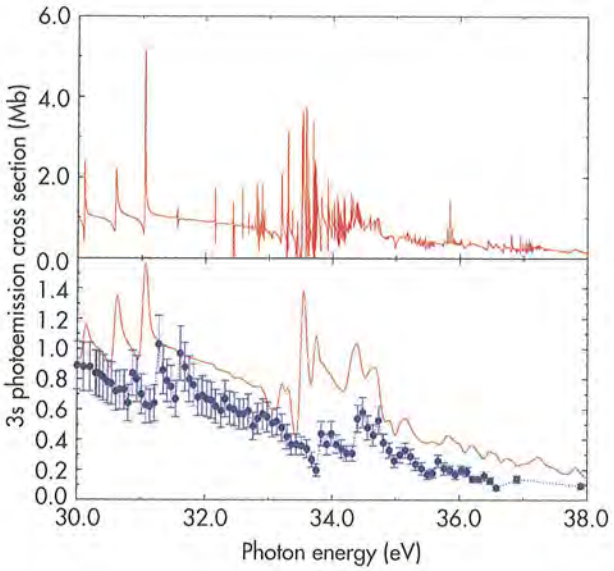
*H. W. van der Hart, JILA*
*C. H. Greene, University of Colorado*

## Research Objectives

To describe in detail the motion of electrons in complex open-shell atoms and to extend the application of our computational approach to more complicated species and to frequencies where the atomic structure is more complicated.

## Computational Approach

For the calculation of complex spectra, we employ the R-matrix approach. In this approach, configuration space is divided into two regions. In the inner region, we use a large basis set to describe all interactions in the atom. After setting up the Hamiltonian, we use a full diagonalization to obtain all the eigenvectors and eigenvalues of the Hamiltonian. These eigenvectors and eigenvalues provide the R-matrix. In the outer region, asymptotic solutions for one outgoing electron are obtained. By matching these solutions with the R-matrix, we obtain all the photoionization properties of the atom. All calculations are performed on the J90 cluster.




**Theoretical (red) and experimental (blue) spectra for photoemission of a 3s electron from the Ar ground state. The top figure shows a theoretical spectrum obtained with infinite resolution, while the theoretical results in the bottom figure have been convoluted with the experimental resolution.**

## Accomplishments

We have employed the R-matrix approach for photoionization studies of Ar, with special emphasis on the resonances observed experimentally in the frequency range between 30 and 38 eV. Many excited $Ar^+$ thresholds lie in this region, so that photoionization can leave $Ar^+$ in a wide variety of excited states. To determine the excitation of these $Ar^+$ states, we must obtain a good description of many $Ar^+$ states simultaneously. Consequently, extensive basis sets are required.

In a first study, we have compared our spectra for emission of 3p and 3s electrons with experiment and obtained excellent agreement. The complex resonance spectrum for photon energies between 30 and 38 eV is reproduced in great detail. In addition, we have determined spectra for observing ejected electrons with nearly zero energy, so-called threshold photoelectron spectra. These spectra are strongly affected by the interactions in both Ar and $Ar^+$. The good agreement with experiment shows our success in describing the complex interreactions in Ar.

In a second study, we have emphasized the photoionization cross sections while leaving $Ar^+$ in the $3p^4(^3P)4p$ states. Using fluorescence spectroscopy, experimentalists have provided detailed spectra for these processes. The present calculations reproduce the experimental spectra well, and also provide good predictions for the polarization of the fluorescence. Through frame transformation techniques, we can also determine the influence of relativistic effects on the photoionization spectra.

## Significance

The interactions between the electrons are very significant in complex open-shell atoms and need to be described accurately to predict the atomic spectra reliably. Theoretical calculations are valuable to identify the observed features in experiment. The comparison of theory with experiment also facilitates the identification of relativistic effects in the experimental spectra. Ultimately, we hope that these critical tests will lead to an improved theoretical methodology that can be used to describe the nonseparable quantum mechanical behavior of complex many-body systems.

## Publications

H. W. van der Hart and C. H. Greene, "Multichannel photoionization spectroscopy of Ar: Total cross section and threshold photoelectrons," Phys. Rev. A **58**, 2097 (1998).

# Material Science Theory and Computation for Advanced Light Source Experiments

*M. A. Van Hove and C. S. Fadley, Lawrence Berkeley National Laboratory and University of California, Davis*
*J. Carter, Y. Chen, P. N. Ross, S. Sachs, G. Stone, P. Tang, V. Zhuang, Lawrence Berkeley National Laboratory*

## Research Objectives

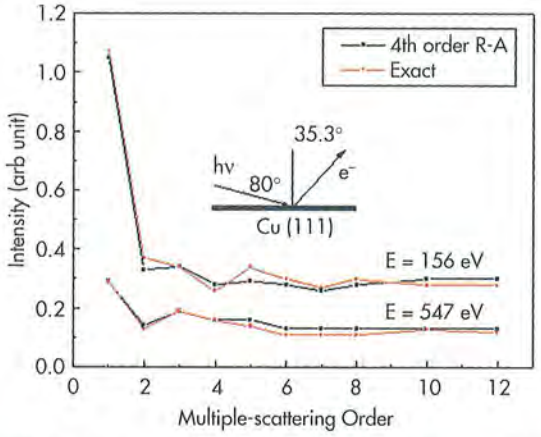
Offer theoretical and computational support to nationwide experimental users of Berkeley Lab's Advanced Light Source (ALS) and other synchrotron facilities in the U.S. and abroad. Develop computational capabilities that permit experimentalists to plan and simulate future experiments, to rapidly evaluate and fine-tune ongoing experiments, and to fully analyze and refine finished experiments. For example, develop methods to deal with the complex electron multiple scattering processes that underlie experimental techniques like photoelectron diffraction and holography, x-ray absorption spectroscopies, and spectromicroscopies.

## Computational Approach

Computational methods utilize NERSC capabilities to tackle problems of unprecedented scale and to open up the field to research on new classes of materials. Further extensions of existing methods and new techniques are introduced in response to the needs and requests of synchrotron radiation users.

## Accomplishments

A new code, the MSCD Package (Multiple Scattering in Cluster Diffraction), was developed and implemented for the interpretation of photoelectron diffraction measurements. The sequential version of the code has been implemented on supercomputers and Sun workstations in UNIX, as well as on PC and Macintosh desktop computers. Extensive comparisons of code performance on the Cray T3E and on cluster parallel architectures have been conducted under MPI.




**The MSCD Package was used to create this photoelectron diffraction simulation, which shows calculated Cu 3p photoelectron intensities, as a function of multiple scattering order, from clean Cu(111) in a fixed forward-scattering emission direction, 35.23Y off-normal, and for emission from the third layer. A photoelectron can be scattered once or twice consecutively along this forward-scattering path. The 4th order Rehr-Albers approximation is compared with exact calculations.**

The Fast Fourier Transform approach has been enhanced to permit new and efficient methods for holographic reconstruction of 3D atomic maps of surfaces and interfaces, a valuable method to obtain structural and magnetic detail about materials from photoelectron diffraction and similar data.

Global optimization by means of genetic algorithms has been implemented for parallel processing on the Cray T3E and clusters of workstations. This is an essential step in searching for structural solutions of very complex surfaces.

We have developed a molecular-orbital approach to calculate core-level relaxation energies in photoelectron spectroscopy. This capability is valuable for identifying atomic and molecular species attached to surfaces.

## Significance

The ALS produces a rapidly increasing amount of experimental data that requires advanced numerical treatment and simulation to yield scientifically useful results. Important information can be obtained about the atomic-scale structural, electronic, magnetic, chemical, corrosive, tribological, and biological properties of surfaces and interfaces of materials with technological relevance. Examples include electronic nanostructures, magnetic storage materials, chemical catalysts and sensors, corrosion protection, hard coatings, and biological membranes.

## Publications

Y. Chen, F. J. García de Abajo, A. Chassé, R. X. Ynzunza, A. P. Kaduwela, M. A. Van Hove, and C. S. Fadley, "Convergence and Reliability of the Rehr-Albers Formalism in Multiple Scattering Calculations of Photoelectron Diffraction," Phys. Rev. B, in press.

Y. Chen and M. A. Van Hove, MSCD Package User Guide: Simulation of Photoelectron Diffraction Using Rehr-Albers Separable Representation, http://electron.lbl.gov/mscdpack/mscdpack.html.

Y. Chen, G. Zhuang, P. N. Ross, M. A. Van Hove, and C. S. Fadley, "Equivalent-Core Calculation of Core-Level Relaxation Energies in Photoelectron Spectroscopy: A Molecular-Orbital Approach," J. Chem. Phys., in press.

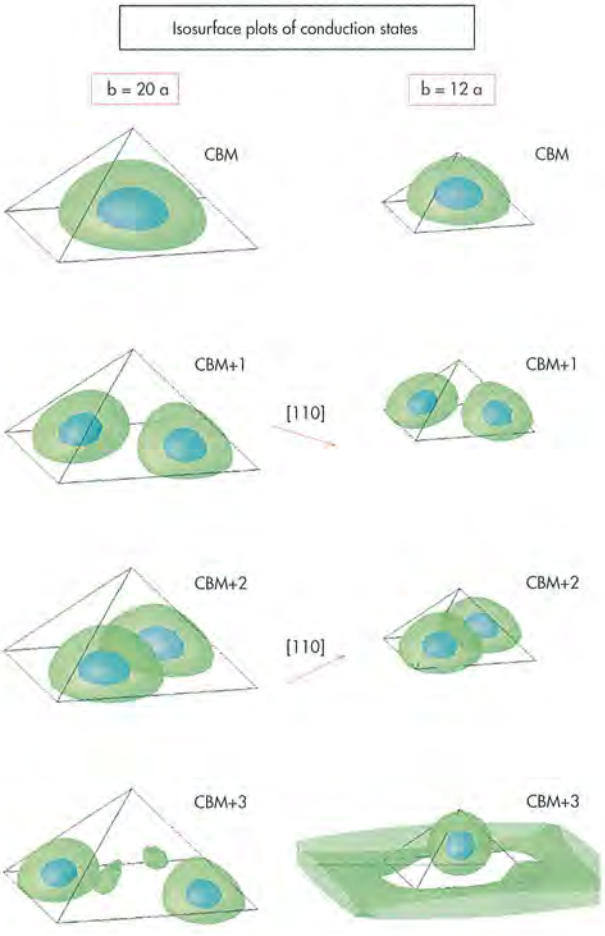
http://electron.lbl.gov/

# Empirical Pseudopotential Calculation of Self-Assembled Quantum Dots

*L.-W. Wang, J. Kim, A. Williamson, and A. Zunger,*
*National Renewable Energy Laboratory*

## Research Objective

Self-assembled, pyramidal semiconductor quantum dots can be formed during the Stranski-Krastanow growth mode in molecular beam epitaxy. Such systems have technological potentials for laser, LED (light-emitting diode), memory, and single-electron devices. Their electronic structures are fundamentally different from bulk systems. New physics emerge because the electron and hole are confined inside the small regions of the quantum dots. We performed state-of-the-art pseudopotential calculations of the quantum dot electronic structures to study this new physics. The systems calculated contain about one million atoms.




**Conduction states (CBM to CBM+3) for different pyramidal quantum dot sizes: "b" is the length of the square of the pyramid base, and "a" is the zinc blende lattice constant.**

## Computational Approach

The empirical pseudopotentials, and their changes with pressure, are fitted to the bulk band structures. The atomic positions are relaxed from the ideal zinc blende positions using the classical valence force-field model. The single-particle Schrödinger's equation is constructed from the relaxed atomic positions and the empirical pseudopotentials. Schrödinger's equation for the million-atom system is solved using the folded spectrum method, making it an O(N) scheme. Parallel fast Fourier transformation on the Cray T3E is used to accelerate this process. The number of computational Flops scales linearly with the number of nodes on the T3E machine up to 256 nodes. Once the single-particle states are obtained, electron-hole coulomb and exchange integrals are computed. This gives the excitonic levels.

## Accomplishments

The parallel code ESCAN has been tested and used extensively for many nanostructure calculations. InAs/GaAs pyramidal quantum dot has been studied for different dot sizes and shapes. Comparing with experimental data, our calculated results help to resolve the shape of the quantum dot, the anisotropy of the polarization, the number of bound electron states, and the level splittings of the electronic structures.

## Significance

Nanoscale heterostructure is the future of semiconductor engineering. The ability to accurately calculate the electronic structure of such a million-atom system is crucial for the understanding of its new physics and for the possible design of such a system. The current approach represents a way to replace the old kp type calculations, which are inadequate for describing many aspects of the system.

## Publications

L. W. Wang and A. Zunger, "Solving Schrodinger's equation around a desired energy: application to silicon quantum dots," J. Chem. Phys. **100**, 2394 (1994).

J. Kim, L. W. Wang, and A. Zunger, "Comparison of the electronic structure of InAs/GaAs pyramidal quantum dots with different facet orientations," Phys. Rev. B, Rapid Commun. **57**, R9408 (1998).

A. J. Williamson, A. Zunger, and A. Canning, "Prediction of a strain-induced conduction-band minimum in embedded quantum dots," Phys. Rev. B, Rapid Commun. **57**, R4253 (1998).

# Electronic Structure of Alloys and Surfaces

*R. E. Watson, M. Weinert, and M. Alatalo,*
*Brookhaven National Laboratory*

## Research Objectives

To understand and predict the relative stability of multicomponent metallic alloys.

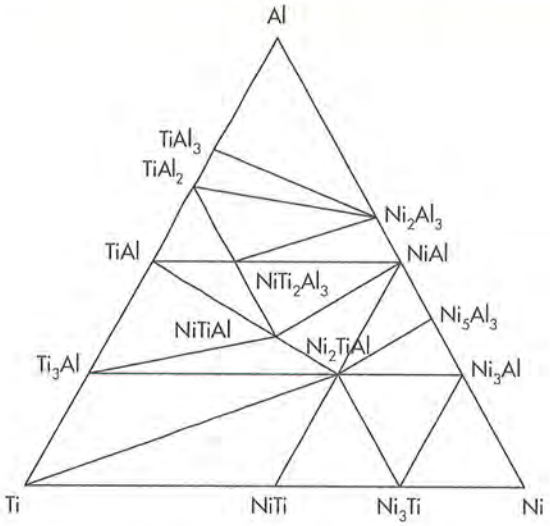
## Computational Approach

The fundamental quantity determining the relative stability of different phases at zero temperature is the heat of formation. The heats for observed and unobserved competing alloy phases are obtained from first-principles local density calculations employing the full-potential linearized augmented Slater-type orbital method. To get a consistent set of heats of formation, all the structural parameters (volume, c/a ratios, internal atomic positions, etc.) must be optimized. The self-consistent solution of the set of effective one-particle equations are solved by a basis of single-particle wave functions expanded in a set of Slater-type orbitals in the interstitial, augmented by numerical solutions of the effective potential in spheres surrounding each atom. The large numbers of calculations needed to adequately investigate the competing alloy compositions, different crystal structures, and structural parameters were done on the cluster of Cray J90s at NERSC.

## Accomplishments

The heats of formation for a large number of binary and ternary transition-metal and aluminum alloys (at various compositions and in a diverse set of crystal structures characteristic of the observed phases) were calculated. The calculated competition among ordered Ni-Ti-Al alloys is shown in the accompanying ternary phase diagram. The triangles connecting different stable phases represent three-phase regions; relatively small changes in the heats of the binaries and/or ternary heats can result in different connections among the phases or even cause phases to disappear. Of the three predicted stable ternary phases inside the triangle, only the NiTiAl phase has not been reported, possibly losing out to as-yet-unconsidered ordered or disordered phases, several of which are currently under investigation.

Experimental heats are available for only $Ni_2TiAl$ and some of the ordered binaries around the perimeter of the triangle. The agreement between experiment and theory is typically a few hundredths of an eV/atom, the same order as the differences among reported experimental values. Similar agreement is obtained for the aluminides of V and of the 4d elements Y to Pd. For nonmagnetic iron alloys, the discrepancy with experiment is an order of magnitude greater, suggesting that the local spin-density approximation underestimates the on-site magnetic energy contribution of bulk Fe to the heat of formation by a factor of 2, and that gradient corrections reduce, but do not remove, this error.




**Calculated phase boundaries for ternary Ni-Ti-Al alloys.**

## Significance

The relative phase stabilities of multicomponent alloys at different compositions and in a diverse set of crystal structures were predicted from first-principles determined heats of formation. Transition-metal aluminum alloys are an important class of technologically important alloys that include super alloys, light-weight structural alloys, and phases displaying shape-memory effects. As a set, these calculated heats can be used to model the phases and precipitates that might form during material preparation, and thus provide guidance for the future development of new materials.

## Publications

R. E. Watson and M. Weinert, "Transition-metal aluminide formation: Ti, V, Fe, and Ni aluminides," Phys. Rev. B **58**, 5981 (1998).

R. E. Watson, M. Weinert, and M. Alatalo, "Ternary transition metal aluminide alloy formation: The $BiF_3$ structure," Phys. Rev. B **57**, 12134 (1998).

M. Weinert and R. E. Watson, "Hybridization-induced band gaps in transition-metal aluminides," Phys. Rev. B **58** (1998).

http://cmth.phy.bnl.gov/elestr.html

# Simulation of Atomic-Level Defects in Ceramics

*W. J. Weber and R. Devanathan,*
*Pacific Northwest National Laboratory*

## Research Objectives

The aim of the present study is to improve our understanding of the production and evolution of atomic-level defects in ion-implanted ceramics and advanced semiconductors, such as silicon carbide (SiC). The simulations are needed because the small time and distance scales of these processes preclude direct experimental observation. The results of our work will be used as inputs for kinetic Monte Carlo simulations and analytical models to extend our knowledge of defect processes to real-world time and distance scales.

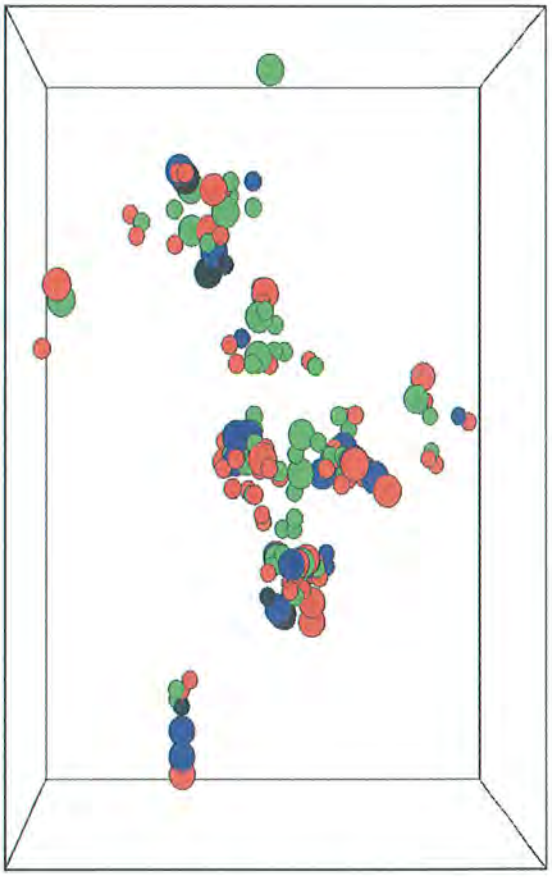
## Computational Approach

Our molecular dynamics code is written in FORTRAN 90 and uses the Parallel Virtual Machine (PVM) message-passing library. This enables the simultaneous calculation of forces acting on several million atoms, using the combined speed and memory of as many as 512 processing elements (PEs). The interactions between atoms are described using a combination of Tersoff and first-principles repulsive potentials. The computer used is the NERSC Cray T3E.

## Accomplishments

We have calculated the energy needed to knock atoms in SiC out of their lattice sites along various crystallographic directions. This value, known as the displacement threshold energy, is a fundamental parameter in radiation damage models and is needed to verify the reliability of our interatomic potentials. Our results show that the threshold energy is 20 and 35 eV for C and Si, respectively, in excellent agreement with experiments and first-principles calculations.

Currently we are simulating several high-energy (10–30 keV) Si recoils along three crystallographic directions in SiC to understand the statistics of the damage cascade. The simulation cell contains 2 million atoms, and each calculation has to be run for more than 20,000 time steps. Our calculations show that anti-site defects are produced by energetic recoils and may play an important role in the amorphization of SiC. In addition, the mixing in the cascade is much less in SiC than in Si, which helps explain the different cascade morphologies of these two materials. The figure shows the distribution of defects in a 10-keV cascade in SiC.



**Vacancies (green), interstitials (red), replacements (blue), and anti-site defects (black) created by a 10 keV Si recoil in SiC. The box shown is about 130 × 90 × 90 Å. The smaller and larger circles represent C and Si defects, respectively.**

## Significance

Silicon carbide (SiC) is an advanced semiconductor that performs better than Si in radiation and high-temperature environments. It has potential applications in space stations, advanced fighter aircraft, proposed fusion reactors, and the petroleum and automotive industries. In addition, SiC-based composite materials are being considered for structural applications in fusion reactors. Both semiconductor doping by ion-implantation and long-term operation in a radiation environment result in the production of atomic-scale defects by the displacement mechanism. The evolution of these non-equilibrium defects determines the ultimate performance of the material. Our study provides much-needed information on the formation and migration of defects in SiC.

# New 3D Parallel GILD EM Modeling and Inversion

*G. Xie and J. Li, Lawrence Berkeley National Laboratory*

## Research Objectives

Three-dimensional electromagnetic (EM) forward modeling and inversion algorithms play an important role in geophysical exploration, oil reservoir management, and environmental site characterization. In this project, we seek to develop a new global integral and local differential (GILD) parallel modeling and nonlinear inversion algorithm, designed to overcome the limitations of conventional inversion. The algorithm and developed software are important for coupled high-resolution imaging of field data in all frequency bands and many data configurations.

## Computational Approach

The new parallel GILD modeling and inversion method consists of five parts:

1. A domain decomposed into subdomain SI and subdomain SII (Figure 1).
2. A new global boundary magnetic integral equation on the boundary and local magnetic differential equations in domain, to be used together (in the modeling step) to obtain the electromagnetic field.
3. A new global magnetic Jacobian volume integral equation in SI and a local magnetic Jacobian differential equation in SII, to be used together in the inversion step to update the electric conductivity and permittivity from the magnetic field data.
4. Subdomain SII naturally decomposed into $4^n$ smaller subcubic domains; the sparse matrix in each subcubic domain can be inverted separately, in parallel.
5. A new parallel multiple hierarchy substructure direct algorithm, a new parallel multiple hierarchy preconditioned conjugate gradient, or Markov chain Monte Carlo (MCMC) approach, to be used to solve the smaller $2 \times 2$ block matrices in SI from domain to the boundary, recursively and in parallel.

## Accomplishments

We have developed the new 3D parallel GILD EM modeling and inversion algorithm. A primary 3D GILD inversion code was tested on a Cray T3D and obtained high-resolution imaging from synthetic and field data. Recently we have been developing a 3D GILD EM modeling and inversion code on the NERSC T3E. The current work involves changing PGHPF to MPI, developing a large-scale GILD parallel modeling and inversion code, GILD@T3E, choosing the optimal regularizing operator and parameter, improving the parallel performance, and making 3D EM images from field data. An example of 2.5D GILD high-resolution resistivity imaging is shown in Figure 2.

## Significance

We are using the new 3D GILD modeling and inversion to develop a high resolution electromagnetic, seismic, and hydrology-coupled GEO-HYDRO imaging. The new high-resolution imaging software will be an essential tool for DOE projects involving oil, gas, coal, geothermal energy, and geophysical exploration; and environmental restoration of contaminated sites and nuclear waste.

## Publications

G. Xie and J. Li, "New 3D nonlinear electromagnetic inversion," in *Three Dimensional Electromagnetics* (Tulsa, OK: Society of Exploration Geophysicists [SEG], 1998).

G. Xie, J. Li, and E. Majer, "New 3D parallel SGILD modeling and inversion," Berkeley Lab Technical Report LBNL-42252 (1998).

G. Xie, J. Li, E. Majer, and D. Zou, "New 3D parallel GILD electromagnetic modeling and nonlinear inversion using global integral and local differential equation," Berkeley Lab Technical Report LBNL-42105 (1998).

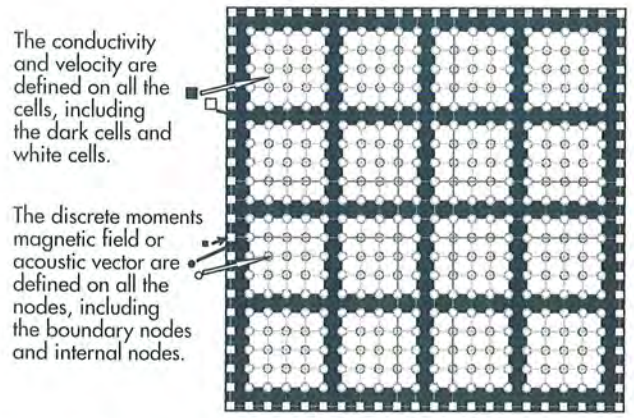



Figure 1. Domain decomposition for SGILD modeling and inversion.

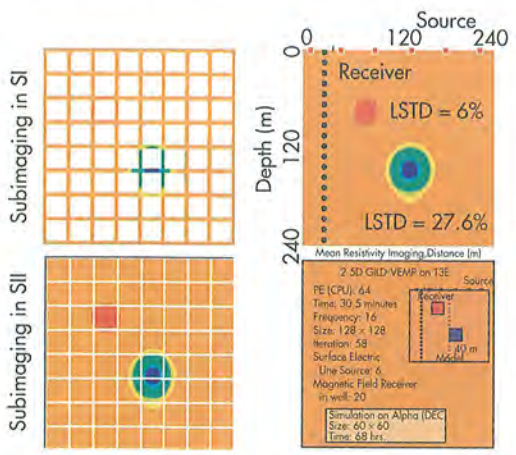



Figure 2. An example of 2.5D electromagnetic SGILD resistivity imaging.

# Investigating Impacts on Tropospheric Ozone Using a Tropospheric/Stratospheric Model

*C. S. Atherton, D. Bergmann, and P. Connell,*
*Lawrence Livermore National Laboratory*

## Research Objective

We are developing a global, three-dimensional atmospheric model, IMPACT, which contains both a prognostic stratosphere and troposphere. IMPACT is driven by meteorology from either a general circulation model or data-assimilated fields. We will use IMPACT to assess impacts of energy-related emissions in the lower and free troposphere, as well as near the tropopause.

## Computational Approach

IMPACT can be run on a variety of platforms, including the Cray C90, J90, T3D, T3E, IBM SP2, and others. Simulations are computationally expensive, due to the large number of chemical reactions involved and stiffness of the equation set. IMPACT has been developed for use on massively parallel computers. It makes use of domain decomposition, high-level communications, variable 3D resolution, and the master-slaves concept.

## Accomplishments

IMPACT has been used to simulate the $^{222}$Rn and $^{210}$Pb cycles, which are tracers that test the model's ability to represent convection, transport, and wet and dry deposition in a physically realistic way. Model results compare well with $^{222}$Rn measurements taken off of the coast of Northern California in 1994.

IMPACT has also been used to study the photochemical cycles of important tropospheric species such as CO, $CH_4$, $NO_x$, OH, and $O_3$. Because IMPACT can be run using actual data-assimilated meteorology, we can compare our model results with observations. Currently, we are comparing model results using a "background" chemistry mechanism and 1997 meteorology with measurements from the NASA SONEX and NOAA NARE campaigns, conducted in the fall of 1997 over the Atlantic Ocean. Our model shows that synoptic-scale events may lead to periods during which North American emissions strongly affect the air quality over the North Atlantic Ocean, as well as periods during which European emissions may contribute significantly.

## Significance

Our model is now being used to simulate actual time periods of sampling campaigns. We are comparing model results with measurements to identify areas for model improvement. Our model can also predict the effect different regions have on air quality on regional, hemispheric, and global scales. Because of this, we can also predict how future changes in emissions will affect air quality on these same scales.

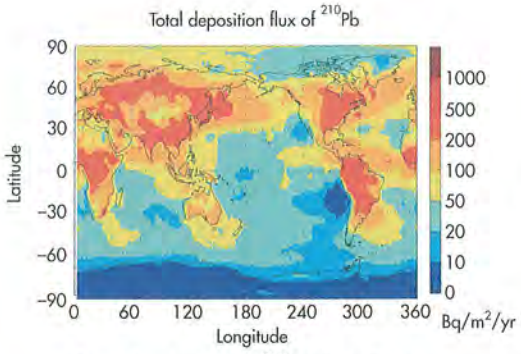
## Publications

C. Atherton, D. Bergmann, C. Chuang, P. Connell, J. Dignon, D. Kinnison, D. Proctor, D. Rotman, and J. Tannahill, "IMPACT: A three-dimensional model for combined tropospheric and stratospheric chemistry studies," Joint International Symposium on Global Atmospheric Chemistry, Seattle, (IGAC/CACGP) August 1998.

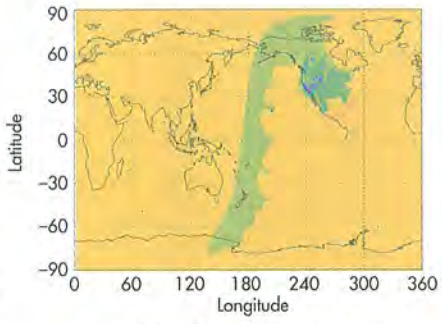
C. Atherton, D. Bergmann, B. Chatfield, C. Chuang, P. Connell, J. Dignon, D. Kinnison, D. Proctor, D. Rotman, and J. Tannahill, "Fate of continental emissions: Three-dimensional global modeling results for 1997," submitted to the American Geophysical Union Fall Meeting, San Francisco, December 1998.

C. Atherton, D. Bergmann, P. Connell, J. Dignon, and D. Rotman, "Using global models and measurements to characterize the North American atmosphere," submitted to the American Meteorological Society 79th Annual Meeting, Dallas, TX, January 1999.

http://www-ep.es.llnl.gov/www-ep/atm/ASD/asd.html




Annual wet and dry $^{210}$Pb deposition




Net odd-oxygen production

**Results of IMPACT predictions for the $^{222}$radon/$^{210}$lead cycle and the photochemical oxidant cycle: (a) the total annual wet and dry deposition predicted for $^{210}$Pb, in Becquerels/m$^2$/year, and (b) predicted net odd-oxygen production (related to the formation rate of ozone), ppbv/hr, near the surface on October 22, 1997, at 1800 GMT.**

# Predictability of the Coupled Ocean/Atmosphere System

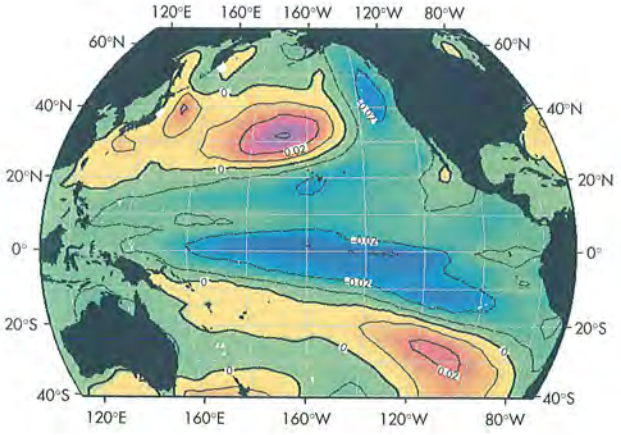
*T. P. Barnett, N. Schneider, and D. W. Pierce,*
*Scripps Institution of Oceanography*

## Research Objectives

Variability of the climate on interannual to decadal time scales is of paramount importance to human society, encompassing such variations as persistent droughts and flooding or spans of unusually warm or cold years. Obviously, it would be of great benefit to be able to predict such changes in long-term precipitation or temperature patterns. This project is aimed at understanding how predictable the coupled ocean/atmosphere system is on such time scales.

## Computational Approach

The investigations start with a 100-year run of a fully coupled ocean/atmosphere general circulation model. This provides the base "climate" that we seek to predict. We then perform ensemble studies by starting at specific times within that 100-year control run, slightly perturbing the initial conditions in various ways, and letting the system evolve forward in time. The perturbations mimic the effect of making predictions of the real Earth's climate with somewhat unknown initial conditions, and of the other unpredictable short-term influences of weather. To the extent that the system evolves in the same way as the control run despite the small perturbations, the system is potentially predictable. Finally, we are investigating the physics of the longer-term variability in the control run to see what processes contribute to that variability; an understanding of these mechanisms might lead to other avenues to explore for predicting such fluctuations.




**The strongest empirical orthogonal function (EOF) of sea surface temperature anomalies, 10-year low-pass filtered, in the coupled ocean/atmosphere general circulation model. This pattern is similar to observed conditions, and shows that the coupled model faithfully captures the large-scale patterns of low-frequency climate variability. This pattern is associated with changes in winter temperature and precipitation over much of North America.**

## Accomplishments

The investigations of the physical mechanisms of the variability have shown that in this model, the majority of the oceanic variance in the mid latitudes can be explained by stochastic atmospheric forcing. There remain, however, tantalizing peaks at a period of 20 years in the cross spectra of atmospheric forcing and ocean variables off the coast of Japan. This suggests that some part of decadal variance might indeed be governed by coupled interactions and hold some predictive potential. The exact dynamics involved are currently under investigation.

In addition, the coupled integration has yielded a strong decadal mode in the tropical Pacific Ocean that involves advection of anomalous temperature in the oceanic thermocline from 1020N to the equator, and a shift of centers of deep convection and concomitant wind stress, thermal, and freshwater forcing in the atmosphere. The details of this new mode are currently being explored.

## Significance

The significance of the work, from an end-user's perspective, is still evolving. To the extent that specific mechanisms of variability, such as the decadal mode described above, can be reliably identified in nature, an understanding of their workings might contribute to more accurate forecasts of seasonal to yearly rainfall and temperatures over various parts of the globe. It will, however, take more time and work before such an increase in predictive skill can be realized.

## Publications

T. P. Barnett, D. W. Pierce, M. Latif, D. Dommenget, and R. Saravanan, "Interdecadal interactions between the tropics and midlatitudes in the Pacific basin," Geophysical Research Letters (submitted, 1998).

T. P. Barnett, D. W. Pierce, N. Schneider, and R. Saravanan, "On the origins of the Pacific decadal oscillation," Geophysical Research Letters (submitted, 1998).

D. W. Pierce, T. P. Barnett, N. Schneider, and R. Saravanan, "Interactions between the Pacific Ocean tropics and midlatitudes on decadal time scales," J. Climate (in press, 1998).

http://meteora.ucsd.edu/

# Modular Ocean Model Code Developments

*C. H. Q. Ding, R. K. Owen, and H. Anand,*
*Lawrence Berkeley National Laboratory*
*R. Pacanowski and V. Balaji,*
*Geophysical Fluid Dynamics Laboratory*

## Research Objective

The goal of this project is to develop the Geophysical Fluid Dynamics Laboratory's (GFDL's) Modular Ocean Model (MOM) so that it will run effectively and efficiently on massively parallel high performance computers for large-scale, high-resolution, century-long ocean simulations. Techniques and software tools that are developed are expected to be relevant and useful to the entire climate research community.

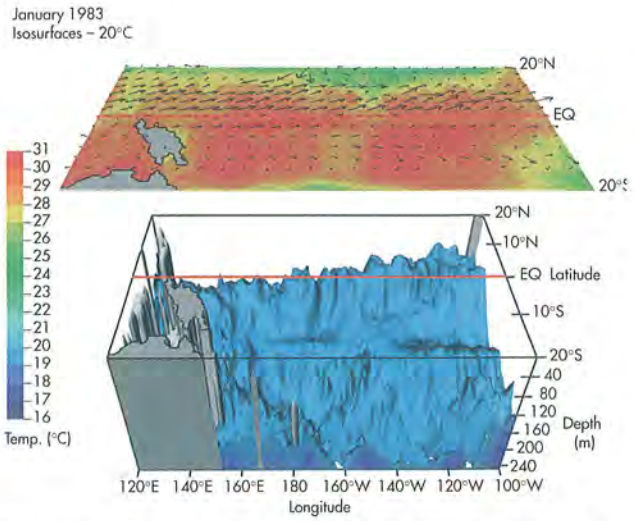
## Computational Approach

MOM uses finite-difference methods to solve primitive equations, including flow, energy, heat, and other tracer components on regular grids. The initial scalable implementation of MOM version 3 (MOM3) achieves moderate parallelism through one-dimensional domain decomposition, i.e., distributing the latitude dimension among the processors. MOM development efforts to date have focused on data input/output (I/O) and the implementation of scalable I/O. Bit-reproducibility of results is also a requirement in any parallel development of MOM.

## Accomplishments

Systematic runs on the Cray T3E indicated good scaling to a larger number of processors for the three-dimensional baroclinic and tracer portions of the model. These arrays ran 30 times faster on 32 processors than they did on one processor. However, the two-dimensional barotropic portion of the model did not scale as well (15 times faster on 32 processors). The barotropic portion is solved by an explicit free surface method. The scaling discrepancy was due to a larger-percentage communications overhead for two-dimensional arrays.

The snapshot part of data I/O in MOM3 was reimplemented, speeding up this part dramatically (by a factor of 50). The old I/O scheme, inherited from a memory-limited environment, wrote out field configurations one latitude row at a time. The flexibility of the common data format netCDF resolved the problem of index switching between data in memory and data in disk files. In the new I/O scheme, index switching is done first, then the entire three-dimensional configuration is written in one shot. This reduces the file system overhead significantly and results in the 50-fold speedup.




**GFDL scientists used MOM for a data assimilation experiment employing 1983 El Nino data.**

With the assistance of S. Luzmoor of SGI/Cray and G. Davis of Unidata, several important problems concerning the netCDF library were resolved, making it ready for use in MOM3 and other climate-related research. In the parallel distributed memory T3E environment, arrays defined with the unlimited dimension suffered from synchronization and overwrite problems, which were fixed. NetCDF was interfaced with the new Cray file system, so that a subset of processors can now open a global file; before, all processors had to open the file (which was often inconvenient). These innovations demonstrated that netCDF can be used efficiently in a real, large-scale application.

## Significance

GFDL scientists are preparing for a large-scale, eddy-resolving southern ocean simulation. This unprecedented high-resolution, decade-long simulation depends critically on the efficiency of the MOM3 codes we are developing.

Climate researchers worldwide also use MOM for climate and ocean modeling. This community will benefit from running MOM on state-of-the-art, high performance computers, as well as common platforms and workstations—made possible by efficient use of cache-based processor architectures, significantly improved data I/O, and a more convenient user interface.

## Publications

http://www.gfdl.gov/~kd/MOMwebpages/MOMWWW.html
http://www.nersc.gov/research/SCG/cding/mom

# Protein Fold Prediction in the Context of Fine-Grained Classifications

*Inna Dubchak, Chris Mayor, Sylvia Spengler, and Manfred Zorn, Lawrence Berkeley National Laboratory*

## Research Objectives

A key to understanding the function of biological macromolecules, e.g., proteins, is the determination of the three-dimensional structure. Large-scale sequencing projects produce a massive number of putative protein sequences in contrast to the much slower increase in the number of known three-dimensional protein structures. This creates both a need and an opportunity for extracting structural knowledge from sequence databases. Predicting a protein fold and implied function from the amino acid sequence is a problem of great interest and importance.

## Computational Approach

We have developed a neural network (NN) based expert system which, given a classification of protein folds, can assign a protein to a folding class using primary sequence. It addresses the inverse protein folding problem from a taxonometric rather than threading perspective. Recent classifications suggest the existence of 300 to 500 different folds. The occurrence of several representatives for each fold allows extraction of the common features of its members.

Our method (1) provides a global description of a protein sequence in terms of the biochemical and structural properties of the constituent amino acids; (2) combines the descriptors using NNs, allowing discrimination of members of a given folding class from members of all other folding classes; and (3) uses a voting procedure among predictions based on different descriptors to decide on the final assignment.

The level of generalization in this method is higher than in the direct sequence-sequence and sequence-structure comparison approaches. Two sequences belonging to the same folding class can differ significantly at the amino acid level, but the vectors of their global descriptors will be located very close in parameter space. Thus, utilizing these aggregate properties for fold recognition has an advantage over using detailed sequence comparisons.

## Accomplishments

In an attempt to simplify the fold recognition problem and to increase the reliability of predictions, we approached a reduced fold recognition problem, when the choice is limited to two folds. Our prediction scheme demonstrated high accuracy in extensive testing on the independent sets of proteins. In order to expand the protein database for machine learning and increase efficiency of the recognition, we are porting the Stuttgart Neural Network Simulator (http://www-ra.informatik.uni-tuebingen.de/SNNS/) to the T3E. As a first step, SNNS was compiled and run on the NERSC C90 and J90. The fold predictor is made available on the web, where users can submit a sequence and receive a report with a detailed prediction of possible folds for the submitted sequence.

## Significance

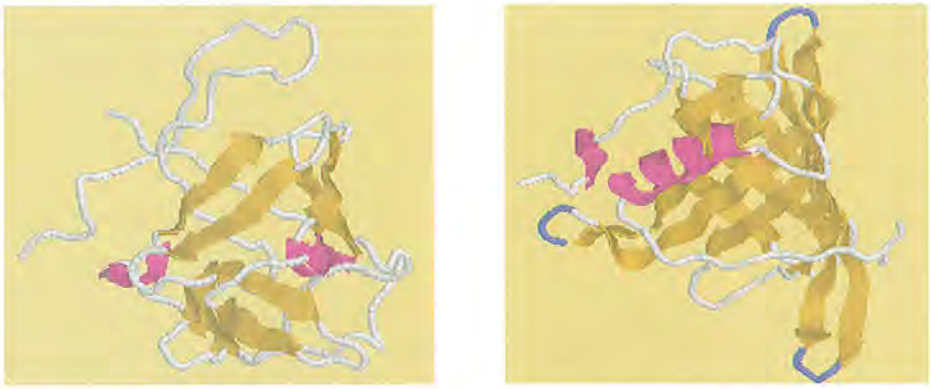
The prediction procedure is simple, efficient, and incorporated into easy-to-use software. It has been applied to fold predictions in the context of fine-grained classifications such as the 3D_ali database and the Structural Classification of Proteins (SCOP) database.

## Publications

I. Dubchak, I. Muchnik, C. Mayor, and S.-H. Kim, "Recognition of a protein fold in the context of the SCOP classification," Proteins (submitted, 1998).

I. Dubchak, I. Muchnik, and S.-H. Kim, "Prediction of folds for proteins of unknown function in three microbial genomes," Microbial and Comparative Genomics **3**, 171–175 (1998).

http://devnull.lbl.gov/prot/mayor/predict/frames/index.html



**Sample fold predictions: (left) representative of beta-trefoil fold; (right) representative of lipocalin fold.**

# Major Improvements in the Simulation of Tropical Stratospheric Winds

*K. Hamilton, R. J. Wilson, and R. Hemler,*
*Geophysical Fluid Dynamics Laboratory*

## Research Objective

To investigate the behavior of the Earth's stratosphere and mesosphere and to determine the controlling dynamical mechanisms through simulation with an atmospheric general circulation model.

## Computational Approach

The GFDL SKYHI model is a comprehensive atmospheric general circulation model that has been used extensively to investigate the dynamical and chemical behavior of the Earth's troposphere, stratosphere, and mesosphere. The model has been designed to execute interchangeably on both shared-memory, parallel vector, and distributed memory cache-based processors.

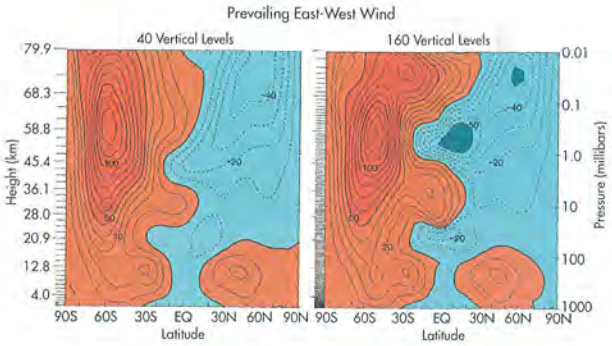
A series of control integrations is continuing on GFDL's 26-processor T932/26-512 and 40-processor T3E/40-128 systems using various versions of the SKYHI model. To date, the experiments run on in-house systems include an integration of 20 years with a 3° × 3.6° 40-level model, two years with a 1° × 1.2° 40-level version, two years with a 1° × 1.2° 80-level version, and seven months with a 0.33° × 0.4° 40-level version.

All of the experiments are capable of being run on the T932 system. The experiments with 1° × 1.2° horizontal resolution up to 80 vertical levels are currently being executed on the in-house T3E. However, one additional study with 160 vertical levels was required in order to determine the sensitivity of the model solution to even higher vertical resolution. Because this model resolution required more memory capacity than was available on the GFDL T3E, a two-month experiment was performed on the NERSC T3E.

## Accomplishments

The 1° × 1.2°160-level and the 0.33° × 0.4° experiments represent integrations at unprecedented spatial resolution (at least for global climate-simulation models). Preliminary analysis of these new integrations has concentrated on the simulation of the large-scale circulation in the middle atmosphere. Overall, the extratropical simulation appears to improve with finer grid spacing, but the effects of increasing horizontal resolution are more significant than vertical resolution.

Results from the SKYHI model experiments indicate that the tropical middle atmospheric simulation is extremely dependent on the vertical resolution employed. In all the simulations with 40 vertical levels, the east-west winds in the lower stratosphere are nearly constant in time, in contrast to the behavior of the observed winds, which exhibit a strong equatorially centered oscillation with a period between 24 and 30 months. This observed oscillation is known as the Quasi-Biennial Oscillation (QBO) and is an important feature of the real atmosphere that has been found to be absent in previous general circulation model simulations. When the vertical resolution of the experiment is increased, the simulated stratospheric winds exhibit much more realistic behavior, including a strong, long-period oscillation and the formation of strong vertical wind shears. This appears to be a spontaneous, internally generated oscillation and closely resembles the observed QBO in many respects, although the simulated oscillation has a period less than that of the real QBO.




**Comparison of zonally averaged east-west wind fields, from south to north pole, in SKYHI model simulations with 40 and 160 vertical levels. The higher-resolution solution (right) shows dramatically increased wind shear near the equator in the middle atmosphere compared to the winds in the low-resolution result (left).**

## Significance

The finding that increased vertical resolution produces far more realistic winds in the tropical middle atmosphere is an important discovery that opens up the possibility of alleviating one of the most serious and widespread problems in atmospheric simulation.

## Publications

K. Hamilton, R. J. Wilson, and R. S. Hemler, "Climatology of the middle atmosphere simulated with high vertical and horizontal resolution versions of a general circulation model: Improvements in the cold pole bias and generation of a QBO-like oscillation in the tropics," Journal of Atmospheric Sciences (submitted, 1998).

# A Global Optimization Strategy for Predicting Protein Structure

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

## Research Objectives

We are developing a joint global optimization approach based on sampling, perturbation, smoothing, and biasing that has been quite successful working directly on the potential energy surfaces of small homopolymers, homopeptides, and recently, α-helical proteins. Our overall strategy is to make good predictions of secondary structures by neural network techniques, and then manifest them as soft constraints to use within both a local optimization algorithm and as guidance within a global optimization framework.

## Computational Approach

The use of soft constraints permits partial solution to the global optimization problem within a local optimization context by quickly refining α-helices and β-sheets when they are predicted with even moderate accuracy. The small-subspace global optimization techniques are concentrated on regions predicted to be coil, a category for which it is not possible to define a soft constraint, and should be particularly effective in resolving these regions.

## Accomplishments

The developed strategy was parallelized and run on the T3E at NERSC using between 16 and 128 processors. A conservative estimate of the number of FLOPs needed to generate these results is

$$(10^2\ N \log N\ \text{Flops/EF}) \times (10^4\ N \times M)\text{EF}$$

where N is the number of atoms, EF is the number of energy and force evaluations, and M is the size of the coil subspace, typically 2–10 degrees of freedom.

In the last year we have explored different parameterizations of the global optimization methods and tested their effectiveness on the prediction of a 70-amino-acid protein, uteroglobin (see figure). We have just begun a second all-helical target which is 104 amino acids, and we have several more helical protein targets to further test the robustness of our optimization approach. We have received follow-on funding from DOE to tackle the more difficult folding class of β-sheet proteins.

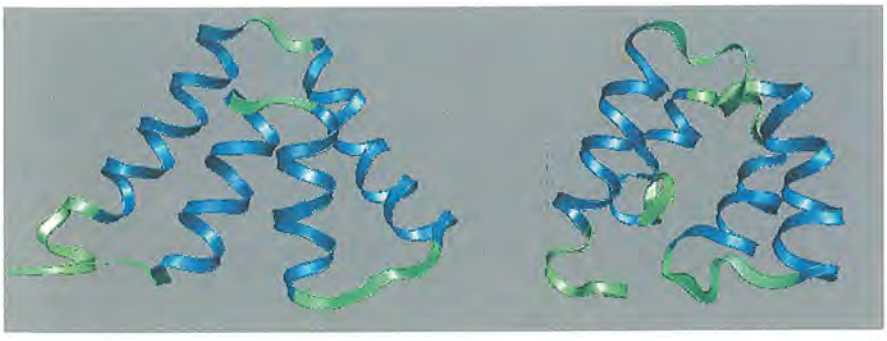
## Significance

The protein folding problem and the prediction of protein structure are the grand challenges in molecular biology. Understanding how and why proteins perform their evolved function is necessary both for reengineering defective proteins indicated in disease and for rational design of synthetic proteins relevant for biotechnical applications. The logical progression from amino acid sequence to protein structure to protein function makes timing critical for solving the protein structure prediction problem. As the Human Genome Project advances beyond mapping to sequencing the genome, we will be faced with an enormous database of amino acid sequences and a demand for protein structures for which x-ray diffraction and NMR methods will be inadequate.

## Publications

S. Crivelli, T. Phillips, R. Byrd, E. Eskow, R. Schnabel, R. Yu, and T. Head-Gordon, "A global optimization strategy for predicting protein tertiary structure: α-helical proteins," Proteins: Structure, Function, Genetics (submitted, 1998).

http://polygon.lbl.gov/~thg/



**Global optimization prediction from sequence (right) and crystal structure (left) of the α-chain of uteroglobin. Methods like these can also be adapted to use soft constraint directives predicted by fold recognition algorithms to refine protein structures.**

# Simulated Replication of Carcinogen-Damaged DNA

*B. E. Hingerty, Oak Ridge National Laboratory*
*S. Broyde, New York University*

## Research Objectives

In this project, we study carcinogen-damaged DNA in order to model replication in the presence of an enzyme.

## Computational Approach

Molecular dynamics calculations using the program AMBER were performed for carcinogen-damaged DNA in the presence of a replicating enzyme. Calculations employing a number of computers were performed, with the Cray C90 at NERSC playing a key role in these computations.

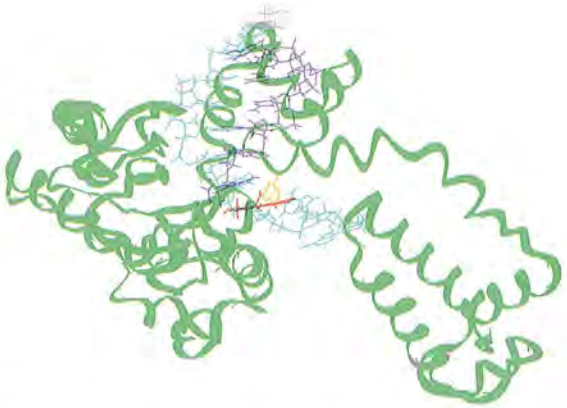
## Accomplishments

Recently we reported on a molecular-dynamics simulation (with the program AMBER) for the major adduct of the tumorigenic member of the pair in a base-sequence context that models an arm of a DNA replication fork. The simulation included aqueous solvent and a mammalian replication enzyme. Very intensive molecular-dynamics calculations were performed for a total of 12,000 atoms (including about 2,000 water molecules)—the first dynamics simulation done for carcinogen-damaged DNA modeling replication in the presence of an enzyme.

In this simulation, a structure evolved in which the activated tumorigenic benzo[a]pyrene adduct formed hydrogen bonds with a key amino acid residue of a polymerase enzyme shown to be essential for faithful and efficient replication. When this residue, argenine 283, is replaced by other amino acids, the enzyme makes replication errors and is markedly slowed down. These are the same effects that are induced by the activated benzo[a]pyrene adduct, suggesting that the adverse biological effects of the adduct may stem at least in part from its compromising the central role of a key amino acid residue associated with the polymerase required for faithful and efficient replication.

## Significance

Many polycylic aromatic hydrocarbons (PAH), environmental pollutants that are mutagenic and tumorigenic, are activated to mirror image pairs of diol epoxides. Each member of the pair can react with DNA to form a covalent reaction product known as an adduct. Such adducts can cause mutations when the DNA replicates, which may finally lead to tumors. However, a fascinating observation has puzzled researchers for decades: even though both members of the pair can react with DNA to the same site, the tumorigenicity of one member is always much greater than that of the other. A structural distinction has long been sought as the underlying origin to the biological difference. Benzo[a]pyrene, present in automobile exhaust and tobacco smoke, is the prototype PAH which manifests this intriguing phenomenon.



**Structure of a DNA replication fork damaged by a tumorigenic environmental carcinogen within a replicating enzyme. Water molecules have been deleted for clarity. Color code is: replication enzyme, green; parent-strand DNA, cyan; daughter-strand DNA, magenta; carcinogen, red; carcinogen-damaged guanine, yellow.**

## Publications

N. E. Geacintov, M. Cosman, B. E. Hingerty, S. Amin, S. Broyde, and D. J. Patel, "NMR solution structures of stereoisomeric polycyclic aromatic carcinogen-DNA adducts: Principles, patterns, and diversity," Chemical Research in Toxicology **10**, 111–146 (1997).

B. Feng, A. Gorin, B. E. Hingerty, N. E. Geacintov, S. Broyde, and D. Patel, "Structural alignment of the (+)–trans-anti-benzo[a]pyrene-dG adduct positioned opposite dC at a DNA template-primer junction," J. Biochemistry **36**, 13769–13779 (1997).

S. B. Singh, W. Beard, B. E. Hingerty, S. H. Wilson, and S. Broyde, "Interactions between DNA polymerase beta and the major covalent adduct of the carcinogen (+)–anti-benzo[a]pyrene diol epoxide with DNA at a primer-template junction," J. Biochemistry **37**, 867–877 (1998).

# AMIP-II Reanalysis—Global Atmospheric Analyses for 1979–1997

*Masao Kanamitsu, Wesley Ebisuzaki, and Jack Woollen,*
*National Centers for Environmental Prediction*
*Gerald Potter and Michael Fiorino,*
*Lawrence Livermore National Laboratory*

## Research Objectives

Use the historical observations to make better analyses of the atmospheric state for the years 1979–1997 and provide analyses for the NCEP/DOE Atmospheric Model Intercomparison Project-II (AMIP-II).

## Computational Approach

Describing the three-dimensional state of the atmosphere is difficult, as there are many more degrees of freedom in the atmosphere than observations made on any given day. The data assimilation system works by having an atmospheric general circulation model create a "first guess" and then finding the best analysis which minimizes the sum of the weighted fits to the first guess, the observations, and the divergence tendency.

The atmospheric general circulation model is pseudo-spectral, as some computations are computed in spectral space, others in grid space. In grid space, the atmosphere is discretized into 192 latitudinal × 94 meridional × 28 vertical (505,344) points. The calculations were solved using vectorized Fortran code running on the NERSC C90 computer.

## Accomplishments

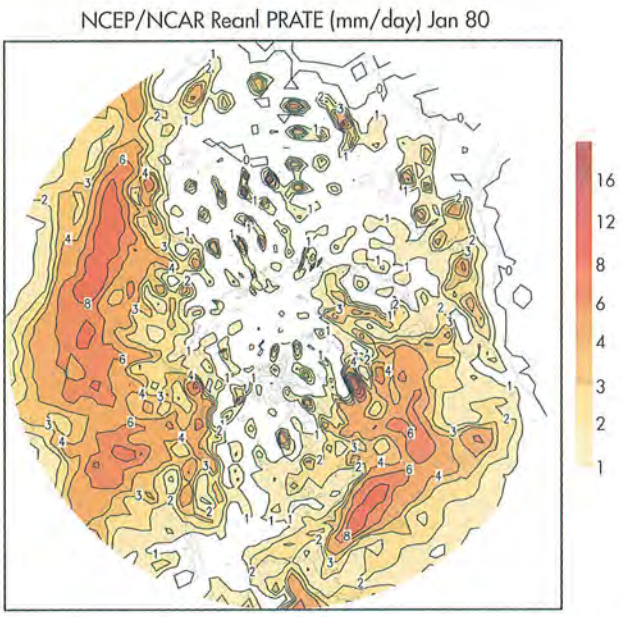
Analyses from January 1979 to November 1984 have been made. These analyses fix many of the serious problems in the earlier NCEP/NCAR Reanalysis. In addition, the use of more realistic cloud and radiation code has produced better estimates of the radiative fluxes than the NCEP/NCAR Reanalysis, when compared to the available satellite data.

## Significance

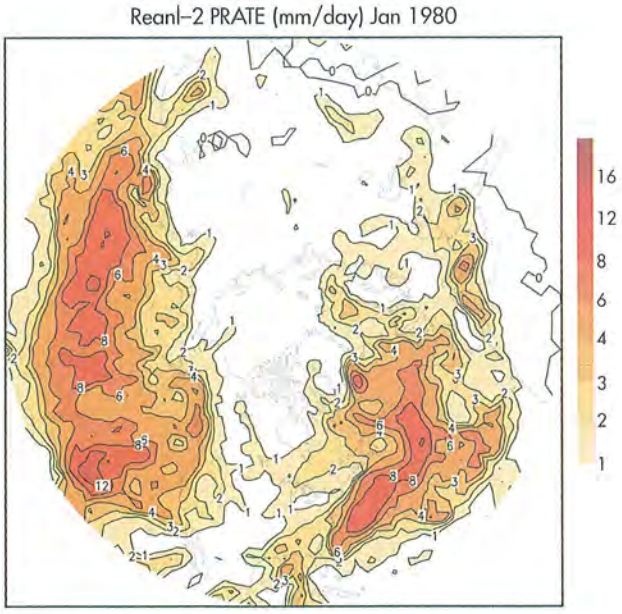
Analyses of the atmospheric state are an important dataset for understanding the atmosphere. The analyses are used by researchers conducting diagnostic studies as well as those trying to predict future states of the atmosphere. There are three sets of analyses covering the satellite era made with modern data-assimilation systems: ERA-15 from the European Center for Medium Range Weather Forecasts (ECMWF), the NCEP/NCAR Reanalysis, and the DAO Reanalysis from NASA. This new AMIP-II Reanalysis replaces the NCEP/NCAR Reanalysis.

## Publications

http://wesley.wwb.noaa.gov/reanalysis2




**January 1980 precipitation rate from the NCEP/NCAR Reanalysis. Note the "spectral snow" problem caused by the poor approximation used in calculating the horizontal diffusion of moisture.**




**January 1980 precipitation rate from the NCEP/DOE AMIP-II Reanalysis. Note the improvement from using a more accurate horizontal moisture diffusion.**

# Seasonal Hydroclimate Predictions for the Western United States

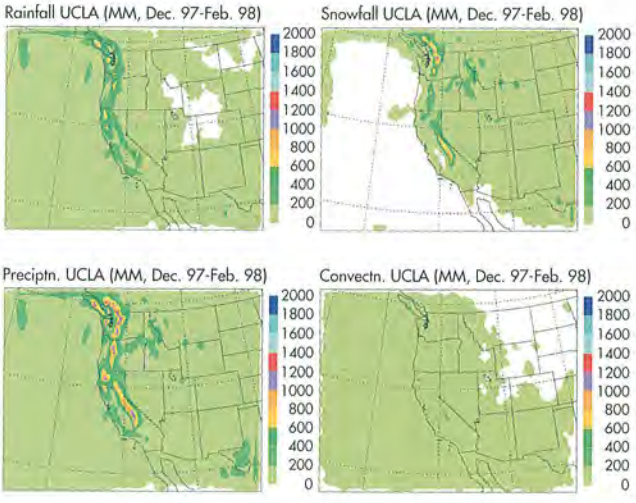
*J. Kim and N. L. Miller,*
*Lawrence Berkeley National Laboratory*

## Research Objectives

Seasonal-scale hydroclimate predictions are important for improving water resources management and assessment, and preparation for natural disasters (e.g., flooding and landslide potential). Seasonal climate prediction is a challenging task due to the chaotic behavior of global numerical models. The main objective of this collaborative research is to examine the potential for seasonal-scale predictions and application of seasonal forecast data toward impact assessments such as streamflow and water budget.

## Computational Approach

In partnership with the National Center for Environmental Prediction (NCEP), University of California (Scripps Institution of Oceanography, UCLA), and the National Weather Service (NWS), we have nested the Regional Climate System Model (RCSM) within the UCLA General Circulation Model (GCM). The NCEP has provided seasonal-scale tropical sea surface temperature (SST) anomaly forecasts for the 1997–1998 winter season, when the intense El Niño event occurred. The UCLA-GCM has simulated multiple realizations at a 2.5° and 2° resolution in the zonal and meridional directions, respectively. The RCSM was nested using two different resolutions, 20 × 20 km and 36 × 36 km, to examine the effects of domain size and spatial resolution. In addition to the seasonal predictions, a diagnostic simulation using the NCEP global analysis was performed and evaluated for a reference simulation.




**Predicted precipitation at a 36 × 36 km resolution for December 1997–February 1998. The large-scale data are from a 2.5° × 2° UCLA-GCM seasonal forecast.**

## Accomplishments

We have produced two predictions and one diagnostic simulation over the western United States. The UCLA-GCM successfully predicted large-scale circulation patterns during December 1997 and February 1998. However, the GCM did not simulate synoptic-scale fields as accurately during the winter. Due to the characteristics of the GCM fields, the RCSM yielded better predictions over the larger domain than the small domain, despite the lack of spatial resolution. The reference simulation successfully simulated streamflow at the Russian River.

## Significance

Seasonal hydroclimate predictions using a physically based model are crucial for improved decision making in water resources management, preparation for natural disasters, agriculture, etc. Despite its significance, this work is still in its early stage and is an internationally recognized growth area. Impact assessment requires very high-resolution information, and the computational requirements increase to the third power as the resolution increases (e.g., doubling the spatial resolution requires about 8 times the computational load). Hence, high performance computing is a crucial component to successful improvements in seasonal hydroclimate research.

## Publications

J. Kim, N. Miller, J. Farrara, D. Cayan, and K. Mo, "Winter-season hydroclimate study for the western U.S. using the Regional Climate System Model (RCSM)," *Proceedings of the 11th Conf. on Applied Climatology* (in press, 1999).

N. Miller, J. Kim, J. Farrara, K. Mo, and D. Cayan, "Short-term and seasonal streamflow predictions for a California Coastal basin during the 1997–1998 winter," Proceedings of the 14th Conf. On Hydrology (in press, 1999).

http://ccs.lbl.gov/RCSM/

# Theoretical Calculation of Water Vapor Continuum Absorption

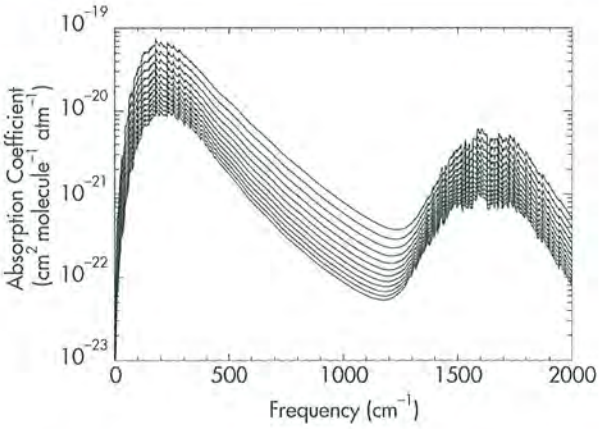
*A. Lacis, Goddard Institute for Space Studies*
*Q. Ma, Columbia University*
*R. Tipping, University of Alabama*

## Research Objectives

To calculate the water vapor continuum absorption from a first-principles theoretical formalism, valid for all frequencies from microwave through visible, and applicable over the full range of atmospheric pressures and temperatures.

## Computational Approach

We have improved the computational efficiency and convergence rate of our previous far-wing formalism for computing continuum absorption due to $H_2O$-$H_2O$ and other molecular systems. In our new formalism, the eigenfunctions of the orientation of the system, rather than the states themselves, are chosen as the complete set of basis functions in Hilbert space. With this new approach, the computational task is transformed from the previous procedure of diagonalization of large matrices to carrying out multidimensional integrations over the continuous orientational variables.




**The absorption coefficient as a function of frequency for $H_2O$-$H_2O$ calculated at 10-K intervals from T=220 K to T=330 K, from top to bottom, respectively.**

## Accomplishments

The new formalism has been applied to linear molecular systems such as $CO_2$-$CO_2$ and $CO_2$-$N_2$, and converged results have been obtained. We have also obtained successful convergence for systems involving symmetric-top and asymmetric-top molecules such as $H_2O$-$H_2O$ and $H_2O$-$N_2$. Detailed computations of self-broadened $H_2O$ continuum absorption have been carried out from the microwave to visible wavelengths for a broad range of atmospheric temperatures. Given that experimental measurements of absorption coefficients for frequencies close to band centers and those in the window regions vary by many orders of magnitude, the agreement between theory and experiment is excellent, being best in the window regions where the quasi-static theory is valid, but underestimating the measured continuum absorption near band centers.

## Significance

The new formalism more readily accommodates the utilization of more realistic interaction potentials involving water molecules (for which no detailed representation is currently available). The short-range anisotropic potential interactions that we have been able to include make the total potential more realistic, and thus lead to better agreement with observations. Accurate representation of the water vapor continuum absorption, and its dependence on temperature, is important for accurate radiative transfer modeling in climate energy balance applications, as well as in the remote sensing of surface and atmospheric temperatures from satellite platforms.

## Publications

Q. Ma, R. H. Tipping, and C. Boulet, "A far-wing line shape theory which satisfies the detailed balance principle," J. Quant. Spectrosc. Radiat. Transfer **59**, 245–257 (1998).

Q. Ma, R. H. Tipping, G. Birnbaum, and C. Boulet, "Sum rules and the symmetry of the memory function in spectral line shape theories," J. Quant. Spectrosc. Radiat. Transfer **59**, 259–271 (1998).

Q. Ma and R. H. Tipping, "The distribution of density matrices over potential-energy surfaces: Application to the calculation of the far-wing line shapes for $CO_2$," J. Chem. Phys. **108**, 3386–3399 (1998).

# Unfolding Pathway for a Beta Hairpin Fragment of Protein G

*Vijay S. Pande and Daniel S. Rokhsar, University of California, Berkeley and Lawrence Berkeley National Laboratory*

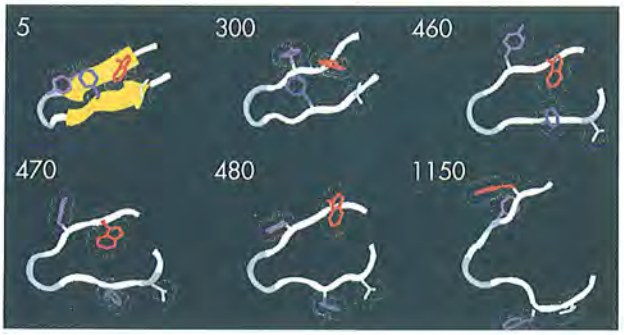
## Research Objectives

To study the unfolding and refolding pathway of a beta-hairpin fragment of protein G using all-atom molecular dynamics simulation. While this fragment is small, it possesses several of the qualities ascribed to small proteins: cooperatively formed beta-sheet secondary structure and a hydrophobic core of packed side chains.

## Computational Approach

This 16-residue peptide folds rapidly and cooperatively to a conformation with defined secondary structure and a packed hydrophobic cluster of aromatic side chains. Since the beta-hairpin is small, its unfolding can be studied in much more detail than the larger proteins whose high temperature unfolding have been examined previously. Using simulations a few nanoseconds in duration, we studied complete unfolding events at temperatures as low as 400°K, and the initial stages of unfolding at 350° and 370°K (77° and 97°C). The availability of many simulations over a range of temperatures permitted the determination of the complete unfolding pathway as well as an extrapolation of this pathway to refolding conditions.

We then tested the hypothesis that refolding under physiological conditions occurs by the reverse of the high-temperature unfolding mechanism. The computationally long time scale for refolding makes a full simulation at low temperature unfeasible. However, we were able to simulate the refolding of the beta-hairpin peptide from conformations in its transition state ensemble. The critical advance that made this possible is analysis techniques that have been developed in the study of lattice models which allowed us to identify the transition states for the various transitions of the unfolding pathway. Even for slow kinetic processes, the actual passage through the transition state can be quite fast (tens of picoseconds); most of the folding time is spent waiting for the fluctuations to reach the transition state. By directly identifying the transition state, we bypassed this time-consuming part of the simulation.




**A typical unfolding trajectory at 400°K demonstrates discrete unfolding steps. Beta-sheet hydrogen bonds (if formed) are shown as sheets, and the hydrophobic core is shown in wireframe with van der Waals radii (TRP red, PHE blue, TYR purple, VAL gray). The time in picoseconds is given in the upper left of each frame.**

## Accomplishments

At high temperatures, we found that the beta-hairpin unfolds through a series of sudden, discrete conformational changes. These changes occur between states that are identified with the folded state, a pair of partially unfolded kinetic intermediates, and the unfolded state. To study refolding at low temperatures, we performed a series of short simulations starting from the transition states of the discrete transitions determined by the unfolding simulations. These simulations showed that refolding at low temperatures can proceed by reversing the unfolding pathway found at high temperatures.

## Significance

The direct simulation of protein folding is a "holy grail" of computational biology. Since straightforward molecular dynamics can typically examine trajectories only tens of nanoseconds in duration, however, the milliseconds needed to fold even small proteins are far too long to simulate. A clever stratagem that allows progress to be made in studying conformational changes in proteins is to instead simulate unfolding, under conditions (high temperature, acid pH, high denaturant) such that the unfolding reaction rate is accelerated into an accessible range. These simulations have yielded insights into the initial stages of unfolding to an expanded conformation, which is assumed to reflect the later stages of refolding. The transition state for this process is in good agreement with experimental determinations of the folding transition state under physiological conditions. Important open questions pertain to the relationship between extremely rapid unfolding at 500°K and the much slower refolding process at physiological temperatures, as well as the underlying physical reason for the surprisingly good agreement between high- and low-temperature transition states.

## Publications

V. S. Pande and D. S. Rokhsar, "Folding pathway of a lattice model for proteins," Proceedings of the National Academy of Sciences (in press, 1998).

http://hubbell.berkeley.edu/
http://marichal.berkeley.edu/

# Nonlinear Stratified Flows: High-Resolution Simulation of Breaking Gravity Waves in the Earth's Atmosphere

J. M. Prusa, Iowa State University
P. K. Smolarkiewicz, National Center for Atmospheric Research
A. A. Wyszogrodzki, University of Warsaw

## Research Objectives

Gravity waves (GWs) are generated in the Earth's atmosphere whenever a parcel of air is disturbed from its hydrostatic equilibrium position. In turn, wave-wave interactions (WWI) and turbulence generated by gravity wave breaking (GWB) force the atmosphere at many scales. At planetary scales, GWB makes a dominant contribution towards reversing the meridional temperature gradient at mesopause altitudes—compared to what would occur due to radiative balance alone. Wave drag induced by GWs is considered to be important in improving subgrid parameterizations for global climate models. At mesoscales, GWs may be a key component in determining the spectral energy of the atmosphere. By using the 512-PE Cray T3E at NERSC, we were able to generate the detailed dynamics of GWB from the mesoscale down to the Kolmogorov scale. These results are being used to detail the mechanisms by which GWs actually influence the mean state of the atmosphere.

## Computational Approach

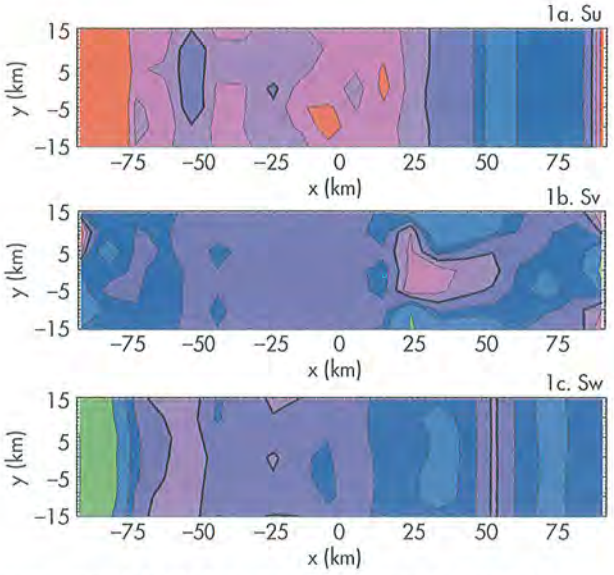
We developed a multiplatform fluid-flow application that runs efficiently on massively parallel machines like the T3E or on scalar processor machines. It solves the anelastic equations of motion in nonorthogonal terrain-following coordinates. The resulting elliptic pressure equation is solved using a conjugate-residual method. Our application has several sets of options to choose from, such as semi-Lagrangian or Eulerian solver, dry or moist model, grid types, turbulence parameterizations, and monotonicity (nonoscillatory) constraints.

## Accomplishments

We simulated three hours of GW dynamics on a computational grid of 544 × 80 × 291 points, corresponding to a physical domain of 200 km (zonal) × 30 km (meridional) × 110 km (vertical). This simulation captured approximately 50 minutes of intense turbulence generated by GWB that was nonstationary, inhomogeneous, and anisotropic. A good idea of this inhomogeneity and anisotropy can be gained from the figure, which shows the zonal ($S_u$), meridional ($S_v$), and vertical ($S_w$) velocity derivative skewness. For isotropic turbulence, $S_u = S_v = S_w \sim 0.5$.

## Significance

Power spectra reveal three distinct subranges in the evolution of GWB: (1) an inertial range turbulence at the highest wavenumbers, (2) a buoyancy range turbulence at mid-scales, and (3) a WWI subrange at the lowest wavenumbers. The last subrange has properties that are consistent with two-dimensional waves that are forcing the basic state. We have conjectured that WWI of two-dimensional GWs (known to be common by direct observation) may be a key dynamical mechanism forcing the atmosphere at the mesoscale. Current efforts are focused on trying to find supporting evidence for this conjecture through direct computation of the turbulent fluxes and structure function statistics.




**Contour density plot of velocity derivative skewnesses in horizontal xy plane at 100 km altitude and $t$ = 155 minutes. The averaging blocks for the Si computations were 10 × 5 × 7.5 km in zonal × spanwise × vertical extent. The region of vigorous wavebreaking/broken waves is $-70 \le x \le 10$ km. Contours are shown at $S_i = -1.0, -0.35, 0.0, 0.35$ (bold), 0.65, and 1.0, with redder hues corresponding to larger values of $S_i$.**

## Publications

J. Prusa, P. K. Smolarkiewicz, and W. W. Wyszogrodzki, "Simulations of gravity wave induced turbulence using 512 PE CRAY T3E," *Proc. 2nd International Workshop on Software Engineering and Code Design in Parallel Meteorological and Oceanographic Applications* (Preprint Vol. NASA GSFC/CP-1998-206860, Scottsdale, Arizona, June 15–18, 1998), pp. 139–151.

———, "Massively parallel computation of gravity wave turbulence in the Earth's atmosphere," SIAM News, Applications on Advanced Architecture Computers (submitted, 1998).

J. Prusa, P. K. Smolarkiewicz, R. R. Garcia, and W. W. Wyszogrodzki, "Evolution of gravity wave spectra at mesopause altitudes," presented at IUTAM Developments in Geophysical Turbulence, National Center for Atmospheric Research, Boulder, Colorado, June 16–19, 1998.

# Cloud Albedo Perturbations on Climate

*S. E. Schwartz and C. M. Benkovitz,*
*Brookhaven National Laboratory*

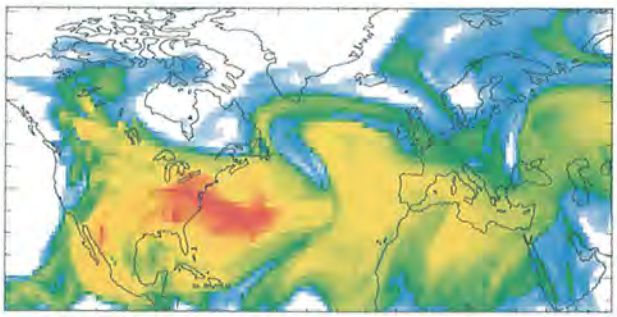
## Research Objectives

In this project we evaluate the magnitude of the perturbation in clear-sky and cloud albedo due to anthropogenic emissions of $SO_2$ associated with fossil-fuel combustion, as a function of time and location. We also systematically examine for evidence of such perturbation, principally in satellite measurements of albedo. This information will permit critical testing of two hypotheses: (1) sulfate aerosol arising from these emissions enhances clear-sky albedo by forming light-scattering aerosol particles, and cloud albedo by increasing the number density of cloud droplets, thus affecting the global radiative balance; and (2) this albedo enhancement causes a global annual average climate perturbation comparable to that of fossil-fuel $CO_2$, but opposite in sign.

In addition, the distribution of the forcing, thought to be confined almost entirely to the Northern Hemisphere and to be rather nonuniform within this hemisphere, will be determined. If the distribution is found to be largely nonuniform, our analyses will also address the question of whether a climate response to this $SO_2$ albedo perturbation may be more readily discernible than that due to $CO_2$.

## Computational Approach

The chemical transport and transformation model has been implemented using FORTRAN. The model solves material balances based on the continuity equations with the application of gradient-transport assumptions. To solve these equations, numerical approximations at any location (x, y, z) are considered mechanistically and dimensionally independent over short periods of time (time step is 1 h) according to the operator splitting technique, also known as the "locally one-dimensional" approximation. Spatial integrals of the transport are approximated using the area-preserving flux form developed by Bott. Dry deposition is represented as the lower boundary condition for the vertical transport. The integration procedure for each transformation term (gas- and aqueous-phase chemical conversions) treats loss terms as exponential decay terms. The C90 computer at NERSC has been used so far to run the model; work is being transferred to the J90.



**Sulfate column burden (vertical integral of the concentration) on July 9, 1986 at 00 UT for secondary sulfate from anthropogenic emissions west of 30°W. White denotes the lowest column burden, red the highest.**

## Accomplishments

A three-dimensional Eulerian transport and transformation model driven by observation-derived synoptic meteorological data has been applied to calculate mixing ratios (MRs) of sulfate and $SO_2$, and wet deposition of sulfate over the North Atlantic and adjacent continental regions for one-month periods in each of four seasons in 1986–87. Model performance is evaluated by comparison of grid-cell average (1.125°) modeled MRs for sulfate (24-h average) and $SO_2$ (6 and 24-h average) in the lowest model level (surface to ca. 65 m) to surface MRs observed at monitoring stations in North America and Europe.

## Significance

Global climate change due to enhanced concentrations of greenhouse gases is of major current concern. Much of the present debate on this issue surrounds the quantitative relation of tempreature change over the industrial era (1850 to present) to models of the forcing of climate change. The greatest uncertainty in this forcing is due to aerosols, light-scattering particles in the atmosphere. This work is directed to developing chemical transport models for such aerosols and evaluating their performance by comparison with observations. Only with such models can one gain confidence in the estimates of this forcing. Work to date has focused on evaluation of model performance by comparison with observations at specific dates and locations.

## Publications

C. M. Benkovitz and S. E. Schwartz, "Evaluation of modeled sulfate and $SO_2$ over North America and Europe for four seasonal months in 1986–87," J. Geophys. Res. **102**, 25305–25338 (1997).

C. M. Benkovitz, R. C. Easter, S. Nemesure, R. Wagener, and S. E. Schwartz, "Sulfate over the North Atlantic and adjacent continental regions: Evaluation for October and November 1986 using a three-dimensional model driven by observation-derived meteorology," J. Geophys. Res. **99**, 20725–20756 (1994).

http://www.ecd.bnl.gov/steve/schwartz.html

# Coupled Parallel Climate Model (PCM) Applications to Climate Change

*Warren M. Washington and Gerald A. Meehl, National Center for Atmospheric Research*
*Albert Semtner, Naval Postgraduate School*
*John Weatherly, Cold Regions Research and Engineering Laboratory*

## Research Objectives

To conduct simulations of climate change with new generation high-resolution climate models.

## Computational Approach

The Parallel Climate Model (PCM) is a coupled climate model that executes on the Cray T3E computer. The atmospheric component is the National Center for Atmospheric Research (NCAR) Community Climate Model; the ocean component is the Parallel Ocean Program with a resolution of 32 levels and 2/3 degree horizontal grid; and the sea ice component is the Naval Postgraduate School model using a resolution of 27 km. The components are interfaced by a flux coupler that passes the energy, moisture, and momentum fluxes between components.

## Accomplishments

Over the past year we were able to obtain a climate simulation for the 1990s. We will use this control experiment for future climate change scenarios with different forcings such as increasing greenhouse gases and the effects of sulfate aerosols. This model has higher-resolution ocean and sea ice components than are used in previous coupled climate model simulations; thus we can see much more realistic eddy structures in the ocean that are closer to the observed patterns.

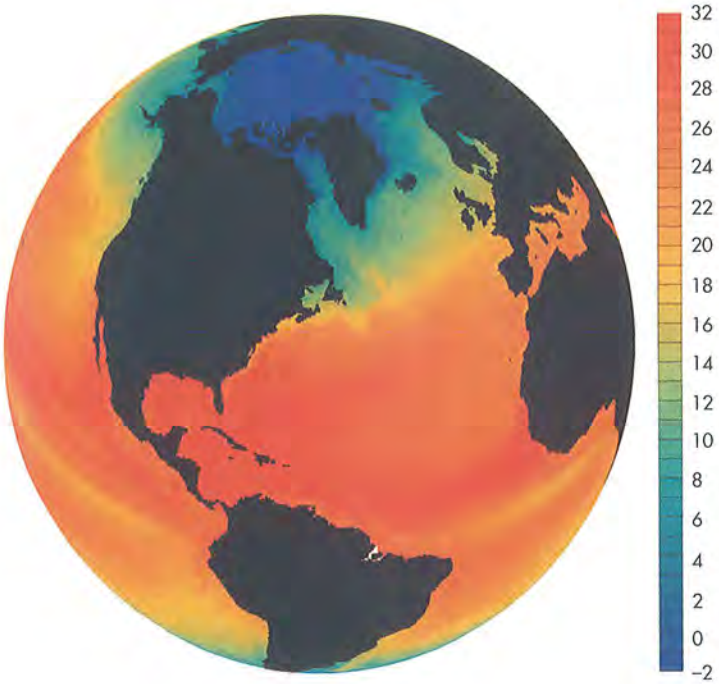
## Significance

Because of an observed warming of the earth's climate that is probably caused by increased greenhouse gases, the Department of Energy is very interested in making better estimates of possible impacts on future states of climate. This requires, in part, better models of the climate system with improved resolution that provides regional impacts.

## Publications

W. M. Washington and J. W. Weatherly, "Simulations with a climate model with high-resolution ocean and sea ice," in *Polar Processes and Global Climate: Draft Summary Report from the Conference on Polar Processes and Global Climate, WMO/ICSU/IOC World Climate Research Programme* (WCRP) (International ACYSYS Project Office, Oslo, Norway, 1997), pp. 250–252.

www.cgd.ucar.edu/ccr/pcm/




**This image depicts the sea surface temperature (Celsius scale) from a coupled simulation with the DOE Parallel Climate Model. Note the Gulf Stream meander pattern and the cooler tropical Pacific and Atlantic surface temperatures caused by upwelling of cold water. Also depicted is the cold water under the Arctic and East Greenland sea ice. (Graphic by Gary Strand, NCAR.)**

# Biomolecular Structure Analysis by Nuclear Magnetic Resonance

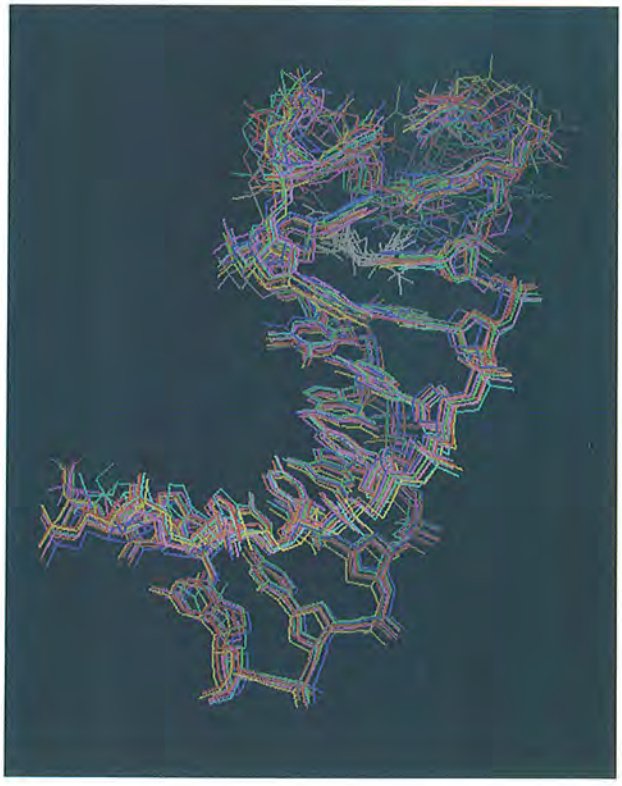
*David E. Wemmer, Lawrence Berkeley National Laboratory*

## Research Objectives

The focus of our work is to understand structure-function relationships in biomolecules and their complexes by applying methods of modern multidimensional nuclear magnetic resonance (NMR).

## Computational Approach

There are two major stages in the analysis of NMR data which rely heavily on computation. The first is optimized transformation of the time domain NMR data into frequency dimensions. To extend resolution, this transformation uses linear prediction or maximum entropy analysis, followed by Fourier transformation. Artifacts are removed from the data using iterative modeling of various sorts. The second stage of the analysis is in conversion of NMR-derived structural restraints, together with knowledge of the covalent structure of the molecule, into sets of coordinates (models) that are consistent with all experimental observations. This can be done through molecular-dynamics calculations in either Cartesian or internal angle spaces. These models are analyzed to determine the structure-function relationships of interest.



A set of NMR-derived structures for the aptamer DNA; arginamide complex is shown.

## Accomplishments

Time allocated in the past year was used to explore both the data analysis and structure refinement steps. Unfortunately, the analysis program PROSA, though functional on other supercomputers, could not load experimental data when run on the Cray C90. However, the real-space refinement program AMBER was run to analyze the structure of an aptamer DNA (one found through an *in vitro* selection for arginine binding) in complex with its target. The results indicate a complex folded structure and demonstrate clear structural changes upon binding. Structures were also calculated for the receiver domain of nitrogen-regulatory protein C (NTRC) from bacteria. This protein is regulated by phosphorylation, and we are trying to determine the structural changes that occur upon phosphorylation. The program DYANA (an angle space dynamics program) was used for refinement of some of the structures. The regions where changes occur were clearly identified, and iterative refinement of the structure is continuing.

## Significance

The systems under study are of fundamental interest, as they are examples of regulatory interactions that occur in complex biological systems. Resulting data aid in understanding regulatory interactions and how they can fail under specific circumstances. The insight gained will also be valuable in future efforts to design new regulatory pathways from the principles used in nature.

## Publications

S. A. Robertson and D. E. Wemmer, "Structural changes in a DNA aptamer upon arginine binding" (in preparation, 1998).

# TRIM Simulation of Plasma Merging and Magnetic Reconnection on the Swarthmore Spheromak Experiment

*M. Brown and D. Auerbach, Swarthmore College*
*D. Schnack, Science Applications International Corporation*

## Research Objectives

Simulate plasma formation, merging, and magnetic reconnection using the adaptive magnetohydrodynamic (MHD) code called TRIM (developed by D. Schnack) in order to directly compare with experimental results from the Swarthmore Spheromak Experiment (SSX).

## Computational Approach

The TRIM code solves the two-dimensional MHD equations on an adaptive triangular mesh. When gradients in field quantities exceed a threshold, a triangular grid element is subdivided for higher resolution. The simulations took about 100 hours on the NERSC C90.

## Accomplishments

Preliminary results demonstrate that TRIM can adequately simulate formation and merging of SSX spheromak plasmas. More quantitative comparison needs to be done, but the time scales and spatial structures appear to closely match what we measure experimentally. In the future, we hope to use the TRIM results with a particle code to see if plasma merging and reconnection is a plausible mechanism for particle acceleration.

## Significance

High-energy particles are a common product of turbulent magnetofluids (fusion plasmas, solar flares, astrophysical plasmas). Magnetic reconnection could be the engine that drives particle acceleration, and could be the source of the hot solar corona and energetic cosmic rays.

## Publications

M. R. Brown, "Experimental studies of magnetic reconnection," Bulletin of the American Physical Society **42** (1998).

http://laser.swarthmore.edu/html/research/SSX/

# Major Computational Applications in Magnetic Fusion

*B. I. Cohen, M. J. Caturla, T. Diaz de la Rubia, A. M. Dimits, A. Koniges, W. M. Nevins, G. D. Porter, M. E. Rensink, T. D. Rognlien, D. E. Shumaker, and X. Q. Xu,*
*Lawrence Livermore National Laboratory*

## Research Objectives

The major simulation codes in LLNL's Magnetic Fusion Program address the physics of fusion plasmas and materials in three areas: (1) anomalous energy and momentum transport in the tokamak core, using gyrokinetic particle-based simulation; (2) the dynamics of energy displacement cascades in vanadium, vanadium alloys, and SiC ceramics, using the molecular dynamics code MOLDYCASK; (3) tokamak edge-region plasmas, modeled by a series of codes using domain-decomposition algorithms on parallel computers. These codes are used to design tokamak divertors that have acceptable heat fluxes on material surfaces and allow pumping of helium ash.

## Computational Approach

The principal computer codes reviewed here are run on massively parallel computers, mostly on the NERSC T3E, and make use of message passing and domain decomposition in most cases. The computational physics algorithms employ state-of-the-art methods in the kinetic simulation of plasmas with particle codes, molecular dynamics simulations, and hydrodynamic simulation.

## Accomplishments

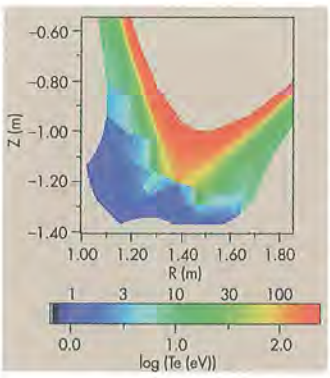
*Gyrokinetic (GK) turbulent transport simulation:* Detailed parameter studies have addressed discharge #81499 in the General Atomics DIII-D tokamak as a base case. Careful comparisons have been made between the results of the fluid and kinetic simulations of shot #81499 and variants to determine parametric dependences and points of agreement between the simulation algorithms.

In the Cyclone Project, a GK flux-tube particle-in-cell (PIC) simulation has been the object of a vigorous study, focusing on its convergence properties with respect to particle number, spatial resolution, and system size. Results indicate strong convergent properties. The GK simulation results concerning turbulent ion thermal diffusivity for the DIII-D discharge are in the range of a factor of 2 to 3 lower than GLF results, with larger differences closer to marginal stability.

The gyrokinetic simulations have also demonstrated the importance of flow shear in reducing drift-wave turbulence in tokamaks, as observed in experiments. In particular, a new phenomenon in which zero-transport states occur for values of the temperature gradient significantly greater than the linear marginal value has been found.

*Neutron interactive materials:* The MOLDYCASK code was converted from PVM to MPI in FY98 and has been used to investigate the primary damage state from recoil cascades in vanadium and SiC. The simulations provide the database for defect production in these materials for input into kinetic Monte Carlo simulations of damage accumulation and microstructure evolution over macroscopic length and time scales.

*Edge plasma simulation:* For the UEDGE transport code, we have generalized the basic domain-decomposition algorithm used in our parallel version to include multiply-connected regions of the edge plasma. This allows simulation of realistic toroidal geometry for devices. An algorithm is also included for calculating the electric fields that are believed important for suppressing turbulence and that contribute significantly to in/out divertor asymmetries. Within the last year, we have developed and parallelized the first 3D global-turbulence simulation code BOUT in a realistic toroidal x-point geometry spanning the region including the separatrix.




**Two-dimensional hydrodynamic simulations with the UEDGE transport code accurately predict the electron temperature in detached plasmas near the divertor plate in the General Atomics DIII-D tokamak experiment. A false-color plot of the electron temperature as a function of vertical height Z and major radius position R is shown for data from the UEDGE simulation for shot number 87506.**

## Significance

The simulation and modeling research described above has been successful in developing a deeper understanding of the physics, analyzing experiments, aiding efforts to improve experimental performance, and designing new experiments.

## Publications

R. S. Averback and T. Diaz de la Rubia, "Displacement damage in irradiated metals and semiconductors," Solid State Physics **51**, 281–401 (1998).

T. D. Rognlien and D. D. Ryutov, "Analysis of classical transport equations for the tokamak edge plasma," Contr. Plasma Phys. **38**, 152 (1998).

X. Q. Xu and R. H. Cohen, "Scrape-off layer turbulence theory and simulations," Contributions to Plasma Physics **38** (1998).

# High-Current Beam Studies for Heavy-Ion Fusion

*A. Friedman, D. P. Grote, S. M. Lund, J. J. Barnard, W. M. Sharp, and G. D. Craig, Lawrence Livermore National Laboratory*
*I. Haber, Naval Research Laboratory*

## Research Objectives

Simulate heavy-ion induction acceleration to study basic beam physics, analyze beam behavior in experiments, and predict beam behavior in future facilities.

## Computational Approach

Two principal models are used: an envelope equation/fluid model embodied in the code CIRCE, and a particle-in-cell (PIC) model embodied in the code WARP. CIRCE offers rapid synthesis and optimization, but neglects higher-order effects that can lead to beam degradation. WARP provides a fully kinetic description of beam behavior in 2D and 3D. The codes are sometimes linked.

## Accomplishments

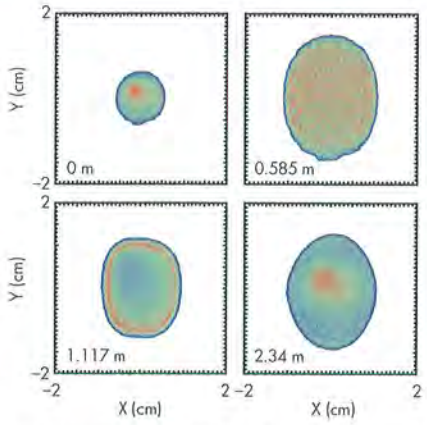
We extended our understanding of high-current beam transport and acceleration and increased the power of our computational tools.

Earlier simulations showed evidence of an instability that drives thermal energy exchange in intense beams initially colder longitudinally than transversely. Recent simulations, coupled with theoretical analysis, have led to a more complete understanding of the mode, which constrains the parameter space available to a fusion driver.

An experiment that accelerates a space-charge dominated beam through a 90-degree bend is under way at LLNL. Extensive simulations have examined the optimization of the envelope match, emittance growth from longitudinal dispersion, injector transients, and the effects of beam nonuniformities (see figure). A complete ring, proposed for the experimental program, has served as a simulation testbed for novel feed-forward beam steering and adaptive control algorithm development.

The HIBALL II final-focus system, including an axially compressing beam, was modeled for the first time self-consistently in 3D. This work validated earlier 2D simulations.

We began simulating the long-term behavior of a beam in a next-step inertial fusion energy facility incorporating hundreds of fundamental lattice periods and using both electric and magnetic focusing (confinement). With ideal linear applied fields and realistic tolerances on transverse misalignments, the beam is seen to suffer little degradation in focusability.




**Contours (in the transverse plane) of the density of a high-current beam at four stations along the LLNL bend experiment. The first frame shows the beam as it exits the diode, reconstructed from experimental measurements at that location. The following frames show a space-charge wave that spreads out and bounces from the edge of the beam, ultimately to reform a high-density spot similar to that at the start. Red denotes highest density, blue lowest.**

A new interface to WARP was built using the Python interpreter/scripting language, which was readily adapted to the parallel environment. This added a fully interactive code-steering capability to the existing parallel code.

## Significance

The principal approach to developing an inertial fusion driver is the heavy-ion induction accelerator. A key challenge, essential to a cost-effective driver, is maintaining the focusability of the intense ion beams (non-neutral plasmas) through numerous manipulations in the presence of the strong, nonlinear self-fields.

## Publications

D. P. Grote, A. Friedman, I. Haber, W. M. Fawley, and J. L. Vay, "New developments in WARP3d: Progress toward end-to-end simulation," *Proc. Int. Sympos. on HIIF,* (Heidelberg, September 1997); Nuclear Instruments and Methods A, in press.

S. M. Lund, J. J. Barnard, G. D. Craig, A. Friedman, D. P. Grote, H. S. Hopkins, T. C. Sangster, W. M. Sharp, S. Eylon, T. J. Fessenden, E. Henestroza, S. S. Yu, and I. Haber, "Numerical simulation of intense-beam experiments at LLNL and LBNL," *Proc. Int. Sympos. on HIIF,* (Heidelberg, September 1997); Nuclear Instruments and Methods A, in press.

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# Transport Barrier Dynamics

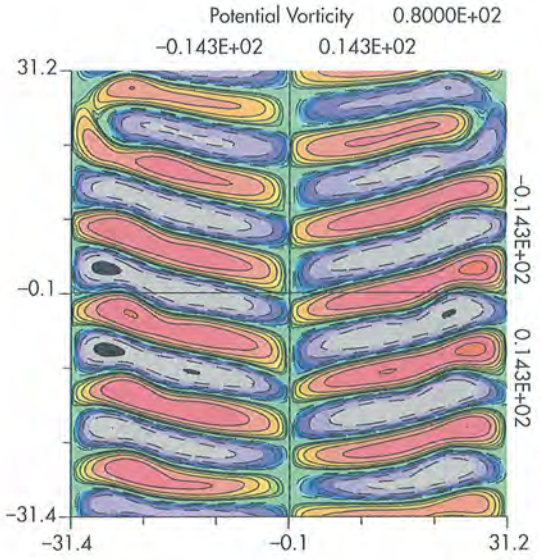
*W. Horton, T. Tajima, P. Zhu, and L. Leonard,*
*University of Texas at Austin*

## Research Objectives

This project develops the theoretical and simulation tools for describing the radial transport in tokamaks under conditions where local radial regions develop fast time-scale dynamics. This occurs in transport models that allow for the bifurcations between different transport mechanisms, as is the general case in both neutral-fluid and plasma-turbulent transport.

## Computational Approach

The parallel processors of the Cray T3E are distributed over the radius of the tokamak plasma to build a high-radial-resolution transport code capable of following the very steep gradients found in the internal transport barriers of high performance tokamaks. The time dynamic in each radial zone is adaptive to the appropriate fast or slow evolution in that particular radial zone.




**Vorticity levels in a 6 × 6 cm box perpendicular to the magnetic field and centered on the minimum q-surface. The ion temperature gradient convection forms a transport barrier with tilted vortices on each side arising from self-consistent E × B flows.**

## Accomplishments

We have developed a model on the Cray T3E that describes the bifurcations occurring in the radial temperature and density profiles in tokamak plasmas. The bifurcations arise from the interaction of the turbulence with the transport profiles through the mechanisms associated with shearing in the radial electric field and the velocity flows. High spatial and temporal resolution algorithms are used to capture the physics of the bifurcations. The space and time scales of the bifurcations are hybrids between the long global transport scales and the mircoscales of the drift-wave turbulence. The present model is built on the ion-temperature gradient driven turbulence; generalizations to include other forms of micro-turbulence are in the planning stages.

## Significance

The problem of bifurcations in the turbulent transport of fluids and plasmas is of wide scientific interest. Observed bifurcations to states with sheared flows in the problem of Bernard convection are relevant to understanding the more complex problem in plasmas. Gaining such an understanding is of key importance for plasma confinement, since several of the large mega-ampere systems find their record fusion performance shots only after making the bifurcation to a high confinement state. The signature for the high confinement state is the formation of an internal transport barrier (ITB). The project will allow several hypotheses for the improved confinement modes to be tested quantitatively. The presence or absence of an internal transport barrier could make the difference in an acceptable fusion power gain for a magnetic fusion reactor.

## Publications

G. Hu and W. Horton, "Minimal model for transport barrier dynamics based on ion-temperature gradient turbulence," Physics of Plasmas **4**, 3262–3272 (1997).

W. Horton, T. Tajima, J.-Q. Dong, J.-Y. Kim and Y. Kishimoto, "Ion transport analysis in a high beta-poloidal JT-60U discharge," Plasma Phys. Control. Fusion **39**, 83–104 (1997).

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http://www.ph.utexas.edu/dept/research/horton

# Stellarator Optimization

*L. P. Ku, D. Monticello, and A. Reiman,*
*Princeton Plasma Physics Laboratory*

## Research Objectives

To identify compact stellarator configurations that have low aspect ratio, good quasi-axisymmetry, and high magnetohydrodynamics (MHD) stability beta limit.

## Computational Approach

We have constructed a configuration optimizer in which the state variables are the Fourier harmonics representing the plasma boundary, and the objective functions are measures of the quasi-axisymmetry and growth rates of the ballooning and kink modes. Constraints such as plasma beta, aspect ratio, profile of rotational transform, etc. can be imposed. The plasma surface is deformed to generate the desired rotational transform, and the quasi-axisymmetry and the stability of the plasma are maximized. The program finds paths to an optimal state using quadratic programming or chi-square minimization techniques. Evaluation of the gradient of the objective functions involves equilibrium calculations, mapping the resulting equilibria to the so-called Boozer magnetic coordinates, and performing stability calculations in the Boozer space. On the Cray C90, each complete function call for the stability calculations takes about 2.5 minutes of CPU time and 35 MW of memory for 33 flux surfaces with about 400 modes. A typical run involves about 600 function calls.

## Accomplishments

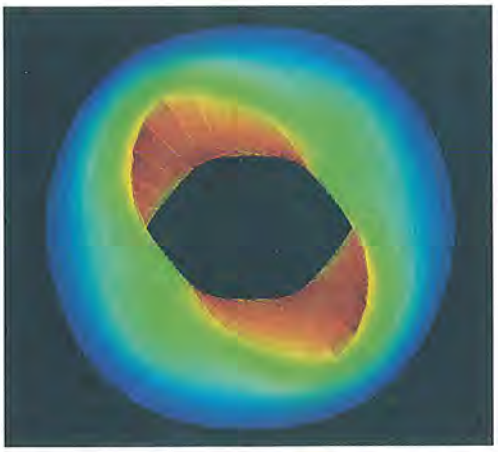
We have been pursuing the design of compact stellarator configurations with aspect ratios (R/a) in the range of 2–4, comparable to those of tokamaks. To provide good particle drift trajectories, we have focused on configurations that are close to quasi-axisymmetric. A wide range of configurations have been studied. These configurations have the fraction of the rotational transform generated externally ranging from 20% to about 50%, and with beta up to 7%. We have explored the MHD and transport properties of these configurations. Methods of stabilizing the external kink modes without a conducting wall have been found. The two illustrations show the boundary shape and the magnetic field strength of a two-field-period, aspect ratio 2.1 stellarator. This configuration has about 40% of the rotational transform generated by the external coils; the remaining 60% is supplied by the bootstrap current.

## Significance

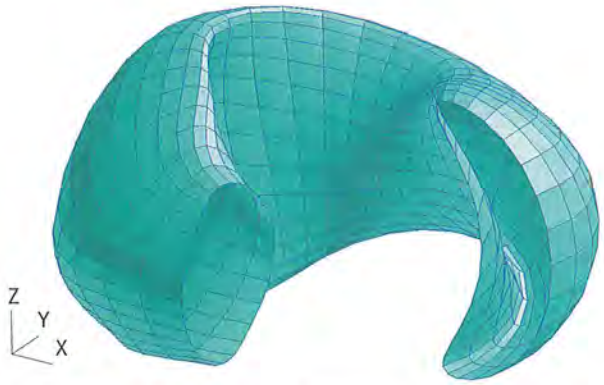
Stellarators are magnetically confined fusion devices with confinement properties similar to those of tokamaks. Both devices have toroidally nested closed magnetic surfaces created by helical (toroidal plus poloidal) magnetic fields. Unlike tokamaks, stellarators primarily use currents in external coils, rather than in the plasma itself, to confine and stabilize the plasma.

Large stellarator experiments are under way in Europe and Japan, and a smaller experiment is under construction at the University of Wisconsin. These programs are important because the similarities and differences between stellarators and tokamaks can be used to improve our understanding of toroidal confinement and to develop an improved reactor concept. Recent studies have shown that stellarators may be competitive with tokamaks as reactors.

Stellarators with improved performance have been designed in recent years by running fast three-dimensional computer codes. Spectral methods have raised the accuracy of the codes to a level where they provide a reliable simulation of the physics. Improvement and further development of these codes will provide us with even more powerful tools to search for interesting and attractive configurations in a very complex and multi-dimensional space.



**A cutaway view of a two-field-period, aspect ratio 2.1 stellarator showing the last closed flux surface.**




**Contours of magnetic field strength on the last closed flux surface of the configuration shown in the left figure, demonstrating the good toroidal symmetry.**

# Gyrokinetic Simulations of Collisional and Turbulent Transport in Fusion Plasmas

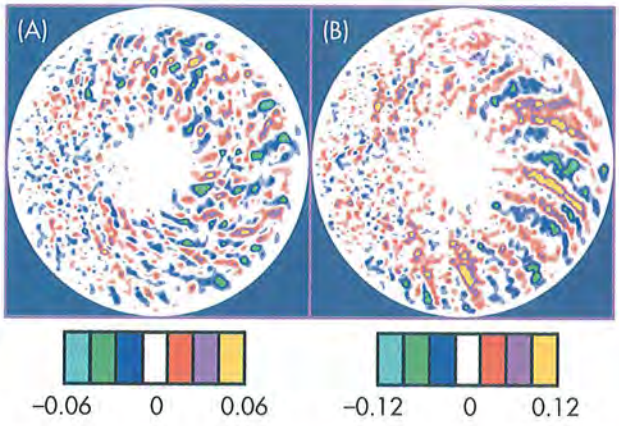
*Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang, and R. B. White, Princeton Plasma Physics Laboratory*

## Research Objectives

The primary purpose of this project is to develop a gyrokinetic particle code capable of simulating transport processes in realistic tokamak fusion plasmas, to use the code to enhance our physics understanding of particle and energy confinement, and to compare the simulation results with the measurements from magnetic fusion experiments.

## Computational Approach

The Gyrokinetic Toroidal Code (GTC) was implemented as a platform-independent program based on a domain decomposition algorithm using Message Passing Interface (MPI). GTC achieved nearly perfect scalability on two massively parallel processing (MPP) systems, the Cray T3E and the SGI Origin 2000.




**Poloidal contour plots of fluctuation potential ($e\Phi/T_i$) in the steady state of nonlinear global simulation with E × B flows included (a) and with the flows suppressed (b). This comparison shows the key mechanism of transport reduction by turbulence-generated E × B flows through the breaking of turbulent eddies, and consequently, the reduction of the radial decorrelation length and associated fluctuation level.**

## Accomplishments

We have developed a general geometry parallel gyrokinetic toroidal code to study both collisional and turbulent transport processes in magnetically confined toroidal plasmas. In the area of collisional transport, we have resolved the apparent contradiction that ion thermal transport levels in enhanced confinement tokamak plasmas have been observed to fall below the "irreducible minimum level" predicted by standard neoclassical theory. In turbulence simulations, linear poloidal flow damping simulations exhibit an asymptotic residual flow in agreement with recent analytic calculations. Nonlinear global simulations of ion-temperature-gradient instabilities in toroidal magnetized plasmas provide key first principles results supporting the physics picture that turbulence-driven fluctuating E × B flows can significantly reduce turbulent transport. Finally, the outstanding differences in the flow dynamics observed in global and local simulations are found to result from profile variations.

## Significance

Our simulation effort has finally enabled us to make contact with existing machine experiments. With the increase in computing power and addition of new physics into the code, we expect gyrokinetic particle simulation to have a significant impact on fusion research in the future.

## Publications

Z. Lin, T. S. Hahm, W. W. Lee, W. M. Tang, and R. B. White, "Turbulent transport reduction by zonal flows: Massively parallel simulations," Science **281**, 1835 (1998).

Z. Lin, W. M. Tang, and W. W. Lee, "Neoclassical transport in enhanced confinement toroidal plasmas," Phys. Rev. Lett. **78**, 456 (1997).

W. W. Lee and R. A. Santoro, "Gyrokinetic simulation of isotope effects in tokamak plasmas," Phys. Plasmas **4**, 169 (1997).

http://w3.pppl.gov/~zlin/

# Design of Optimized Three-Dimensional Magnetic Fusion Confinement Geometries

*D. A. Spong, S. P. Hirshman, and J. C. Whitson,*
*Oak Ridge National Laboratory*
*P. M. Valanju and B. Miner, University of Texas*

## Research Objectives

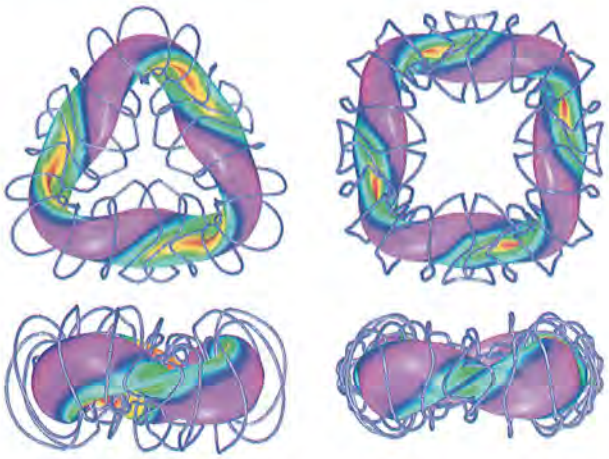
Stellarators rely on three-dimensional shaping of the outer magnetic surface to provide good plasma confinement and stability without the need for the externally driven currents that are necessary in tokamaks. The flexibility offered by three-dimensional shaping opens up a vast design space of possible configurations. The design of stellarator devices with desirable properties relies strongly on high-performance computing, both with respect to the nonlinear, multiparameter space optimizations and in the evaluation of the transport and stability properties of the resulting configurations.

## Computational Approach

Our stellarator optimization is built around the three-dimensional plasma equilibrium code VMEC. VMEC calculates the magnetic structure within the plasma volume based on a specification of the outer magnetic surface shape. From this magnetic field structure, a variety of optimization targets are evaluated, such as the longitudinal adiabatic invariant (determines plasma confinement), the Mercier criterion (determines plasma stability), the aspect ratio (determines compactness of the device), the rotational transform, etc. The outer plasma surface shape (which is characterized by 20–30 Fourier amplitudes) is then varied, using a Levenberg-Marquardt optimization loop to achieve overall minimization of the target functions in a root mean squared sense. As a second step, modular magnetic field coil geometries that will produce the required outer magnetic surface shape are determined. Following the optimization, the confinement of the configuration is evaluated in more depth, using particle simulation techniques. The optimizer is written in Fortran-90, extensively uses dynamic memory allocation techniques, and runs on the Cray C90 and J90 computers. The Monte Carlo particle simulation currently runs on the J90, but is being adapted to run in parallel on the T3E using MPI (Message Passing Interface).

## Accomplishments

This project has led to compact magnetic configurations that provide improved plasma confinement and stability over previous approaches. These efforts are part of the National Compact Stellarator Experiment (NCSX) project and are expected to lead to the construction of proof-of-principle (POP) and concept exploration (CE) devices within the next few years. The POP device will be based on the quasi-axisymmetric optimization technique, while the CE device will be based on the quasi-omnigenous (QO) approach (see figure).



**Top and side views of 3- and 4-field-period optimized low-aspect-ratio stellarators based on the quasi-omnigenous approach. Filamentary magnetic field coils are shown in light blue. The coloration of the magnetic surface is proportional to the local magnetic field strength.**

## Significance

This work contributes to the development of innovative new magnetic fusion concepts that will avoid the disruptive current-driven instabilities of the tokamak and thus lead to improved, more reliable reactors. These configurations should also offer improved confinement, heating efficiency, and a more compact design than more conventional stellarator designs.

## Publications

S. P. Hirshman, D. A. Spong, J. C. Whitson, D. B. Batchelor, B. A. Carreras, V. E. Lynch, and J. A. Rome, "Transport optimization and MHD stability of a small-aspect-ratio toroidal-hybrid stellarator," Phys. Rev. Lett. **80**, 528 (1998).

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# Three-Dimensional Magnetohydrodynamics Studies of Tokamak Fueling

*H. R. Strauss, New York University*
*W. Park, Princeton Plasma Physics Laboratory*

## Research Objectives

Tokamaks are the leading confinement concept for magnetic-fusion energy. The strong magnetic field in the donut-shaped tokamak confines the ionized hydrogen isotopes as they are heated to temperatures of over 10,000 eV and undergo fusion reactions. One of the objectives of present-day tokamak research is to develop efficient means of injecting cold fuel into the core of the tokamak to replace what is being burned. Recent experimental results indicate that if pellets of cold fuel are injected from the outside of the tokamak (the low field side), they are immediately expelled without reaching the center, while if the pellets are injected from the inside (i.e., the hole of the donut, or the high field side) the fuel does reach the high-temperature center where it is needed. Our objective was to reproduce this effect in a 3D simulation code to better understand and optimize it.

## Computational Approach

We use the MH3D code, which is a very flexible code system for solving the magnetohydrodynamics (MHD) equations in three space dimensions and time. Existing code options allow several representations of a plasma, ranging from a conducting fluid to a collection of interacting charged particles with long mean-free-paths. The most efficient way to represent general spatially localized perturbations is to use an unstructured numerical mesh. We call the recently developed unstructured-mesh, finite-element version of the MH3D code "MH3D++." It has been used to model both inside and outside pellet injection.

## Accomplishments

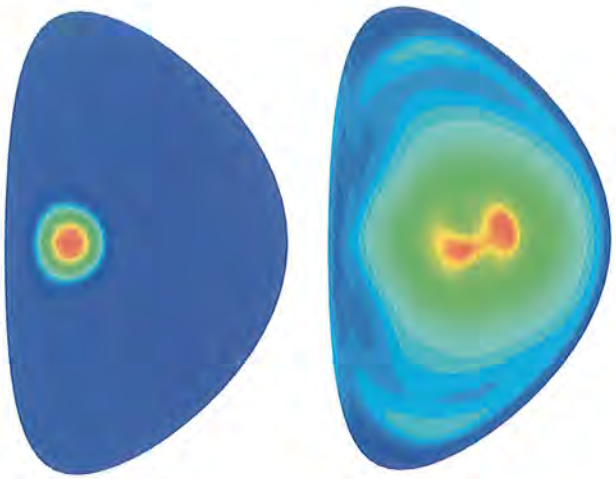
Nonlinear 3D simulation results show that the MHD forces will accelerate pellets, causing those injected on the low field side of a tokamak (i.e., the outside) to be expelled, and those injected on the high field side to be transported to the plasma center. This can also have the secondary effect of reconnecting the magnetic field into a reverse shear configuration. These computational results are in qualitative agreement with the experimental results from the ASDEX tokamak, which have shown that pellets injected on the inboard, low major radius edge suffered less loss, and were absorbed more completely into the plasma.

## Significance

Computational simulations provide a bridge between theory and experiment, helping to predict and optimize performance in future tokamak experiments.

## Publications

H. R. Strauss and W. Park, "Magnetohydrodynamic effects on pellet injection in tokamaks," Phys. Plasmas **5**, 2676 (1998).



**Simulated penetration of a fuel pellet, localized in three dimensions, into a tokamak.**

# Analysis of Data from Experiment E895 at the Alternating Gradient Synchrotron

*Dieter Best, Gulshan Rai, and Hans-Georg Ritter,*
*Lawrence Berkeley National Laboratory*

## Research Objectives

The physics goal of experiment E895 at Brookhaven National Laboratory's Alternating Gradient Synchrotron (AGS) is to study multiparticle correlations—especially collective effects—as well as particle production and other phenomena in a variety of heavy ion collisions (up to Au + Au) over a range of incident beam energies.

## Computational Approach

E895 relies heavily on the HPSS mass storage system and NERSC's Parallel Distributed Systems Facility (PDSF). All the raw data—consisting of several thousand files of about 500 MB each (about 2 TB total)—are stored on HPSS. The data analysis proceeds as follows: A UNIX shell script copies raw data from HPSS to the PDSF data vaults using FTP, making maximum use of the available disk space. A second shell script checks all workstations for active jobs. When an inactive workstation is found, a job is started and assigned to work on one of the raw data files. This way many files are analyzed in parallel. The output per job is around 100 MB, which is copied back to HPSS.

## Accomplishments

The total data at beam energies 2 and 4 AGeV were analyzed in 1998, along with about 10–20% of the data at 6 and 8 AGeV. The data processing will continue for at least another year. Concurrently a large number of simulated data will be analyzed for calibration purposes. Preliminary results for E895 have been presented at many conferences worldwide. Manuscripts on directed and radial flow will be submitted shortly to Physical Review Letters.

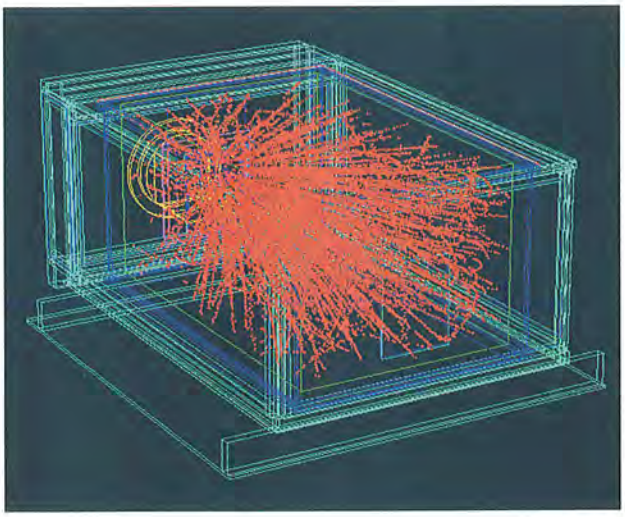
## Significance

E895, which began at the Equation of State Time Projection Chamber (EOS TPC) in the Berkeley Lab Bevalac, charts new territory at the AGS in two important respects. First, we can measure and identify most produced particles and nuclear fragment species over a substantial fraction of 4 pi solid angle. Second, our measurements will build upon the detailed excitation functions already measured by the EOS TPC and seamlessly extend them up to the higher beam energies.

## Publications

N. N. Ajitanand et al., "Collective flow in Au + Au collisions between 2–8 AGeV at AGS," Nuclear Physics A 638, **451** (1998).

http://cnr2.kent.edu/~e895/



**This central Au on Au collision at 4 GeV/nucleon kinetic energy comes from the January 1996 run of E895. Ionization clusters in the EOS Time Projection Chamber are shown in red. In this event, some 18,000 clusters are distributed over the 2+ million pixels of the TPC.**

# Semilocal String Formation

*Julian Borrill, University of California, Berkeley, and Lawrence Berkeley National Laboratory*

## Research Objectives

To model a possible state of the universe only a hundred billionth of a trillionth of a trillionth of a second ($10^{-35}$ second) after the Big Bang.

## Computational Approach

Using NERSC's Cray T3E, we were able to perform the first full three-dimensional simulations of semilocal string formation. We used a staggered leapfrog discretization of the quantum field equations on a $256 \times 256 \times 256$ periodic lattice. The illustrations show isosurfaces of the flux energy density measured as a fraction of the theoretical peak value.

## Accomplishments

Our simulations have shown that non-topological semilocal defects can be energetically stabilized by the back reaction of their gauge field on their scalar sector. We have also seen that the number density of semilocal strings formed depends on the relative strengths of the gauge to the scalar couplings, $\beta$, ranging from one-third the number density of topological cosmic strings for $\beta = 0.05$, to the classical stability analysis prediction of no semilocal string for $\beta \geq 1$.

## Significance

Semilocal strings are "worms" of energy that arise from a complex interaction of quantum matter and force fields during a phase transition, such as the fracturing of a unified force into its constituents in the very early universe.

The strings originate as open segments, with a north magnetic monopole on one end and a south monopole on the other. When two oppositely-oriented ends meet, the monopoles annihilate, forming either a closed loop (if the ends belong to the same string) or a longer segment (if the ends belong to different strings). In the first case, the string loops shrink under their own tension and rapidly disappear. In the second case, however, the strings build up into longer and longer objects, ultimately spanning the universe.

If semilocal strings do persist, then they would be a possible source of the primordial density perturbations needed to seed the formation of the gravitationally bound astronomical objects we observe today—from planets to clusters and superclusters of galaxies. In certain models they would also provide a mechanism for baryogenesis, generating the slight asymmetry between matter and antimatter in the early universe that allows us to exist today.

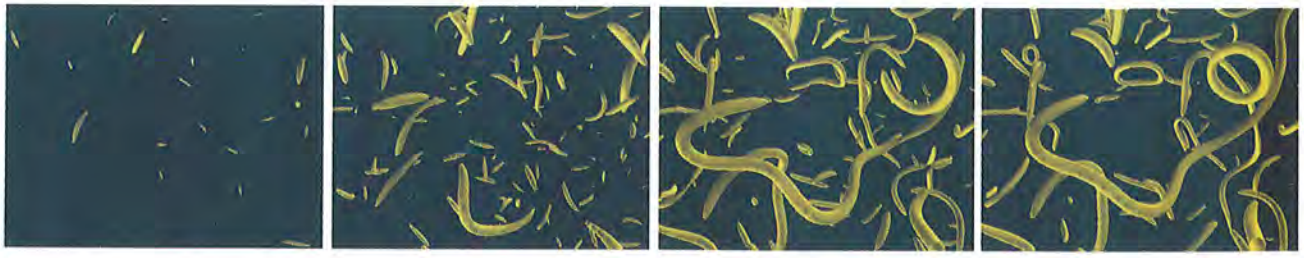
## Publications

Ana Achucarro, Julian Borrill, and Andrew R. Liddle, "The formation rate of semilocal strings," Phys. Rev. Lett. (submitted, 1998).

———, "The formation of non-topological string networks," Physica B (in press, 1998).

Julian Borrill, Ana Achucarro, and Andrew R. Liddle, "The rate of formation of semilocal strings," in *Proceedings of PASCOS-98* (World Scientific, 1988).

http://cfpa.berkeley.edu/~borrill/defects/semilocal.html



**A series of images from the simulation of semilocal strings evolving after the Big Bang. (Images by Kevin Campbell, NERSC Visualisation Group)**

# Three-Body Bound State Calculations Without Angular Momentum Decomposition

*C. Elster and W. Schadow, Ohio University*

## Research Objectives

The objective is to carry out few-nucleon calculations without the traditionally employed angular momentum decomposition.

## Computational Approach

The discretized Faddeev equation for a bound state (neglecting spin degrees of freedom) is an integral equation in 3 variables on a typical grid of $90 \times 109 \times 42$ (momentum magnitudes p,q, and angle between the momentum vectors). The eigenvalue equation for the bound state is solved iteratively by using Lanczos-type techniques, here the power method. The numerical treatment can be divided into two steps, namely calculation of the kernel, i.e., setting up the integral equation, and the iteration (on average 5) of the equation to obtain the eigenvalue. For the kernel, a two-body t-matrix (with the two-nucleon interaction as driving term) is obtained by solving a system of linear equations of the form $A \times x = b$, where A is typically a $4000 \times 4000$ matrix. This system is solved for about 100 different vectors b. The calculated t-matrix is then interpolated to the variables needed in the Faddeev equations. The interpolations are performed using cubic Hermite splines. The number of required interpolations is typically $1.8 \times 10^8$.

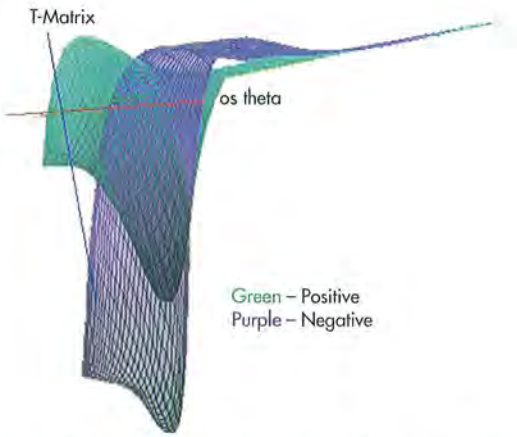
## Accomplishments

As a first test for the numerical accuracy of the solution of the Faddeev equation as a function of vector variables, we determined the energy eigenvalue of the bound system and compared our result with the one obtained in a traditional Faddeev calculation carried out on a partial wave truncated basis. We achieved excellent agreement (5 significant figures) between the two approaches, as well as excellent agreement with calculations in the literature.

For a stringent test of the three-dimensional wave function obtained from the Faddeev amplitude, we inserted it into the 3N Schrödinger equation and evaluated the accuracy with which the eigenvalue equation is fulfilled throughout the entire space where our solution is defined. We found that within the physical relevant momentum region, namely the magnitudes of the Jacobi momenta less than 10 $fm^{-1}$, the 3N Schrödinger equation is fulfilled with high accuracy by our numerical solution.

## Significance

Nuclear scattering at intermediate energies of a few hundred MeV requires quite a few angular momentum states in order to achieve convergence of scattering observables. Presently employed computational methods for 3N scattering at higher energies, using conventional partial-wave expansions, have intrinsic limitations, since with increasing energy the number of channel quantum numbers strongly proliferates, leading to increasing numerical difficulties with respect to accuracy and storage requirements.




**The real part of the half-shell two-nucleon t-matrix, T(q, $q_0$, x, E), as function of q and the angle x = cos(theta) between the momentum vectors q and $q_0$ at center-of-mass energies E = 25 MeV (green) and E = –25 MeV (purple). The vector $q_0$ describes the momentum of the incident nucleon. The employed nucleon-nucleon interaction is of Malfliet-Tjon type.**

This work represents an alternative computational approach by solving the Faddeev equations directly in a three-dimensional (3D) form in momentum space. The incorporation of the boundary conditions for three-body scattering does not change for 3D solutions of the Faddeev equations. In the integral from in momentum space, which we are using, they are automatically included. This approach will allow us to extend the investigations concerning the importance of three-nucleon forces in a computationally sound way to the energy regime up to 300 MeV, a regime of current experimental efforts at the Indiana University Cyclotron Facility (IUCF), the Kernfysisch Versneller Instituut (KVI), and the Research Center for Nuclear Physics (RCNP).

## Publications

C. Elster, W. Schadow, A. Nogga, and W. Glöckle, "Three body bound state calculations without angular momentum decomposition," Few-Body Systems (submitted, 1998).

C. Elster, W. Schadow, H. Kamada, and W. Glöckle, "Shadowing and antishadowing effects in a model for the n+d total cross section, Phys. Rev. C (in press, 1998).

http://xxx.lanl.gov/ps/nucl-th/9805018
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# Topics in Nonequilibrium Field Theory

*S. Habib, L. Bettencourt, G. Lythe, and C. Molina-Paris, Los Alamos National Laboratory*
*H. Mabuchi, California Institute of Technology*
*K. Shizume, University of Tsukuba*
*B. Sundaram, City University of New York*

## Research Objectives

Nonequilibrium field theory covers a variety of topics such as transport theory of quantum fields, nonequilibrium phase transitions, the nucleation and transport of topological defects and other nonlinear coherent structures, as well as fundamental issues such as the quantum-classical transition and the coherent control of quantum systems. Specific examples of current interest involving nonequilibrium dynamics of field theories include electroweak baryogenesis and topological transition rates, post-inflationary reheating in the early universe, and chiral condensates and evolution of the quark-gluon plasma in heavy-ion collisions. Due to advances in high-performance computing, quantitative attacks are now possible on a host of outstanding, but until recently quite intractable, problems in quantum field theories under nonequilibrium conditions. We are studying selected problems in the areas of baryon number violation, Relativistic Heavy Ion Collider physics, nonequilibrium phase transitions, quantum transport, and cavity quantum electrodynamics (QED), all of which share common features from the perspective of nonequilibrium quantum field theory.

## Computational Approach

We use several computational techniques in our research effort. Homogeneous and inhomogeneous mean-field dynamics codes solve for the evolution of a mean field self-consistently coupled to quantum fluctuations. These codes exist for Landau-Ginzburg theories, QED and scalar QED, and the linear sigma model. Applications include dynamics of phase transitions, disoriented chiral condensates, and soliton transport. The next class of codes are Langevin solvers for field theories in one, two, and three dimensions. They feature automatic inclusion of global and gauge constraints as well as extensive diagnostics for tracking nonlinear coherent structures such as domain walls and vortices. Finally, we have a suite of Schrödinger and master equation solvers based mainly on spectral split-operator methods. Applications include fundamental studies of quantum dynamics, quantum chaos, soliton transport, decoherence, cavity QED, and atomic optics.

## Accomplishments

In FY98, we concentrated to a large extent on porting code to the T3E. In addition, we completed three research projects on statistical mechanics of a new field theory, the quantum-classical transition in chaotic systems, and a new method to compute Lyapunov exponents.

**Field intensity profiles of a model for a two-dimensional superfluid at low temperature. The quasi-circular features are vortices, which evolve in time under the effect of their own interactions and interactions with the surrounding heat bath. The two vortices closest to each other have opposite charges and will annihilate each other in the course of the evolution.**

## Significance

In our work to date, we have shown that very high resolution simulations allow for the possibility of using new methods to study statistical mechanics of field theories, demonstrated how the classical limit of certain chaotic systems is obtained from quantum dynamics via decoherence, and developed a new, accurate method for the characterization of classically chaotic systems.

## Publications

A. Khare, S. Habib, and A. Saxena, "Exact thermodynamics of the Double Sinh-Gordon Theory in 1+1-dimensions," Phys. Rev. Lett. **79**, 3797 (1997).

S. Habib, K. Shizume, and W. H. Zurek, "Decoherence, chaos, and the correspondence principle," Phys. Rev. Lett. **80**, 4361 (1998)

G. Rangarajan, S. Habib, and R. D. Ryne, "Lyapunov exponents without rescaling and reorthogonalization," Phys. Rev. Lett. **80**, 3747 (1998)

http://gita.lanl.gov/people/salman/nersc

# Quantum Chromodynamic Quark Model Analysis of Hadron Elastic and Transition Form Factors

Chueng-Ryong Ji, Ho-Meoyng Choi, Ted Horton, and Daniel Arndt, North Carolina State University
Alex Pang, University of British Columbia

## Research Objectives

The main objective of this project is to calculate the form factors of hadrons and compare them with experimental data. For the lower and higher momentum transfer regions, we use a quantum chromodynamic (QCD) motivated relativistic quark model and perturbative QCD, respectively.

## Computational Approach

To simplify the spinor algebra, we have devised techniques which avoid manipulating any non-abelian matrices but instead involve only ordinary algebraic terms. We implemented our technique in Maple.

## Accomplishments

We have calculated various transition form factors and radiative decays of pseudoscalar, vector, and axial vector mesons using the light-front quark model. We extended the calculation to cover the analysis of mass spectra and mixing angles of meson nonets.

## Significance

Finding evidence of the quark and gluon effects inside hadrons and nuclei is one of the most significant goals of experiments at the Thomas Jefferson National Accelerator Facility (JLab). Our work provides theoretical guidance to achieve this goal.

## Publications

A. Szczepaniak, C.-R. Ji, and A. Radyushkin, "A consistent analysis of the O($\alpha_s$) corrections to the pion elastic form factor," Phys. Rev. D **57**, 2813 (1998).

S. J. Brodsky, C.-R. Ji, A. Pang, and D. Robertson, "Optimal renormalization scale and scheme for exclusive processes," Phys. Rev. D **57**, 245 (1998).

H. M. Choi and C.-R. Ji, "Relations among the light-cone quark models with the invariant meson mass scheme and the model prediction of $\eta$-$\eta'$ mixing," Phys. Rev. D **56**, 6010 (1997).

http://www.physics.ncsu.edu/people/ji.html

# Computational Nuclear Theory

*Volker E. Oberacker and A. Sait Umar, Vanderbilt University*

## Research Objectives

Describe theoretically the structure of atomic nuclei far from the stability line. Study the dynamics of nuclear fission, in particular viscosity of nuclear matter, via prompt muon-induced fission. Simulate relativistic heavy-ion collisions in a (3+1) dimensional classical string model.

## Computational Approach

In the nuclear structure project, we solve a set of self-consistent Schrödinger equations (HF + BCS / HFB) on a 2D lattice (axial symmetry) using the Cray J90; high accuracy is achieved by utilizing the Galerkin method with B-Splines. In the muon-induced fission project, we implement the time-dependent Dirac equation on a 3D Cartesian lattice using the B-Spline collocation method on the C90 and J90. The classical string calculations in (3+1) dimensions are solved using Monte Carlo techniques on the J90.

## Accomplishments

The main challenge for the theory of exotic nuclei near the proton or neutron drip lines is that the outermost nucleons are weakly bound (implying a large spatial distribution) and that these states are strongly coupled to the particle continuum. For these reasons, the traditional basis-expansion methods fail to converge. We overcome these problems by representing the nuclear Hamiltonian on a lattice. We have achieved high accuracy (on a moderate-size lattice) in calculating nuclear observables with the B-Spline Galerkin method. In the muon-induced fission project, we have demonstrated a correlation between the nuclear viscosity and a measurable quantity (muon attachment).

In the classical string simulations, we have for the first time added structure functions for the nucleons, and have also added mass quantization.

## Significance

The nuclear quantum many-particle problem represents a numerical challenge. Our mean-field nuclear structure calculations are carried out in connection with current and future experiments at DOE facilities such as the Oak Ridge Holifield Radioactive Ion Beam Facility (HRIBF) accelerator and the proposed ISOL (Isotope Separation On-Line) facility. The classical string model simulations provide the theoretical background for experiments to be carried out at Brookhaven's Relativistic Heavy-Ion Collider (RHIC).

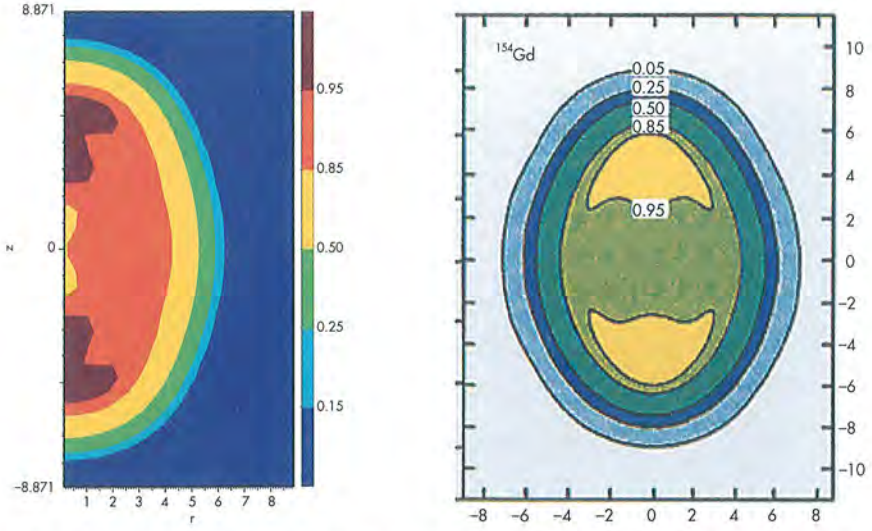
## Publications

D. R. Kegley, V. E. Oberacker, M. R. Strayer, A. S. Umar, and J. C. Wells, "Basis spline collocation method for solving the Schroedinger equation in axially symmetric systems," J. Comp. Phys. **128**, 197 (1996).

V. E. Oberacker et al., "Prompt muon-induced fission," in *Proceedings of the International Conference on Fission and Properties of Neutron-Rich Nuclei* (World Scientific, Teaneck, NJ, 1998).

D. E. Malov, A. S. Umar, and D. J. Ernst, "Hadronic structure functions as distributions of classical strings," Phys. Rev. C (submitted, 1998).

http://compsci.cas.vanderbilt.edu/NERSC.html
http://compsci.cas.vanderbilt.edu/QSM/qsm.html




**Proton density for 154Gd: (left) calculated with the 2D Skyrme Hartree-Fock + BCS pairing code; (right) measured charge distribution.**

# Transport Studies of Space-Charge Dominated Beams

*M. Reiser, R. A. Kishek, Institute for Plasma Research*

## Research Objectives

The focus of this research is on the transport of intense beams in the space-charge dominated regime, especially in circular geometries. The goal is to understand the mechanisms that affect the quality of such beams after transport through a realistic focusing lattice.

## Computational Approach

The main tool employed is the 3D and 2D3V versions of the particle-in-cell (PIC) code WARP, developed by Lawrence Livermore National Laboratory. We run mainly on the J90 cluster and the C90 machine, although we plan to move to the T3E for more intensive runs. The Crays are primarily used for long runs where the long-term (multi-turn) characteristics of the ring are under investigation.

## Accomplishments

Self-consistent simulations are used to examine and characterize the design of the University of Maryland Electron Ring. The PIC code is used to address highly nonlinear and complex issues that are inaccessible to simpler accelerator codes. These issues include the magnet fringe fields, image forces from the walls, and dispersion, among other things. All of these are important in the regime in which our ring is to be operated. Design sensitivities have been explored and show that, for reasonable deviations of the beam parameters from nominal design values, the emittance growth is acceptable and allows at least 20 turns for the maximum beam current (more turns can be achieved with lower currents). This is so even in the presence of known lens nonlinearities. Studies of the interaction of dispersion (caused by the bends) with the space charge show good agreement with latest analytic theories. These theories in turn will assist us in designing a dispersion-matching system if needed. Simulations of a prototype injector experiment have assisted in refining the experimental configuration. The simulations agree very well with the latest experimental observations and even reproduce the transverse density waves seen in the experiment. The evolution of these density waves is currently under investigation.

## Significance

An increasing number of applications, from heavy-ion fusion to high energy colliders (e.g., muon colliders, electron beam injectors for linear colliders, antiproton storage rings, and spallation neutron sources), demand higher-intensity beams, which places those beams in the space-charge dominated regime. Our simulation and experimental program offers a low-cost approach for understanding the complicated physics arising from such beams.

## Publications

S. Bernal, P. Chin, R. Kishek, Y. Li, M. Reiser, J. G. Wang, T. Godlove, and I. Haber, "Transport of a space-charge-dominated electron beam in a short-quadrupole channel," Phys. Rev. Special Topics: Accelerators and Beams **1** (1998).

R. A. Kishek, I. Haber, M. Venturini, and M. Reiser, "PIC code simulations of the space-charge dominated beam in the University of Maryland Electron Ring," in *Proceedings of the Workshop on Space-Charge Physics in High Intensity Hadron Rings* (Shelter Island, NY, 1998).

M. Reiser, S. Bernal, A. Dragt, M. Venturini, J. G. Wang, H. Onishi, and T. Godlove, "Design features of a small electron ring for study of recirculating space-charge dominated beams," Fusion Engineering and Design **32-33**, 293 (1996).

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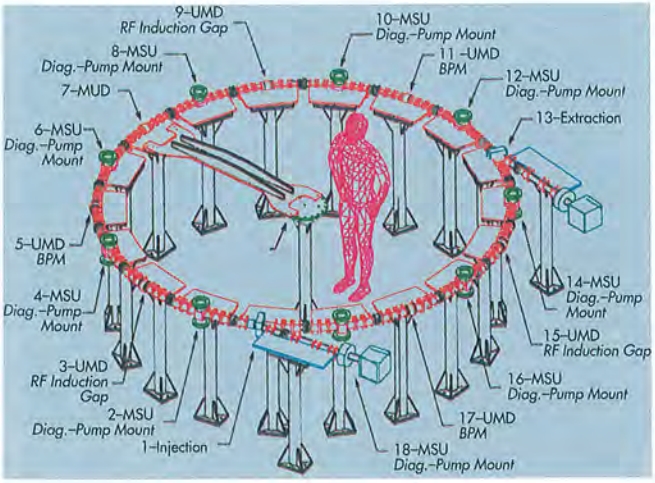



**Three-dimensional view of the University of Maryland Electron Ring.**

# Applications of Lattice QCD to Thermodynamics of Hadronic Matter and Properties of Hadrons

*D. K. Sinclair, J.-F. Lagae, and G. T. Bodwin,*
*Argonne National Laboratory*
*J. B. Kogut, University of Illinois*
*S. Kim, Sejong University*

## Research Objectives

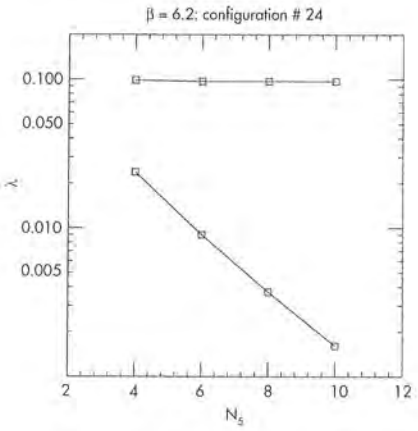
Application of improved actions for lattice quantum chromodynamics (QCD) to the study of the transition of hadronic matter to a quark-gluon plasma at high temperature. Development of such improved actions (with particular emphasis on the fermionic part of the action). Application of nonrelativistic QCD methods to studies of heavy quarkonium.

## Computational Approach

QCD is simulated on a discrete space-time lattice (lattice QCD) by formulating it as a molecular-dynamics problem and solving its time evolution numerically. A stochastic driving term is applied periodically to ensure ergodicity and rapid progress through phase space. The Dirac operator that describes quark propagation is inverted numerically using a conjugate gradient method. These computations have been ported to the T3E using the natural parallelism associated with the lattice and the locality of its interactions.

## Accomplishments

We are studying the properties of a new action for the quarks in lattice QCD—domain-wall fermions—where the 4-dimensional quarks are the boundary values of a 5-dimensional fermion field. This formulation formally has exact chiral symmetry as the 5th dimension becomes infinite. We are studying the low-lying eigenmodes of this theory at high temperatures, and the way the Atiyah-Singer index theorem is realized as the extent of the 5th dimension is increased. In addition we are studying mesonic excitations of the plasma phase. Preliminary results look promising.




**Lowest 2 eigenvalues of the domain-wall Dirac operator as functions of the 5th dimension on a configuration of topological charge 1.**

We have continued our simulations of lattice QCD, with an extra 4-fermion term allowing us to use massless quarks. This has enabled us to identify the 2-flavor finite-temperature phase transition and confirm that it is second order. The masslessness of the quarks has enabled us to extract preliminary values of one of the critical indices at this transition, and to get a clearer picture of the behavior of mesonic excitations as we cross this transition.

Our earlier calculations of the decay rates of S- and P-wave bottomonium have been extended to include the effects of light "sea" quarks. Earlier calculations in the quenched approximation predicted decay rates appreciably lower than experiment. Preliminary results indicate that the inclusion of light quarks is adequate to correct this.

Last year we introduced a new action for staggered quarks. Preliminary indications on small lattices indicated that this greatly reduced the flavor symmetry breaking at modest lattice spacing. We have now performed extensive calculations on a larger lattice, indicating that it does indeed considerably reduce flavor symmetry breaking, and we have quantified this improvement.

Finally, we have extended our studies of the low-lying eigenmodes of the staggered quark Dirac operator at high temperatures to larger lattices, and are checking the Atiyah-Singer index theorem, measuring the topological charge with an improved cooling scheme, and observing how the chirality density of the quark fields tracks the topological charge density of the gluon fields.

## Significance

The finite-temperature phase transition is expected to be observed in relativistic heavy ion collider experiments. It is also important for the understanding of the early universe. These measurements also allow us to understand the underlying dynamics of QCD. Improved actions allow the use of coarser lattices, thus reducing the computing requirements for simulations. Bottomonium decay rates can be compared with experiment. We also predict the decay rates for as yet unobserved decays.

## Publications

J.-F. Lagae and D. K. Sinclair, "Domain wall fermions at finite temperature," e-print hep-lat/9809134 (1998).

J. B. Kogut, J.-F. Lagae, and D. K. Sinclair, "Thermodynamics of lattice QCD with chiral four fermion interactions," Phys. Rev. D **58**, 034504 (1998); e-print hep-lat/9809052.

J.-F. Lagae and D. K. Sinclair, "Improved staggered quark actions with reduced flavour symmetry violations for lattice QCD," e-print hep-lat/9806014 (1998).

# Cosmic Microwave Background Data Analysis

*George Smoot and Julian Borrill, University of California, Berkeley, and Lawrence Berkeley National Laboratory*
*Andrew Jaffe, University of California, Berkeley, and UC Space Sciences Laboratory*

## Research Objectives

To develop the novel computational techniques necessary to extract fundamental cosmological parameters from cosmic microwave background (CMB) datasets.

## Computational Approach

Computing the maximum likelihood of signal to noise is the limiting step in extracting cosmology from CMB observations. Recent successful flights of the MAXIMA and BOOMERanG balloon-borne detectors have produced the largest CMB datasets to date. Both experiments plan to fly again in 1999, to be followed by the MAP and Planck satellites in 2001 and 2007. Over that time the maps produced will grow from tens of thousands to millions of points, and the time it takes to analyze them with the algorithms we currently use will correspondingly increase from hours to millions of years (see table). More efficient algorithms must be developed to process future datasets.

## Accomplishments

In the first year of this project we have developed a full-scale parallel implementation of the map-making and maximum likelihood analysis algorithms on the NERSC T3E. We are now using them to process data from the MAXIMA-1 and BOOMERanG North America flights, providing both insights into the cosmos and benchmark results against which to measure the performance of the new algorithms we will have to develop.

## Significance

The cosmic microwave background (CMB) is the faintest echo of the Big Bang. It is what is left over when all the radiation from astronomical objects is subtracted from what we observe. Despite the CMB's stunning uniformity—isotropic to a few parts in a million—it is the tiny perturbations in the CMB that contain its unprecedented view of the early universe. Already present before gravitationally bound objects had formed, these temperature differences are an imprint of the primordial density fluctuations that seeded everything from planets to galaxy clusters and superclusters. As such they promise to be an exceptionally powerful discriminant between competing cosmological models.

Given a map of the sky temperature, and knowing the statistical properties of noise that went into it, we can now calculate the most likely underlying signal, and by how much it is the most likely.

## Publications

George Smoot and Douglas Scott, "The cosmic background radiation," European Physical Journal C **3**, 1 (1998); astro-ph/9711069.

J. R. Bond, A. H. Jaffe, and L. Knox, "Radical compression of cosmic microwave background data," Astrophysical Journal (submitted, 1998); astro-ph/9808264.

Julian Borrill, "Power spectrum estimators for large CMB datasets," Physical Review D (in press, 1998); astroph/9712121.

http://aether.lbl.gov/
http://cfpa.berkeley.edu/group/cmbanalysis/

### Computational Resources for CMB Analysis

| Dataset | Map Size | Memory | Flops | Serial Time | T3E Time (Nodes) |
|---|---|---|---|---|---|
| BOOMERanG N. America | 30,000 | 15 GB | $5 \times 10^{15}$ | 8 months | 40 hours (64) |
| MAXIMA-1 | 40,000 | 25 GB | $10^{16}$ | 16 months | 40 hours (128) |
| MAXIMA-2 | 80,000 | 100 GB | $10^{17}$ | 13 years | 4 days (512) |
| BOOMERanG Antarctica | 120,000 | 240 GB | $3 \times 10^{17}$ | 40 years | 6 days (1024) |
| MAP | 1,000,000 | 16 TB | $2 \times 10^{20}$ | 25,000 years | |
| Planck | 10,000,000 | 1600 TB | $2 \times 10^{23}$ | 25,000,000 years | |

**Computational resources required to analyze CMB datasets using the quadratic estimator algorithm, assuming 20 signal components and 5 iterations on a single (serial) 250 MHz processor and the indicated number of T3E nodes running at the equivalent of 600 MHz. For an $N_p$ pixel map, the amount of RAM memory needed scales as $N_p^2$, and the number of floating point operations as $N_p^3$.**

# Weak Matrix Elements with Domain Wall Quarks

*Amarjit Soni, Thomas Blum, Christopher Dawson, and Matthew Wingate, Brookhaven National Laboratory*

## Research Objectives

We are in the process of setting up a comprehensive framework for using lattice gauge methods with domain wall quarks (DWQ) for the calculation of weak matrix elements.

## Computational Approach

The basic ingredient in the method is a calculation of the quark propagator. The novel element in our method is that it requires introduction of a fictitious fifth dimension. The T3E-600 and T3E-900 machines at NERSC have been used for these computations.

## Accomplishments

We have demonstrated that DWQ start to exhibit the crucial symmetries of the continuum theory (chiral symmetries) with a modest extent in the fifth dimension, i.e., even when the number of lattice sites in the extra dimension is as few as about 10. In the work finished so far, we have obtained a number of key results including a calculation of the important matrix element $B_K$ and the calculation of the strange quark mass. Our results show that DWQ have significantly improved scaling behavior: the discretization errors are $O(a^2)$ and not $O(a)$. Our data indicate that the good scaling and chiral behavior of DWQ more than compensates for the added cost of the extra dimension.

## Significance

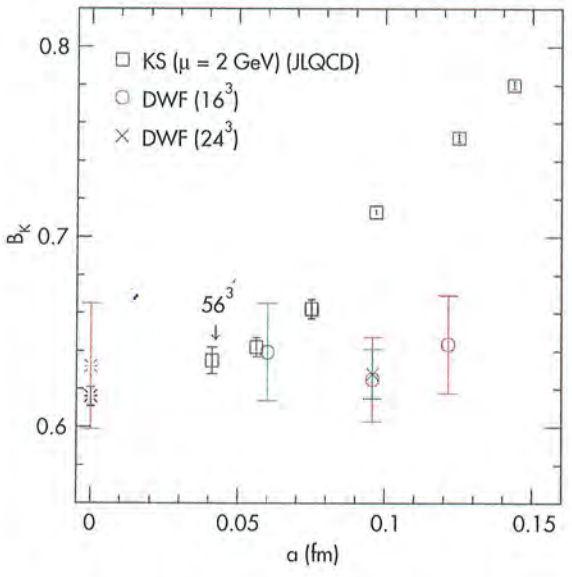
This work opens up an entirely new method for attacking some of the basic challenges in particle physics computations. For many decades, we have not been able to understand the strength of some simple reactions such as $K$ decays to $\pi\pi$. Consequently, we have been unable to test the Standard Model of Elementary Particles through existing data and with improved experiments that are now under way. Using DWQ, we are now in the process of calculating the crucial CP violation parameter $\epsilon'/\epsilon$. Successful completion of this calculation should enable us to test for clues for the new physics that lies beyond the Standard Model.

## Publications

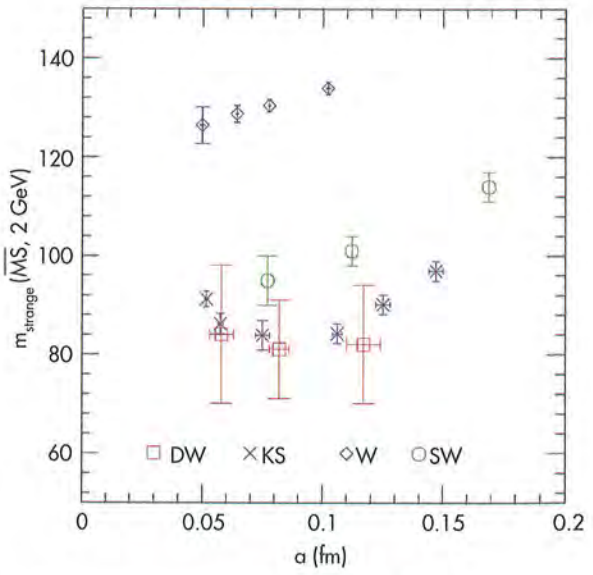
T. Blum and A. Soni, "QCD with domain wall quarks," Phys. Rev. D **56**, 174 (1997). http://publish.aps.org/ejnls/prdfetch/abstract/PRD/V56/P00174_1/

T. Blum and A. Soni, "Domain wall quarks and kaon weak matrix elements," Phys. Rev. Lett. **79**, 3595 (1997). http://ojps.aip.org/prlo/top.html

T. Blum, A. Soni and M. Wingate, hep-lat/9809253.




**The kaon *B* parameter. The Kogut-Susskind result is from the JLQCD research group. DWF indicate improved scaling in this case.**




**The strange quark mass after matching to the $\overline{MS}$ scheme.**

# Testing Improved Actions for Kogut-Susskind Quarks

*Doug Toussaint, University of Arizona*

## Research Objectives

Due to computational limitations, lattice calculations of quantum chromodynamics (QCD) are currently done with grids that are fairly coarse relative to the interesting physics. This causes several kinds of distortion in the results, including a breaking of the symmetry under interchange of different kinds of quarks with the Kogut-Susskind approach to putting the quarks on the lattice. Differences in the masses of various members of the pion multiplet are symptoms of this problem. We are studying variants of the standard discretization designed to reduce these artifacts of nonzero grid spacing.

## Computational Approach

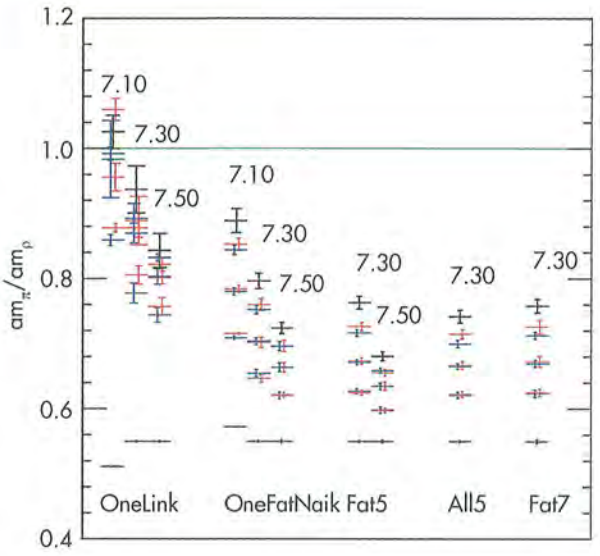
Sample configurations of the gluon field were generated using the refreshed molecular dynamics algorithm. Amplitudes for mesons to propagate in these background fields were computed by the conjugate-gradient algorithm, using a red-black decomposition of the matrix to reduce the size of the problem. The code is the MILC (MIMD Lattice Computation) collaboration's QCD code, which runs on a variety of MIMD (multiple instruction, multiple data) machines, in this case on the NERSC T3E.

## Accomplishments

We have tested several discretizations of the Dirac equation on a set of fairly coarse lattices, and tested four of these discretizations on a finer lattice. Some of the discretizations tested show promise for use in large-scale calculations, reducing the flavor-symmetry breaking by better than a factor of 2. We find that it is necessary to examine the nonlocal pions, as well as the local pions checked in previous studies, to get an accurate picture of the extent of flavor-symmetry breaking.

## Significance

Studies such as this one lay essential groundwork for numerical studies that will eventually compute the properties of strong interactions at high temperatures, the masses of familiar and as-yet-undiscovered strongly interacting particles, and matrix elements necessary for relating fundamental parameters to experimental results.




**Masses of different members of the pion multiplets with various lattice actions. The numbers at the top are the gauge coupling constant, and the labels at the bottom identify the action. The goal is to identify actions for which all of the red and blue lines cluster near the black lines near the bottom.**

## Publications

K. Orginos and D. Toussaint, "Testing improved actions for dynamical Kogut-Susskind quarks," Phys. Rev. D (in press, 1998).

———, "Tests of improved Kogut-Susskind fermion actions," presented at the Lattice-98 Symposium, Boulder, Colorado, July 1998.

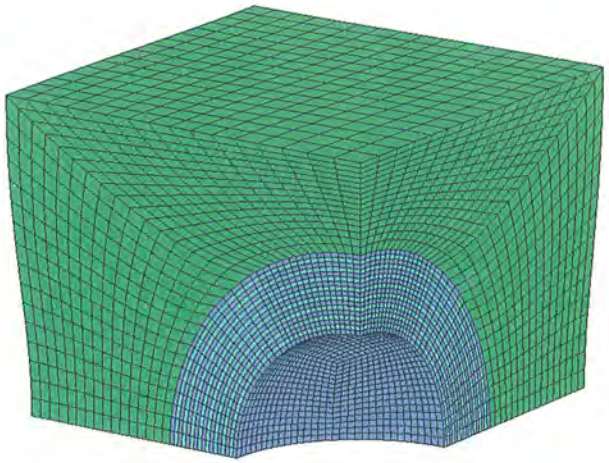
http://www.physics.arizona.edu/~doug

# Parallel Multigrid Solver for Unstructured Finite Element Method Meshes in Solid Mechanics

*Mark Adams and James W. Demmel,*
*University of California, Berkeley*

## Research Objectives

We are interested in the efficient application of the inverse of large sparse operators from unstructured finite element applications. This research will develop scalable algorithms for use in implicit codes for the simulation of complex physical systems, and will develop a prototype implementation of a promising multigrid algorithm for unstructured meshes. This algorithm* has the advantage of the potential robustness of classical (geometric) multigrid methods, but without requiring that the user provide coarse meshes and operators. This solver will thus provide a solution to the largest computational bottleneck of some implicit unstructured finite element codes, such as solid mechanics, and potentially any other sparse finite element discretization.



**This model of a sphere within a soft material with a parameterized mesh is used for scalability studies. The sphere is steel with a Poisson ratio of 0.3, and the soft material is rubber with a Poisson ratio of 0.49 and an elastic modulus $10^{-4}$ that of the sphere. The problem, here discretized to 80,000 degrees of freedom, is run on the number of processors required to keep about 25,000 equations on each processor.**

## Computational Approach

We rely heavily on public domain libraries. We use PETSc for our numerical primitives and parallel code development environment, ParMetis and Metis for our mesh partitioning needs, and FEAP for our finite element "client." All our codes are based on MPI, and our original software is written in C++. We use a Cray T3E for code development testing and numerical studies.

## Accomplishments

To date we have been able to solve systems of up to 5 million degrees of freedom, and we hope to solve a 10-million-degree-of-freedom system in the near future. This past year we extended our work to indefinite systems that arise from contact problems in which the contact constraint is applied with Lagrange multipliers. We also applied our solver to larger problems and non-linear problems in plasticity and finite deformation. We developed a new parallel maximal independent set algorithm that won the best student paper competition at the Fifth Copper Mountain Conference on Iterative Methods.

## Significance

This work has the potential to provide the fastest and most economical solution to the largest and most expensive computational problem in many implicit simulations of complex physical phenomena. These simulations enable testing of products such as automobiles more economically and quickly than laboratory crash testing, and enable performance assessment of products such as nuclear weapons which cannot be laboratory tested.

## Publications

Mark Adams, "Heuristics for the automatic construction of coarse grids in multigrid solvers for finite element matrices," Technical Report UCB//CSD-98-994, University of California, Berkeley (1998).

———, "A parallel maximal independent set algorithm," in *Proceedings of the Fifth Copper Mountain Conference on Iterative Methods* (Copper Mountain, Colorado, April 1998).

http://www.cs.berkeley.edu/~madams/prometheus.html

*Herve Guillard, "Node-nested multi-grid with delaunay coarsening," Technical Report 1898, Institute National de Recherche en Informatique et en Automatique (1993); also independently developed by Chan and Smith.

# Direct Numerical Solution of the Continuum Three-Body Coulomb Problem

M. Baertschy and D. Byrum, University of California, Davis
W. Isaacs and C. W. McCurdy, Lawrence Berkeley National Laboratory
T. Rescigno, Lawrence Livermore National Laboratory

## Research Objectives

Our group's research centers on low-energy electron scattering from small molecules, an important problem in environments such as semiconductor processing plasmas, materials development, and toxic waste remediation. The physically important process of electron impact ionization, where one or more electrons are knocked out of the target by the incoming electron, has not been formally solved for even the simplest case of electron-hydrogen atom scattering. We are developing an approach to this continuum three-body Coulomb problem, and seek the first direct numerical solution without nonphysical approximations.

## Computational Approach

We treat the full 6-dimensional Schrödinger equation for the electron-hydrogen system. Expanding the wave function in angular momentum results in sets of coupled 2D differential equations. The use of exterior complex scaling, whereby the radial coordinates are mapped onto a complex contour, formally turns the infinite range problem into a finite range problem. We discretize the radial coordinates using variable spacing finite differences, resulting in a large sparse matrix problem. We solve the full-coupled problem using an iterative method, the conjugate gradient squared algorithm, with a block-diagonal preconditioner. The angular momentum expansion provides a natural framework for distributing the solution vector across processors. By using a parallel version of SuperLU, a direct sparse solver, to apply the preconditioner, we can also distribute individual angular momentum blocks across several processors. This code was developed on the T3E using MPI.

## Accomplishments

We have developed a code able to generate the numerical wave functions describing electron impact ionization of hydrogen for a range of scattering energies. From these wave functions we can extract scattering cross sections that describe how energy is shared between the two outgoing electrons after ionization.

**A sample partial-wave component of the full e-H wave function. The peaks along the right edge correspond to excitation of the hydrogen atom. The outgoing waves represent ionization flux.**

## Significance

These are the first accurate calculations of electron-hydrogen ionization singly differential (energy sharing) cross sections and, indeed, represent the first "exact" solution to a quantum mechanical three-body Coulomb problem. These calculations lay the groundwork for one approach to incorporate ionization into our group's electron-molecule calculations.

## Publications

C. W. McCurdy and T. N. Rescigno, "Calculating differential cross sections for electron-impact ionization without explicit use of the asymptotic form," Physical Review A **56**, R4369–R4372 (1997).

C. W. McCurdy, T. N. Rescigno, and D. A. Byrum, "An approach to electron-impact ionization that avoids the three-body Coulomb asymptotic form," Physical Review A **56**, 1958–1969 (1997).

T. N. Rescigno, M. D. Baertschy, D. A. Byrum, and C. W. McCurdy, "Making complex scaling work for long-range potentials," Physical Review A **55**, 4253–4262 (1997).

# Adaptive Mesh Refinement in Complex Geometries

*P. Colella, D. Graves, D. Modiano, J. Pilliod, and D. Serafini, Lawrence Berkeley National Laboratory*

## Research Objectives

The goal of this research is to develop library and application software for the solution of partial differential equations in complex geometries of engineering interest with moving boundaries. Our main interest is in the equations related to incompressible, low Mach number and compressible fluid dynamics and combustion problems.

## Computational Approach

Our representation of complex geometry is centered around an embedded boundary method, in which the irregular domain boundary cuts away from a regular, Cartesian mesh. This allows us to use proven high-accuracy solution-adaptive finite difference methods in regions of the domain away from the boundary. Because most of the domain will be away from the boundary, the computational efficiency of the overall algorithm will not be penalized by the additional effort expended at the cut cells.

## Accomplishments

We designed and implemented a library for the representation and manipulation of embedded boundary data. Using this library, we implemented an embedded boundary algorithm to solve Poisson's equation and the diffusion equation, and a solution-adaptive embedded boundary algorithm for high-speed inviscid compressible gas dynamics.

## Significance

This research will enable routine high-resolution simulations of problems in realistic engineering geometries, in applications such as diesel engine cylinder combustion, inkjet printers, explosion dynamics in confined chambers, biological microelectromechanical systems, and industrial burners.

## Publications

M. Day, P. Colella, M. Lijewski, C. Rendleman, and D. Marcus, "Embedded boundary algorithms for solving elliptic PDE's on complex domains," Report LBNL-41811, Lawrence Berkeley National Laboratory (1998).

H. Johansen and P. Colella, "A Cartesian grid embedded boundary method for Poisson's equation on irregular domains," Journal of Computational Physics **147**, 60–85 (1998).

H. Johansen, "Cartesian grid embedded boundary finite difference methods for elliptic and parabolic partial differential equations on irregular domains," Ph.D. thesis, University of California, Berkeley (1997).

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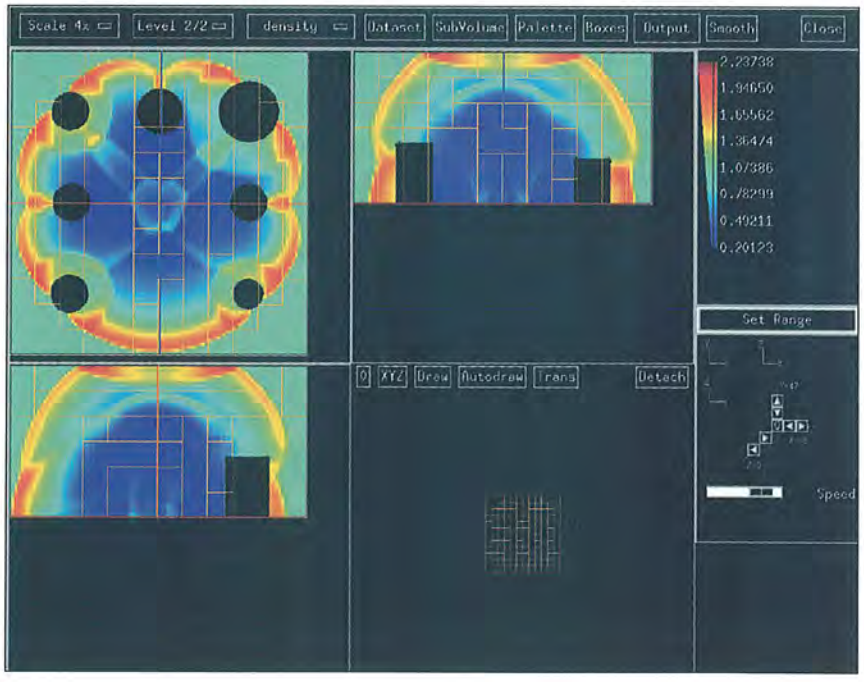



**Solution-adaptive simulation of an explosion in a confined chamber with cylindrical obstacles. Density is shown. Areas of ambient density are blue, areas of higher density are red. The upper left plot is a cross-section at the floor of the room. The upper right and lower left plots are perpendicular vertical cross-sections through the center of the room.**

# A Numerical Study of Acceleration-Driven Fluid Interface Instabilities

*J. Glimm, X.-L. Li, D. Saltz, and D. Sendersky,*
*State University of New York at Stony Brook*

## Research Objectives

When the surface of contact between two distinct materials is unstable, small random disturbances on the surface will develop into interpenetrating structures, such as fingers, jets, droplets, and bubbles. These structures are complex and chaotic, and together they comprise a mixing layer. A scientific theory is required to capture the unresolvable microstructure of mixing layers in a macroscopic framework amenable to computer simulation. The simulation data is crucial, as numerical data reveal far more information than is accessible in physical experiment. We seek to develop such a theory and to demonstrate its validity by comparison with computer simulation and physical experiment.

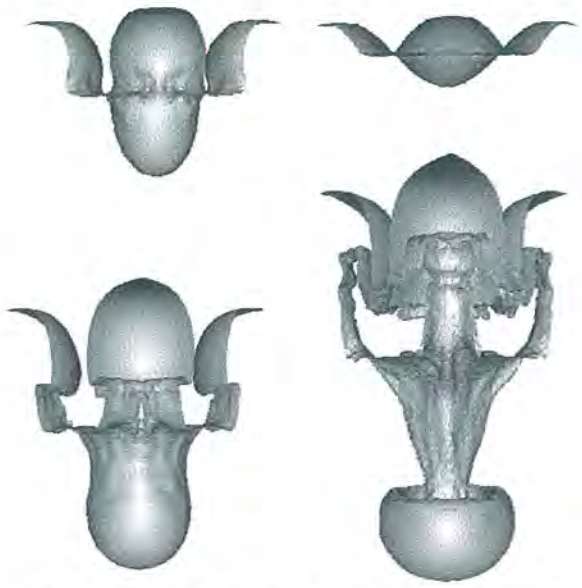
We are studying the fluid mixing layers that form in the late stages of acceleration-driven hydrodynamic instabilities, such as the Rayleigh-Taylor and Richtmyer-Meshkov instabilities. Our major objective is a numerical study of the late-time development of chaotic mixing and turbulence in order to obtain a definitive computational dataset for the validation of two-phase flow and turbulence models.

## Computational Approach

We use a mature, high-resolution, 3D hydrodynamics code, known as FronTier, to perform direct numerical simulations of the formation and growth of fluid mixing layers. The FronTier code is based on front tracking, a numerical method in which surfaces of discontinuity are given explicit computational degrees of freedom; these degrees of freedom are supplemented by degrees of freedom representing continuous solution values at regular grid points. This method is ideal for problems in which discontinuities are an important feature, and especially where their accurate computation is difficult by other methods. The FronTier code has been extensively tested on the NERSC T3E for complex geometry evolution, numerical stability, and data communication.

## Accomplishments

We have made some important progress in the numerical study of the 3D Rayleigh-Taylor and Richtmyer-Meshkov instabilities. First, we have fully implemented a new 3D tracking algorithm, known as the grid-based front tracking algorithm. This robust algorithm has enabled the FronTier code to handle complex 3D interface geometry easily and accurately. We have also tested a hybrid method that mixes the classical grid-free front tracking and the new algorithm. Other important progress has been made in the numerical study of strong shock-contact interactions in the Richtmyer-Meshkov instability. We have modified the interface-interior coupling method to accommodate a numerically accurate passage of the shock front through the interface for any shock strength. This improvement makes it possible for the FronTier simulation of the strong shock-contact interaction in NOVA laser-induced fusion and the study of the 3D Richtmyer-Meshkov instability on the T3E computer.



**Three-dimensional evolution of Rayleigh-Taylor instability from a single Fourier mode.**

## Significance

Mixing layers are of fundamental importance in natural phenomena such as supernova explosions, in industrial settings such as petroleum flow in pipelines, and in technological applications such as inertial confinement fusion (ICF), where they are known to be a major limiting factor in the performance of ICF capsules.

## Publications

J. Glimm, D. Saltz, and D. H. Sharp, "Two-phase modeling of a fluid mixing layer," J. Fluid Mech. (in press, 1998).

J. Glimm, J. W. Grove, X.-L. Li, K.-M. Shyue, Q. Zhang, and Y. Zeng, "Three dimensional front tracking," SIAM J. Sci. Comp. **19**, 703–727 (1998).

J. Glimm, J. Grove, X.-L. Li, D. C. Tan, "Robust computational algorithms for dynamic interface tracking in three dimensions," SIAM J. Sci. Comp. (submitted, 1998).

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

# Endogenous Technological Change in Modeling the Global Energy System

*A. Gritsevskii, G. MacDonald, S. Messner, and N. Nakicenovic, International Institute for Applied System Analysis (IIASA)*

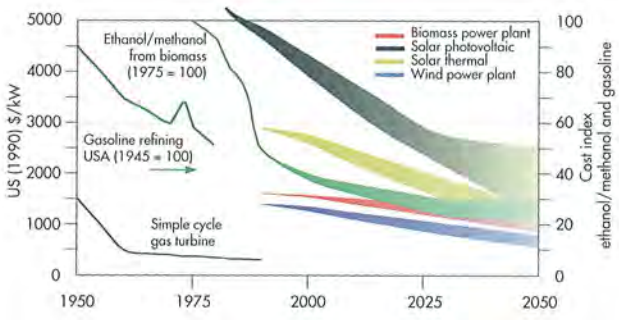
## Research Objectives

The aim of this project is to create a new version of the global energy system model MESSAGE that endogenizes the introduction of advanced energy technologies.

Investment costs of energy technologies decrease as their installed capacities increase, but the relationship is nonconvex and therefore difficult to include endogenously in an energy model. Our work represents a first attempt to combine these nonconvex technological learning effects with a full-sized, global, bottom-up energy-systems model that includes detailed regional resolution and technological representation. The model comprises 11 world regions grouped according to levels of economic development and geographic location. Over 100 technologies from extraction to end-use are also included. The advanced model developed in this project will have the capability to analyze the diffusion of individual technologies, as well as the formation of interactive technology clusters.

## Computational Approach

From a mathematical perspective, the problem is one of a large nonconvex stochastic global optimization. It has a well-specified structure, making a solution feasible. Our algorithm combines a global adaptive search algorithm with a simultaneous stochastic drawing approach that makes it possible to approximate the original problem by sequences of linear optimization problems. Uncertainties play a very important role in the proposed approach and are treated by using a nonsymmetric utility (risk) function. The global optimization algorithm running in parallel was developed specifically for this project.




**Technology learning curves: Cost improvements per unit installed capacity in U.S. dollars (1990) per kW versus cumulative installed capacity in MW for photovoltaics, wind, and gas turbines. Sources adapted from MacGregor et al., 1991; Christiansson, 1995; Grubler, 1998.**

## Accomplishments

During the first stage of the project, a global one-region world model was implemented and tested in the NERSC T3E environment. This model incorporates a technological learning mechanism (increasing returns) for selected technological clusters (mainly hydrogen-based technologies, synthetic fuels, wind, and solar). An extensive set of computer runs was performed in order to identify potential interrelations between technological clusters and their sensitivities to model assumptions, and to develop alternative scenarios of new research, development, and demonstration (RD&D) investments.

## Significance

This experiment (using NERSC computer facilities) represents a unique opportunity to achieve a significant breakthrough in modeling and evaluating alternative strategic long-term energy policies affecting global and regional development and the environment. Results of the proposed experiment have the potential to significantly impact recommendations for national RD&D policies, early investment decisions in new technologies, and, ultimately, the future condition of the global environment.

## Publications

A. Gruebler and A. Gritsevskii, "A model of endogenous technological change through uncertain returns on learning (RD&D and investments)," presented at the International Workshop on Induced Technological Change and the Environment, 26–27 June, International Institute for Applied Systems Analysis, Austria; The Economical Journal (submitted, 1998).

S. Messner, A. Golodnikov, and A. Gritsevskii, "A stochastic version of the dynamic linear programming model MESSAGE II," Energy **21**, 9, 775–784 (1996).

N. Nakicenovic, "Technological change and learning," Perspectives in Energy **4**, 173–189 (1997).

http://www.iiasa.ac.at/Research/ECS/

# Correlated Wave-Functions and Long-Range Order in Lattice Models of Strongly Interacting Electrons

*J. E. Gubernatis, M. Guerrero, and G. Ortiz,*
*Los Alamos National Laboratory*

## Research Objectives

Our objective is to study lattice models of strongly interacting electrons using the constrained-path quantum Monte Carlo (CPMC) method. Of specific interest are those models that might display long-range, superconducting pairing correlations.

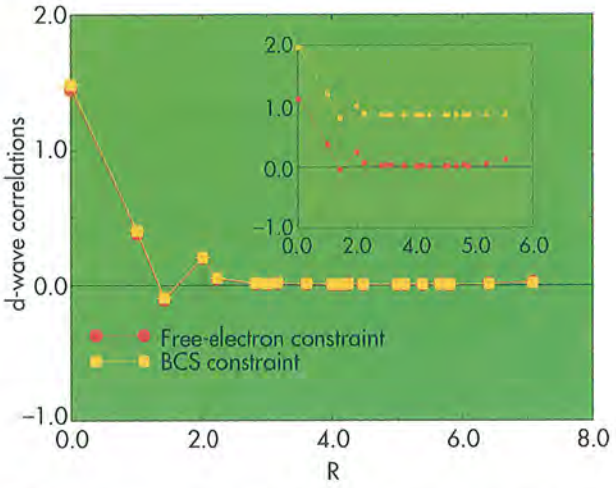
## Computational Approach

We use an improved and parallelized version of the CPMC method. The CPMC method is a zero temperature algorithm that projects a ground-state wave function from a known initial parent state by a branched random-walk in an overcomplete manifold of Slater determinants. The infamous "fermion sign problem," which causes the variances of the computed quantities to grow exponentially with the number of projection steps, is avoided by using only those determinants that satisfy a certain constraint. If the constraining state is the exact ground state, then the solution is exact; otherwise, it is approximate. Mathematical analysis and benchmark calculations indicate that the results are extremely accurate and almost independent of parent-state quality.

## Accomplishments

We developed a formulation of the CPMC method that uses constraining states involving many-body correlations. It allows us to implement a whole family of generalized mean-field states as constraints, including various superconducting ones, and to study potential biases in physics that might be produced by the constraining state. In particular, we focused on the phase diagram of the two-dimensional repulsive Hubbard model, calculated superconducting pairing correlations using a Bardeen-Cooper-Schrieffer (BCS) state as the constraining state, and compared the results with the case where a free-electron state is used. We found that the results are independent of the constraining state and indicate the absence of off-diagonal long-range order (ODLRO) in the d-wave superconducting channel for any hole doping and interaction strength.

This new formulation also gives us added confidence in the method. Presently, we are exploring other models and geometries of strongly interacting electrons, like the n-leg Hubbard ladders, where supposedly an enhancement of superconducting d-wave pairing correlations exists. Another extension of the method that is envisaged is the inclusion of external magnetic fields. Because the states we now want to sample are complex valued, a nontrivial extension of the method is needed to avoid the "fermion phase problem."




**The d-wave superconducting pairing correlation function is a function of distance between the pairs. For two different parent states, free-electron and BCS, the CPMC method gives essentially the same final result. The inset shows the different strengths of the pairing correlations in the parent states.**

## Significance

The lack of clear numerical evidence of ODLRO upon doping suggests that the well-studied two-dimensional repulsive Hubbard model is an inappropriate one to describe the superconducting phase of the high-temperature superconducting materials. Moreover, with the clear numerical evidence of antiferromagnetism at half-filling, this lack also weakens the case that the Hubbard model supports the SO(5) phenomenology.

## Publications

S. Zhang, J. Carlson, and J. E. Gubernatis, "A constrained path quantum Monte Carlo method for fermion ground states," Phys. Rev. Lett. **74**, 3652 (1995).

———, "Pairing correlations in the two-dimensional Hubbard model," Phys. Rev. Lett. **78**, 4486 (1997).

M. Guerrero, G. Ortiz, and J. E. Gubernatis, "Correlated wave-functions and the absence of long range order in numerical studies of the Hubbard model," Phys. Rev. B (in press, 1998).

http://bifrost.lanl.gov/~jeg/jeg.html

# MPP Calculations of Metastability in Materials Science and Stochastic Parallelization

*M. A. Novotny and G. Korniss, Florida State University*

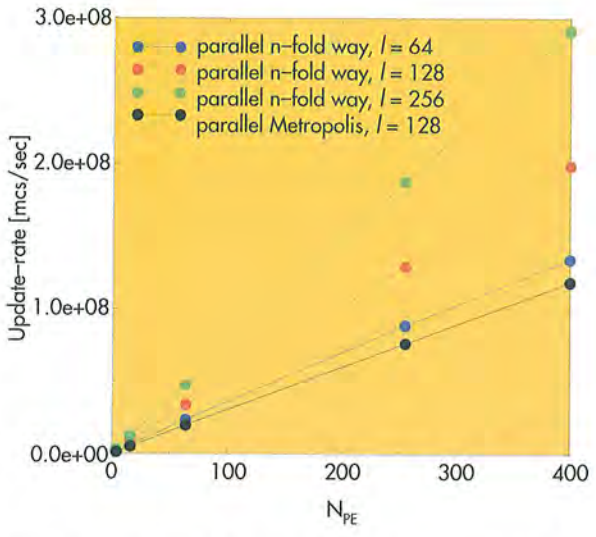
## Research Objectives

We have used both J90 time and T3E time to perform simulations related to magnetization switching of magnetic materials. Although the J90 time is important for our calculations (due to the available libraries and vectorization), we will describe here only our research from the T3E. On the T3E we implemented a massively parallel Monte Carlo algorithm for simulating the metastable decay in the kinetic Ising model. Our goal was two-fold. First, we studied the applicability and efficiency of stochastic parallelization. Second, we investigated the effects of finite (smaller than the system size) observation windows in large systems in the different decay regimes of the model.

## Computational Approach

Lubachevsky presented an efficient method for parallel discrete event simulation without changing the underlying dynamics of the system. He also proposed a way to incorporate a rejection-free (*n*-fold way) version of the standard Metropolis update-scheme, possibly further contributing to speedup.

To study magnetization switching in the two-dimensional Ising ferromagnet, we implemented this algorithm on the Cray T3E parallel architecture and employed the SHMEM-library routines for message passing. We experimented with a synchronous integer-time and an asynchronous continuous-time parallel version of the *n*-fold way algorithm, where each processing element (PE) carries an $l \times l$ block of spins. In general, different PEs have different local simulated times, and the algorithm deals with it in a conservative fashion to ensure causality.




**Update-rate as a function of the total number of processing elements, $N_{PE}$, with fixed block-size *l*.**

## Accomplishments

We found that the asynchronous algorithm with continuous time-increments suits the T3E distributed-memory architecture best, since global barrier synchronization is completely avoided. Despite a relatively low utilization and an intricate relationship between the average simulated time-increment and the size of the spin blocks on each PE, we found that for sufficiently large *l*, the algorithm still outperforms its corresponding parallel Metropolis (non-rejection-free) counterpart. We tested our code up to 400 PEs and found excellent (almost linear) scaling with fixed block size *l* (see figure). We have published a conference paper with preliminary results, and are in the process of writing a longer article.

## Significance

We demonstrated that it is possible to implement an efficient code for stochastic simulation on a distributed-memory machine, where the pattern of communication between the underlying PEs is completely unpredictable. The implementation becomes highly efficient for simulating large systems.

## Publications

G. Korniss, G. Brown, M. A. Novotny, and P. A. Rikvold, "Hard simulational problems in the modeling of magnetic materials: Parallelization and Langevin micromagnetics," in *Computer Simulation Studies in Condensed Matter Physics XI*, edited by D. P. Landau and H.-B. Schuttler (Springer-Verlag, New York, in press, 1998).
http://xxx.lanl.gov/abs/cond-mat/9803118

M. A. Novotny, G. Brown, and P. A. Rikvold, "Computer simulations of thermal switching in small-grain ferromagnets," Mat. Res. Soc. Symp. Proc. (in press, 1998).
http://xxx.lanl.gov/abs/cond-mat/9806083

G. M. Buendia, E. Machado, and M. A. Novotny, "Compensation temperature of a mixed Ising ferrimagnetic model in the presence of external magnetic fields," Mat. Res. Soc. Symp. Proc. (in press, 1998).
http://xxx.lanl.gov/abs/cond-mat/9806063

http://www.scri.fsu.edu/~rikvold/matsci_html/matsci-mag.html

# Nonperturbative Numerical Studies of Equilibrium and Nonequilibrium Lattice-Gas Models in Materials Science

*P. A. Rikvold and G. Brown, Florida State University*

## Research Objectives

We seek to study the structure and dynamics of microscopic models in materials science. Most of our NERSC allocation in FY98 was applied to investigate the evolution of microstructure during processing of multiphase materials, such as phase-separating alloys. Other applications include magnetization switching in magnetic nanoparticles, and adsorption in electrochemical cells. Only the materials-processing project is discussed in detail here.

## Computational Approach

We use Time-Dependent Ginzburg-Landau (TDGL) Langevin-equation simulations to represent the evolving microstructure. Large two-dimensional lattices with between $512^2$ and $5103^2$ nodes, and long simulations on the order of $10^5$ integration steps are required to allow the microstructure domains to become well defined while avoiding finite-size effects. Fast Fourier transforms are employed to determine the scattering intensities of particular microstructures, and the resulting large data sets are saved to enable correlations between different points at different times to be calculated.

## Accomplishments

The large-scale calculations on the Cray J90 have enabled us to simulate statistical fluctuations in models of phase-separating alloys such as $Fe_3Al$. These fluctuations give rise to variations in the scattering intensity of coherent x-rays scattered from the phase-separating material. The intensity variations resemble the "speckle" observed in scattered laser light. However, it is only the recent emergence of high-brilliance synchrotron sources that have made it possible to perform such experiments on optically opaque materials and with atomic resolution. The statistical signatures of nonequilibrium speckle fluctuations that were extracted from our simulations should also be observable in experiments. Furthermore, the data analysis methodology developed for our large data sets should be directly applicable to corresponding experimental scattering data.

## Significance

The microscopic structures that give most materials their characteristic mechanical and transport properties are produced by nonequilibrium processes, such as quenching, annealing, and sintering. Our studies contribute to the understanding of how microstructure evolves and how it can be manipulated by changing the physical conditions during materials synthesis.

## Publications

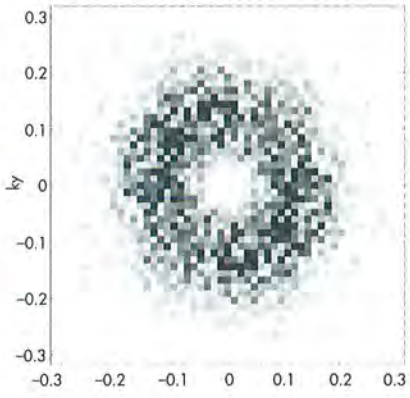
G. Brown, P. A. Rikvold, M. Sutton, and M. Grant, "Speckle from phase-ordering systems," Phys. Rev. E **56**, 6601–6612 (1997).

G. Brown, P. A. Rikvold, and M. Grant, "Universality and scaling for the structure factor in dynamic order-disorder transitions," Phys. Rev. E **58** (in press, 1998).

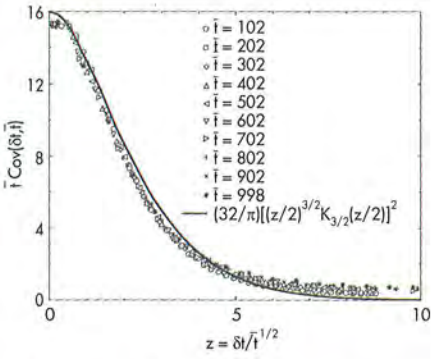
P. A. Rikvold, M. A. Novotny, M. Kolesik, and H. L. Richards, "Nucleation theory of magnetization reversal in nanoscale ferromagnets," in *Dynamical Properties of Unconventional Magnetic Systems*, edited by A. T. Skjeltorp and D. Sherrington (Kluwer, Dordrecht, 1998), pp. 307–316.

http://www.scri.fsu.edu/~rikvold/matsci_html/matsci-mag.html


A typical microstructure for TDGL simulations with conserved order parameter. The light and dark regions represent domains of different composition.




A speckled scattering pattern from simulation with conserved order parameter. Darker shades indicate brighter speckles.




Scaling of speckle two-time correlations for non-conserved order parameter, determined by simulations. The solid line is an analytic result.

# Sparse Linear Algebra Algorithms for MPPs

*Horst D. Simon, Kesheng John Wu, and Osni Marques,*
*Lawrence Berkeley National Laboratory*

## Project Description

Our goal is to develop scalable parallel algorithms to solve large sparse symmetric eigenproblems. Our research addresses several crucial issues for large-scale parallel machines, such as robustness, scalability, and portability.

## Computational Approach

Two approaches to compute eigenvalues using the Lanczos method are currently being evaluated, the shift-and-invert scheme and the thick-restart scheme. Our work uses many software components developed elsewhere; the software we develop is portable and conforms to widely used standards.

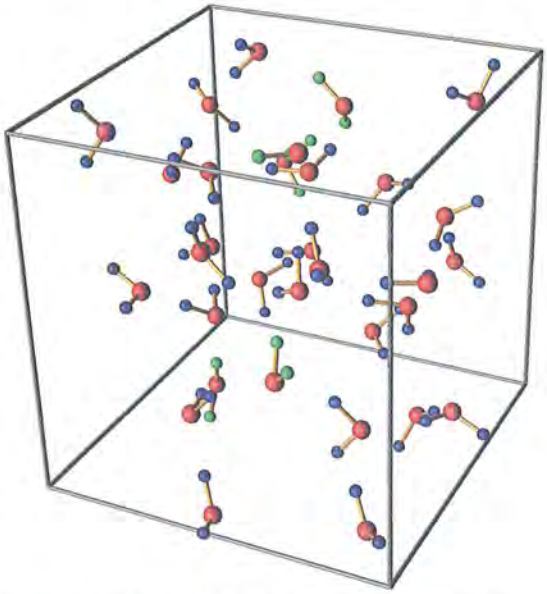
## Accomplishments

We have ported and parallelized the scalar LANSO code by Beresford Parlett. The code runs efficiently on the 512-processor Cray T3E at NERSC and demonstrates very good speed-up. The code is implemented in MPI and is portable to other platforms. This has been demonstrated by testing on a cluster of SMPs.

On symmetric eigenvalue problems, our Lanczos method consistently used less time than the popular ARPACK. In addition to the inherent higher efficiency of the Lanczos algorithm, this speed was due to a new algorithmic technique called "thick restart" (TRLAN). With thick restart, the Lanczos algorithm has the same advantage of reduced storage as ARPACK. The implementation of the TRLAN package has been completed, and a NERSC client is using this algorithm now for materials science research. Using it with other applications, e.g., the partitioning problem, is under investigation.

During 1998, we continued to investigate the use of the Lanczos algorithm in the problem of large text retrieval using latent semantic indexing (LSI). In our theoretical work, we demonstrated the advantages of Lanczos-based LSI, examined the distribution of the singular values, and developed techniques to exploit the features in the distribution. In collaboration with the web search engine Inktomi, we used our algorithm to compute the first 5 singular values of a data matrix of 100,000 terms by 2,559,430 documents. To our knowledge, this is the first time the singular value decomposition of such a large matrix has been computed.

We continued our collaboration with Boeing, which has released the SPOOLES software to NERSC. SPOOLES is a general sparse linear system solver, which is currently being evaluated and tested under a DARPA-funded follow-on project.



**This configuration of molecules in liquid water is used in an *ab initio* computation of nuclear magnetic resonance chemical shifts. Materials science applications such as this will benefit from improved scalable sparse linear algebra algorithms. (Bernd Pfrommer, Francesco Mauri, and Steven G. Louie, UC Berkeley Department of Physics, and Material Sciences Division, Lawrence Berkeley National Laboratory)**

## Significance

Scalable sparse linear algebra algorithms are an essential part of the computer science enabling technology for large-scale computer simulations and intelligent data processing. The algorithms and software being developed enable many applications on a previously unknown scale.

## Publications

Bernd G. Pfrommer, James Demmel, and Horst Simon, "Unconstrained energy functionals for electronic structure calculations," Report LBNL-41735, Lawrence Berkeley National Laboratory (1998); J. Comp. Physics (in press, 1999).

Kesheng Wu and Horst D. Simon, "Thick restart Lanczos algorithm for symmetric eigenvalue problems," Report LBNL-41412, Lawrence Berkeley National Laboratory (1998); SIAM J. Matrix Analysis and Applications (submitted, 1998).

Hongyuan Zha and H. Simon, "On updating problems in latent semantic indexing," Report CSE-97-011, Department of Computer Science and Engineering, Pennsylvania State University (1997); SIAM J. Matrix Analysis and Applications (in press, 1999).

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

# Index of Researchers

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

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