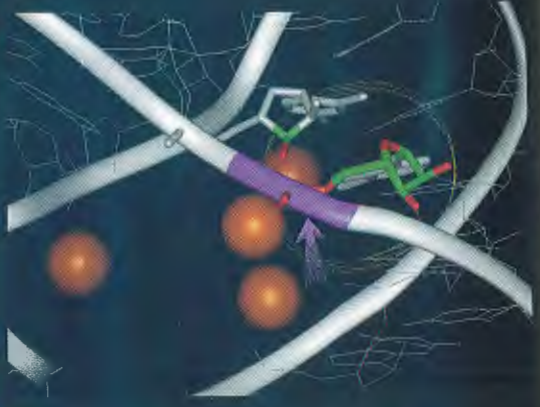
NERSC

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

1999 Annual Report



BERKELEY LAB

Ernest Orlando Lawrence
Berkeley National Laboratory

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

1999 Annual Report

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

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

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

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

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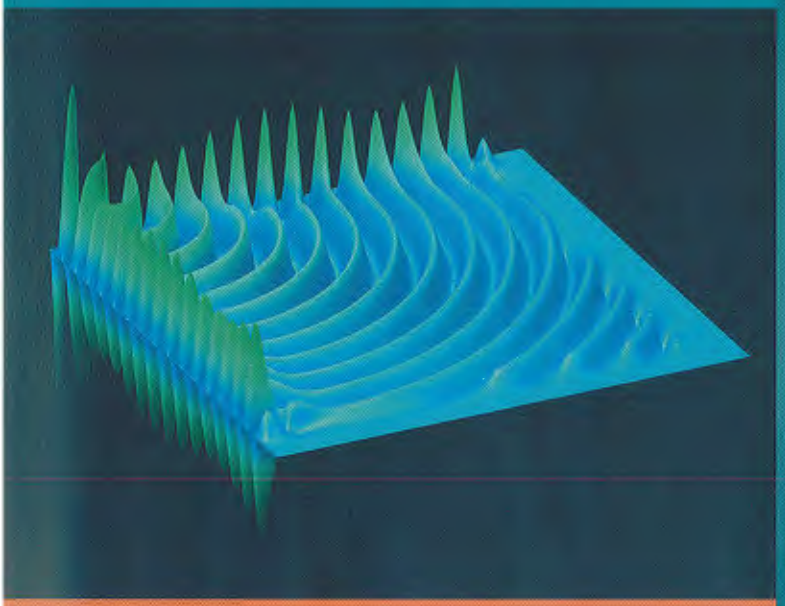
Director's Perspective



Wave functions for the breakup of a system of three charged particles illustrate the first complete solution to a fundamental problem in quantum physics. See pages 6 and 82 for details.

In 1999 NERSC celebrated 25 years of leadership in high performance computing. Looking back over these 25 years, the evolution and growth of computer technology—in particular, high performance computing power—has been truly astonishing. Yet an even more surprising fact is how remarkably constant the original vision of NERSC has remained: to provide a national user community access to a unique scientific facility, by adapting and advancing technology and by delivering excellent services. In the 1990s we have seen significant and sometimes revolutionary changes in how this vision was implemented: the transition to massively parallel supercomputer technology and the addition of intellectual services in 1996 fundamentally reshaped NERSC. From this long-term perspective, 1999 was a typical year for NERSC. While making rapid strides in integrating new technologies, we continued to maintain the highest standards of service, and again enabled our community of users to attain unprecedented new scientific results.

One of the highlights of the year was the successful completion of the NERSC-3 procurement, which will result in the acquisition of an IBM SP with more than 3 Tflop/s peak performance. The machine is arriving at NERSC in two phases. The installation of Phase 1 resulted for the first time in an aggregate computing resource at NERSC of more than 1 Tflop/s. The completion of Phase 2 by the end of 2000 will more than quadruple the amount of computing power available to our users, when compared to our computational resources in 1998.

This year brought us a wealth of scientific results, many of which are documented in this annual report. Most notable is the first cover story in *Science* with both simulation and visualization carried out at NERSC. I expect many more to follow, enabled by NERSC-3 resources. While funding for the Grand Challenge projects is being phased out, this DOE program has forged large-scale collaborations which will last well into the future. Many of the projects have created a software infrastructure, often with help from NERSC staff, which will make it much easier to harness the power of future generations of distributed memory machines. Thus I believe that we are on the verge of harvesting a great scientific return from the investment into highly parallel technology.

Horst D. Simon, Division Director of NERSC

In 1999 DOE announced a new policy of broader scientific peer review for the use of NERSC. A new NERSC Policy Board was established to help chart the future of the facility. Proposals to use NERSC are now subject to peer review, and a Program Advisory Committee (PAC) has been established to conduct the peer review process. I am excited about this major policy change, because the new advisory structure helps to strengthen NERSC's role as a unique facility in the DOE Office of Science, and will improve further the quality of computational science carried out at NERSC.

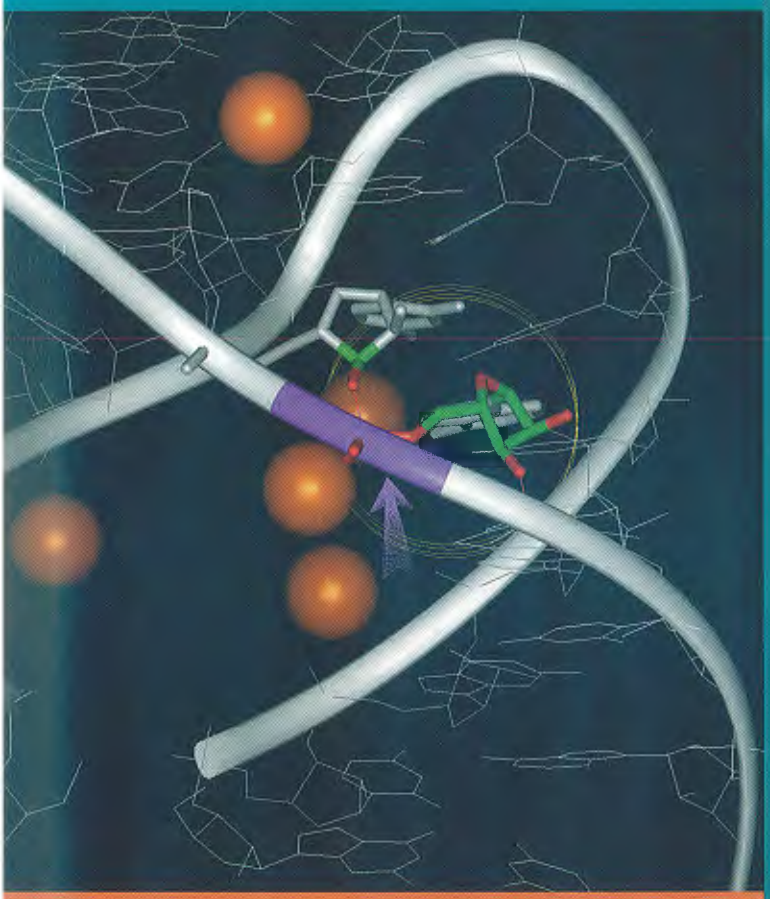
The pace of innovation will continue in 2000. We just welcomed the new Distributed Systems Department into the NERSC Division at Berkeley Lab, and I expect to leverage the new staff's expertise by starting a significant new computational grid project in 2000. The delivery of NERSC-3, Phase 2 will require us to relocate our computational facility to Berkeley Lab's new Oakland facility, which is currently under construction. Moving equipment (again!) and then operating it at the new site with most of our staff remaining in Berkeley will be a challenge. At the same time, we are facing political challenges to maintain and hopefully increase the role of computing in the DOE Office of Science.

With these exciting times ahead of us, I am grateful to our DOE Office of Science sponsors for their continued endorsement of our ambitious plans. I would like to thank our clients, in particular the NERSC Users Group and its executive board members, for their continued support, especially for their willingness to help whenever needed. My special thanks and congratulations, as always, go to the NERSC staff for their skill, dedication, and tireless efforts to make NERSC the best scientific computing resource in the world.

Computational

YEAR IN REVIEW

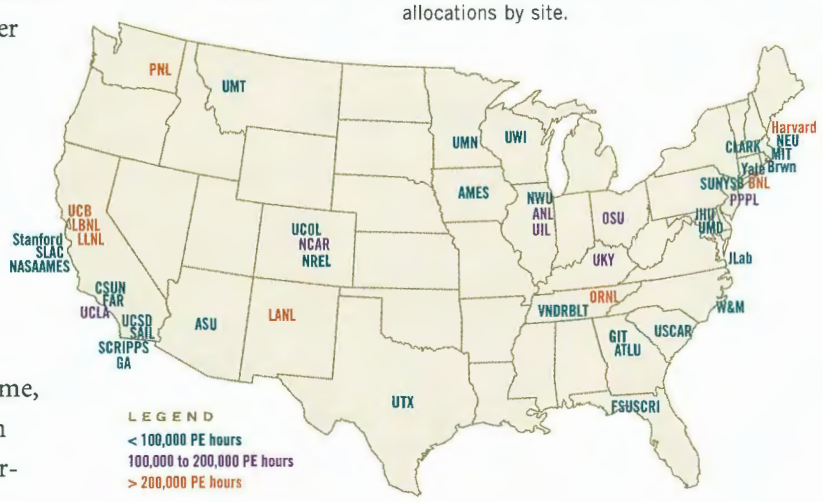
Science



Structure of the hammerhead ribozyme, with the RNA backbone represented by a white ribbon. See page 48 for details.

In 1999 NERSC celebrated its 25th year of innovation. As America's first supercomputer center to support a nationwide user base, and the model for those that followed, NERSC pioneered many of the supercomputing practices taken for granted today, including remote access, time sharing, interactive use, multitasking, high performance data storage and retrieval, high performance networking, on-line documentation, 24-hour support for users, and intellectual resources. At the same time, NERSC has consistently provided its users with some of the most powerful and advanced supercomputers available anywhere.

Figure 1: NERSC FY99 massively parallel processing (MPP) allocations by site.



Our anniversary year was marked by significant scientific and mathematical achievements by our nationwide clients and our staff, as well as a new policy that makes NERSC accessible to even more researchers. This section of the Annual Report describes some of those achievements as well as the peer review policy that will help ensure the quality of computational science in the future.

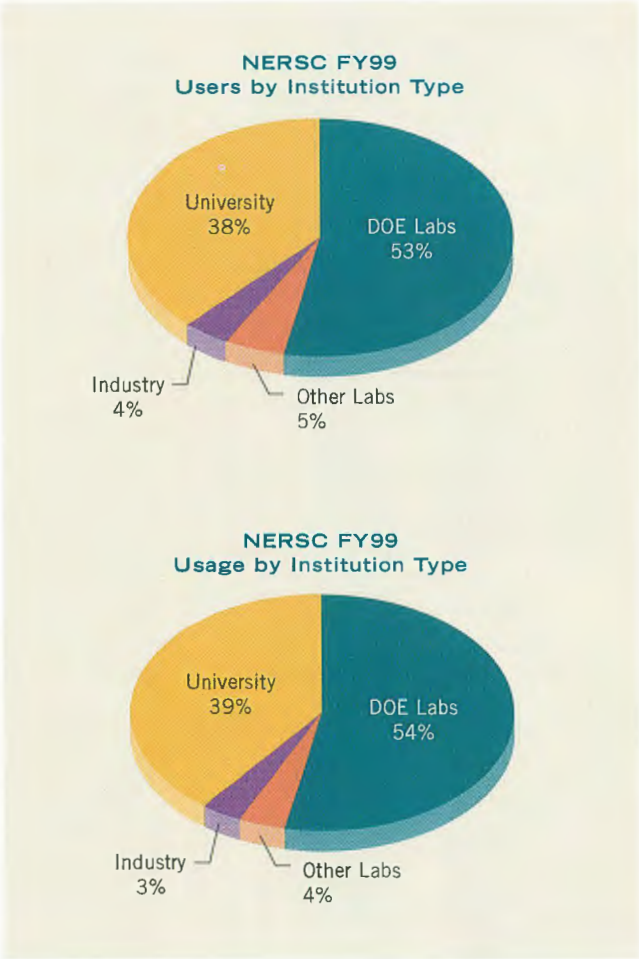
Research by NERSC Clients

As a national facility for scientific research funded by the Department of Energy, Office of Science (DOE SC), NERSC annually serves about 2,400 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).

Advanced Scientific Computing Research

DOE's Office of Advanced Scientific Computing Research supports a number of projects in computer science and applied mathematics, including work on turbulent flows by NERSC's Center for Computational Sciences and Engineering (p. 10). Another research group is developing increasingly accurate simulations of acceleration-driven fluid interface instabilities, a field

Figure 2: Percentage of NERSC users and usage (computing time) by institution type.

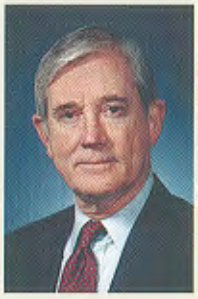


Shared Memories: Reflections on NERSC's 25th Anniversary

Bill McCurdy
Associate Laboratory Director for Computing Sciences
Lawrence Berkeley National Laboratory

The idea that interactive scientific computing could be provided to a national community from a central facility was truly revolutionary. The early NERSC center achieved that goal and built the modern aesthetic of supercomputing, which allows scientists to interact with the machines as though they were in the same room, visualizing and manipulating results immediately.

Al Trivelpiece
Director, Oak Ridge National Laboratory



As the Director of the Office of Energy Research ... I created some uproar by allocating 5 percent of the time available on the fusion computer system for projects in ER other than fusion. The idea of having a high performance computing resource available for [all] ER programs took hold and led indirectly to NERSC.

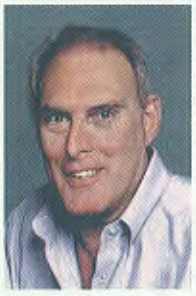
James Decker
Deputy Director, DOE Office of Science

Looking back over my nearly 25 years of involvement with NERSC, I think that it has been an outstanding success. It has made significant contributions to all of our research programs.

Steven Jardin
Princeton Plasma Physics Laboratory
Chair, NERSC Program Advisory Committee

One of the greatest things about NERSC is how they are always able to keep the computing environment seemingly unchanged as it evolves in major ways.... As new generation computers, networks, and file storage systems were brought in, the transitions have been made in such a seamless manner that our production work was virtually uninterrupted.

Sid Karin
Director, San Diego Supercomputer Center
National Partnership for Advanced Computational Infrastructure

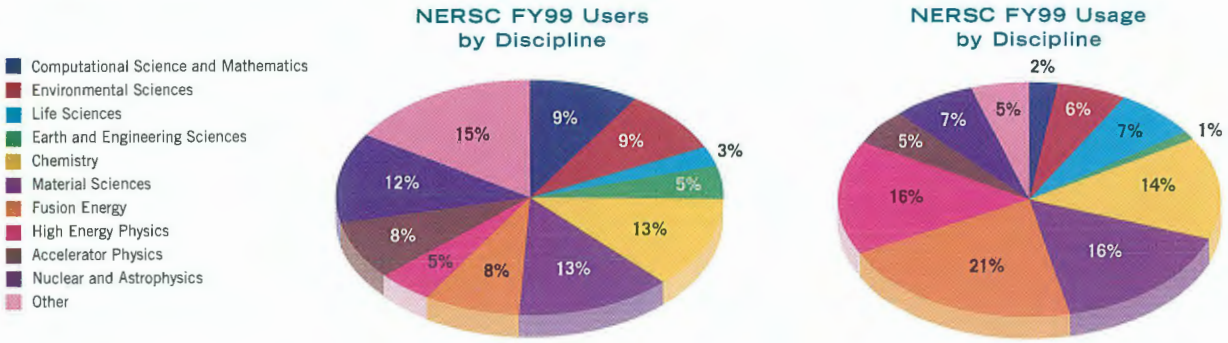


NERSC has remained at the forefront of supercomputing ... for all of its history. In the early days there was little competition for the leadership role. Today there are many more respectable participants, yet NERSC remains among the leaders. This is a remarkable sustained accomplishment.

Bastiaan Braams
Courant Institute of Mathematical Sciences,
New York University
Chair, NERSC Users Group Executive Committee

[NERSC] provided the U.S. fusion community with supercomputer access of a kind that was envied everywhere and that created a national collaboratory for fusion theory before the name "collaboratory" had been invented.

Figure 3: NERSC users and usage by scientific discipline.



with applications ranging from astrophysics to climatology to mechanical engineering. Still other researchers are applying new numerical methods to simulate the unusual magnetic and electrical properties of condensed matter; one of their goals is to identify experimental probes that would signal the appearance of novel phenomena.

Development of improved scalable linear algebra algorithms (such as a sparse direct linear system solver) for MPP systems is another major focus of OASCR-funded research. Early versions of a variety of scalable algorithms developed on NERSC systems are already in use for computational chemistry, earthquake modeling, electronics engineering, and astrophysics data analysis. Experimental software for information retrieval has successfully passed preliminary tests on a collection of more than half a million full-text documents; future applications will test image retrieval as well.

Basic Energy Sciences

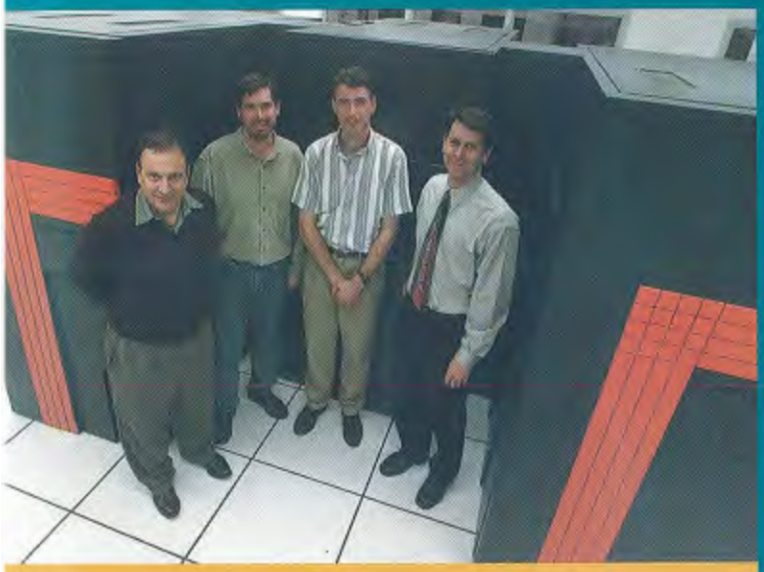
NERSC provides computational support for a large number of materials sciences, chemical sciences, geosciences, and engineering research projects sponsored by DOE's Office of Basic Energy Sciences.

Two computational chemists who use NERSC resources—Peter Cummings of the University of Tennessee and Oak Ridge National Laboratory, and David Dixon of Pacific Northwest National Laboratory—were among the scientists featured in a *Chemical & Engineering News* cover story, "Bridging Chemistry and Engineering" (April 26, 1999). The article demonstrated that, with the help of high performance computers, computational chemistry has become sophisticated enough to have real-world engineering applications, especially in the early stages of process design.

Cummings's research includes the search for surfactants that can be used along with supercritical carbon dioxide as an environmentally friendly replacement for organic solvents. To work successfully with supercritical CO_2, the surfactant molecules would have to display the unusual behavior of organizing themselves as reverse micelles (polar heads in, organic tails out) around water molecules. Cummings and his colleagues achieved the first atomistically detailed molecular dynamics simulation of micellization, in which all the water molecules were scavenged within a nanosecond (see page 30). The researchers hope their efforts will help chemists understand how these surfactants work and aid in the selection of possible new candidates.

Dixon, according to the *C&EN* cover story, is "pushing the accuracy envelope. His concern it to try to get the accuracy of his predications down to less than 1 kcal per mole, which is needed in many engineering applications. Accuracy is particularly critical in calculating values for quantities that have never been measured experimentally." Dixon and his research group are developing and testing methods for reliably predicting the energetics and kinetics of chemical processes without recourse to empirical parameters, thus minimizing the expensive experimental measurements needed to model complex systems such as the combustion of hydrocarbon fuels (see page 31).

Researchers Solve a Fundamental Problem of Quantum Physics



Tom Rescigno, William Isaacs, Mark Baertschy, and Bill McCurdy found the solution to the problem of the scattering of three charged particles in a quantum system.

Visualizations by Mark Baertschy of UC Davis and Terry Ligocki of the NERSC/Berkeley Lab Visualization Group graced the December 24, 1999 cover of *Science*. The images show a representative radial wave function of two electrons in the collision of an electron with a hydrogen atom. (©1999 by the American Association for the Advancement of Science. Used with permission.)

For over half a century, theorists have tried and failed to provide a complete solution to scattering in a quantum system of three charged particles, one of the most fundamental phenomena in atomic physics. Such interactions are everywhere; ionization by electron impact, for example, is responsible for the glow of fluorescent lights and for the ion beams that engrave silicon chips.

Now, a research team using NERSC's Cray T3E and the IBM Blue Pacific computer at Lawrence Livermore National Laboratory have obtained a complete solution of the ionization of a hydrogen atom by collision with an electron, the simplest nontrivial example of the problem's last unsolved component. Bill McCurdy, Berkeley Lab's Associate Laboratory Director for Computing Sciences, along with his longtime collaborator Thomas Rescigno, a staff physicist at Livermore Lab, and their co-authors, doctoral candidate Mark Baertschy of UC Davis and postdoctoral fellow William Isaacs of Berkeley Lab, reported their findings in the December 24, 1999, issue of *Science* magazine.

Their breakthrough employs a mathematical transformation of the Schrödinger wave equation that makes it possible to treat the outgoing particles not as if their wave functions extend to infinity—as they must be treated conventionally—but instead as if they simply vanish at large distances from the nucleus. "Using this transformation we compute accurate solutions of the quantum-mechanical wave function of the outgoing particles, and from these solutions we extract all the dynamical information of the interaction," says McCurdy.

The method developed by McCurdy and colleagues allows the calculation of a highly accurate wave function for the outgoing state that can be interrogated for details of the incoming state and interaction in the same way an experimenter would interrogate a physical system. Comparison with real scattering experiments proves the accuracy of the new method. The experimental data points match the graph of the calculated cross sections with astonishing exactitude (see page 83).

In other research, the replacement of electronics by faster optical devices is being furthered by the computational design of photonic band gap materials, whose applications include waveguides that can bend electromagnetic waves with bending radii of only a single wavelength. Advances in semiconductor quantum dot research this year included the first *ab initio* calculation of the capacitance of nanocrystal quantum dots, and calculation of the electronic and optical structures of million-atom quantum dots. This research may usher in a new generation of nanoscale devices such as lasers, sensors, photovaltaics, and data storage media.

Basic research under way in chemistry and materials science includes incorporating quantum mechanical effects into simulations of chemical reaction dynamics, calculating the electronic structures of reactive chemical systems, and investigating the atomic and electronic structures of ceramic/metal interfaces. With an eye to energy efficiency, computational scientists are simulating reaction pathways in the process of soot formation and conducting scaling studies to improve the fidelity of combustion simulations. Studies of particulate dynamics in filtration and granular flow are relevant to the extraction of water or oil from underground reservoirs as well as commercial filtration processes used in purification and manufacturing. And the successful imaging of subducting tectonic plates, ocean ridges, and velocity anomalies at the base of the Earth's liquid core, based on computational analysis of global seismic data, is offering new insights into the inner structure of our planet.

Biological and Environmental Research

DOE's Office of Biological and Environmental Research is a major supporter of global climate studies as well as computational medical and biological research. These fields are claiming a growing share of NERSC resources.

The highly respected climate research group led by Warren Washington of the National Center for Atmospheric Research has developed a new, state-of-the-art global climate model. Their 300-year control experiment simulates El Niño and La Niña events that are remarkably close to observed patterns (see page 50). They are now conducting historical simulations to calibrate the model. Results of their simulations of future climate change scenarios will be provided to the Intergovernmental Panel on Climate Change and the U.S. National Assessment of the Potential Consequences of Climate Variability and Change.

The DOE Center for Research on Ocean Carbon Sequestration, which is jointly managed by Lawrence Berkeley and Lawrence Livermore national laboratories, has begun using NERSC resources to provide the scientific basis for understanding the efficacy and environmental impacts of various strategies for ocean carbon sequestration, including biological fertilization and direct injection of CO_2 into the deep ocean.

Other climate research at NERSC includes continuing work on the comparison and diagnosis of climate models; the first three-dimensional, high-resolution simulations of decaying stratified turbulence on a rotating sphere; an improved model for three-dimensional global atmospheric chemistry simulations; and preliminary simulations of Southern Ocean eddy dynamics to understand their contribution to global ocean systems. (Also see page 9 below for a discussion of NERSC staff involvement in climate research.)

Medical and biological researchers are using NERSC resources to develop a new technique for recognition and classification of protein folds in genomes; to simulate enzyme reactions relevant to the development of new antibacterial agents; to conduct atomic-scale studies of enzyme catalysis, which may eventually lead to ribozyme-based therapies for certain viruses and cancers; and to search for new scintillator crystals to be used in medical imaging and physics research.

Fusion Energy Sciences

Research funded by the Office of Fusion Energy Sciences is flourishing on massively parallel systems. Steady improvements in computational techniques and codes have resulted in simulations realistic enough to compare with experiments. These simulations have elucidated a variety of experimental results and have helped improve the performance of experimental devices.

The theoretical picture of toroidal ion temperature gradient-driven turbulence was simplified considerably this year by the discovery of a simple fit for the dependence of the thermal flux on the temperature gradient. Researchers also demonstrated a new scheme to reduce heat transport by slightly rippling the equilibrium temperature profile, which generates short-scale zonal flows and thus reduces the heat transport.

Another significant accomplishment was the development of a practical formulation for real tokamak geometry that could be simply incorporated into both gyrokinetic and gyrofluid linear and nonlinear codes. In addition, non-adiabatic electron physics and electromagnetic effects were added to several tokamak turbulence codes. Including electrons extends the applicability of the model to describe particle transport as well as heat transport, and provides a more relevant description of the physics of ion temperature gradient driven modes, since trapped electrons are known to enhance the growth rate of the underlying instability. Another milestone is a new computational approach that explains the previously apparent discrepancy between experimental observations and theoretical calculations using magnetohydrodynamics equations.

The NIMROD fusion plasma code, which provides for flexibility in both physics and geometry, is maturing rapidly and has more than doubled its performance in the last year. It is being applied to a wide variety of challenging simulations. Significant progress is also being made in simulations of beam dynamics for heavy-ion fusion. And stellarator simulations have helped develop feasible experimental designs with more compact plasmas; if successful, these designs could significantly improve the economics of fusion power.

High Energy and Nuclear Physics

High performance computing continues to have a major impact on the field of high energy and nuclear physics, ranging from theoretical studies, to the design of next-generation experimental facilities, to the storage and analysis of massive data sets from experiments.

In nuclear physics, quantum Monte Carlo methods have made it possible to computationally study nuclear systems with realistic nuclear interactions, taking into account the vast amount of nucleon-nucleon scattering data. These interactions produce large spatial, spin, and isospin correlations between the nucleons. These correlations can play an important role in a variety of intriguing processes, ranging from the scattering of electrons by nuclei to the reactions that produce solar neutrinos. Quantum Monte Carlo studies of nuclear structure have produced results that follow the experimental data more closely than do empirical formulas.

In high energy physics, lattice QCD (quantum chromodynamics) researchers provide theoretical calculations that are useful in interpreting experimental results and that suggest improved experiments to test the Standard Model of elementary particles. Due to steady improvements in algorithms and computational techniques, and rapid increases in computing resources, QCD calculations are now having an important impact on high energy physics. For example, this year physicists computed the weak matrix elements responsible for the longstanding puzzle of weak kaon decays, in which two seemingly similar decay processes proceed at very different rates.

The Computational Accelerator Physics Grand Challenge has had a significant impact on the design of several accelerators, including the Next Linear Collider (NLC), the Accelerator Production of Tritium, and the Spallation Neutron Source. Simulations of the NLC resulted in an improved linac design with a higher acceleration gradient, saving $100 million over the original design. Another group of accelerator researchers is testing the feasibility of various plasma-based accelerator concepts. If plasma-based accelerator technology is successfully developed, it could lead to miniaturized tabletop accelerators, which could have an impact as widespread as miniature lasers.

Over the past two years, 6 terabytes of data for the STAR detector at Brookhaven National Laboratory were simulated on NERSC's T3E. These data were invaluable for understanding the detector response of STAR and for

developing analysis algorithms. Mechanisms were developed to efficiently transport large volumes of STAR data over the network between computing facilities spread across the country. As a result of these efforts, STAR is now confident that the first data can be reliably handled and efficiently processed to extract the physics.

NERSC is also playing a major role in the storage and analysis of cutting-edge astrophysics data. The successful analysis of the massive set of cosmic microwave background (CMB) data collected during the 1997 BOOMERANG test flight has raised high expectations for the results from the 1999 BOOMERANG long-duration flight, which are currently being analyzed. The CMB contains detailed cosmological information and may answer many fundamental questions about the universe, such as its geometry and expansion rate. In addition, the Supernova Cosmology Project is using NERSC resources to analyze data from the most successful search for nearby supernovas in history. They discovered 35 supernovas, 20 before or at maximum light. Analysis of these Type Ia supernovas will help calibrate high-redshift supernovas and ascertain possible systemic biases in the extraction of cosmological parameters from redshift data.

Research by NERSC Staff

NERSC is an active partner in many of the scientific and applied mathematical research projects that make use of our facilities. Our staff develop and adapt computational approaches, algorithms, and software to help scientists get the best performance and results out of our advanced systems. And our ACTS Toolkit (http://acts.nersc.gov/) provides software tools and resources for developing high performance scientific applications.

Some recent examples of staff research in the areas of climate modeling, combustion modeling, earth sciences, and materials science, are discussed below.

Chris Ding (front) and Helen He (standing) of NERSC's Scientific Computing Group are collaborating on the parallel version of the MOM3 ocean model with scientists from GFDL. R. K. Owen (back) and Harsh Anand Passi of NERSC's User Services Group, along with Steve Luzmoor of SGI/Cray, ported the netCDF common data format library to the T3E, which helped streamline input/output in MOM3.

Climate Modeling

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.

Input/output improvements, made possible by the flexibility of the common data format netCDF, have already enabled the snapshot part of the code to run 50 times faster on a parallel machine than on a single processor. NERSC's innovative integration of the netCDF library into MOM has improved data accessibility and facilitated data sharing, while also demonstrating that netCDF can be used efficiently in a real, large-scale application.

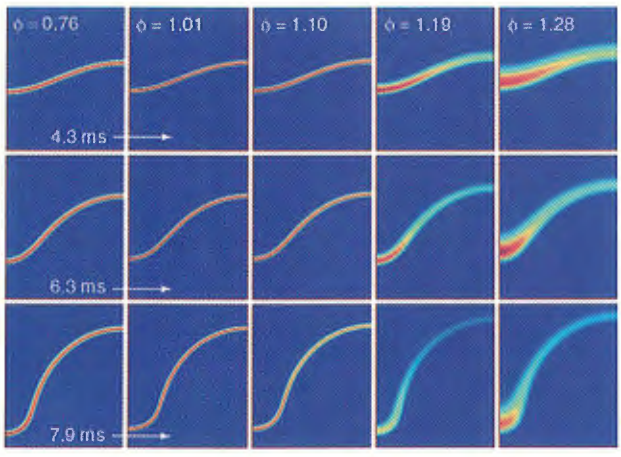
In addition, a standalone module for in-place remapping of a multidimensional array on a distributed-memory computer has reduced the memory requirements on a single processor by half.

The algorithms and software modules developed in this project can be used in the I/O of other climate models in addition to MOM. And the in-place global remapping algorithm can be used in grid-based climate models for polar filtering, spectral transforms, and I/O subsystems.

Combustion Modeling

As computing tools become more powerful, computational simulation will play an increasingly important role in the design of combustion devices such as more efficient gasoline engines or less-polluting diesel engines. Researchers in NERSC's Center for Computational Sciences and Engineering (CCSE) are working toward a key component of this goal with the development of high-fidelity numerical simulation capabilities applied to turbulent combustion processes such as furnaces and engines.

One of the most difficult issues in the modeling of turbulent combustion is the coupling between chemical kinetic processes and the small-scale eddies in the flow. The computational challenge arises from the need to resolve numerically a wide range of spatial and temporal scales associated with the flow field, while at the same time employing complex models for the fundamental chemical processes. CCSE is developing an adaptive block-structured refinement approach which allows overall computational effort to be focused in localized, time-evolving regions of the domain, such as the zone near a burning flame. By minimizing unnecessary computation in less critical regions of the domain, they can incorporate more detail in the fluid and chemistry components of the model. Implementing such software requires a variety of design and implementation expertise, including software infrastructure design, detailed algorithm development, physical model validation, parallel computing, and complex visualization issues. CCSE recently tested their methodology on a set of vortex-flame interactions, an important prototype for premixed turbulent combustion. They studied the effect of fuel stoichiometry on the interaction of a counter-rotating vortex pair with an initially flat premixed methane flame. The simulation was based on a well-diagnosed, highly reproducible, two-dimensional vortex-flame experiment by Q.-V. Nguyen and P. H. Paul at Sandia National Laboratories. This experiment posed a challenge to existing numerical combustion models, which could not correctly predict the time-dependent behavior of a number of intermediate species produced by the combustion process. CCSE's simulation was the first to reproduce some key results of the experiment.



A vortex-flame interaction simulation by NERSC's Center for Computational Sciences and Engineering (CCSE) was the first to reproduce some key experimental results. For a detailed description of this image, see page 76.

CCSE conducted numerical simulations using a configuration similar to the Sandia vortex-flame experiment, in terms of fueling characteristics and the strength and shape of the imposed vortices. Simulations over a range of inlet stoichiometry and vortex characteristics indicated that the vortex not only stretches and strains the flame, but also scours material from the cold region in front of the flame. The scouring effect is strongly dependent on the spatial distribution of various key flame radicals, and therefore is strongly affected by the inlet fuel equivalence ratio. This latter observation helped to explain previously observed computational results which seemed to otherwise disagree with experiment, and underscores the benefit of efficient computing methods that can provide results over a range of

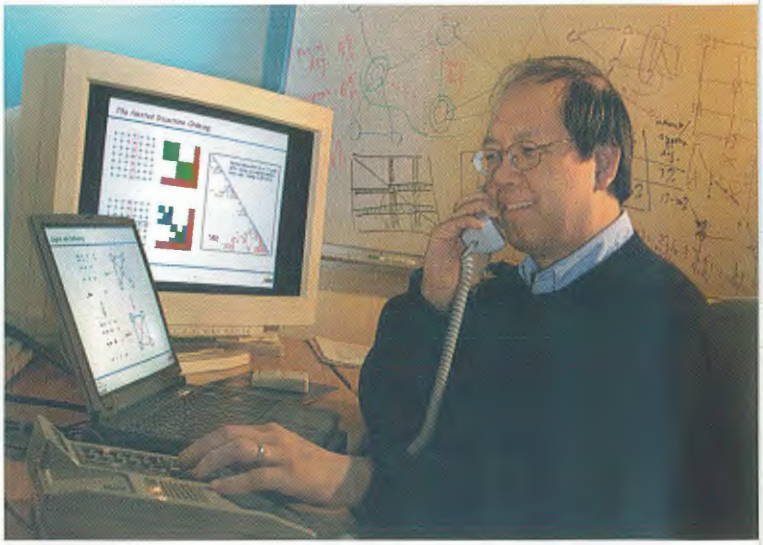
similar scenarios. CCSE is continuing research to further improve the fidelity of the detailed fluid dynamical simulations, and is working with combustion chemists at UC Berkeley and LBNL's Environmental Energy Technologies Division to develop more complete chemical mechanisms for combustion.

Earth Sciences

For challenges ranging from cleaning up groundwater contamination to increasing the flow from oil and natural gas fields, understanding the movement of liquids and gases in the subsurface is essential for earth scientists, and computer simulations give them insight into otherwise inaccessible regions. The Earth Sciences Division at Berkeley Lab has developed a code for simulating multiphase flow and transport processes in fractured-porous media. Called TOUGH2 (Transport of Unsaturated Groundwater and Heat), the code can model one-, two-, and three-dimensional flows of multiple phases, such as gas, aqueous liquids, and oil, and multiple components, such as water, air, organics, and radionucleides. The code is used by over 150 organizations in more than 20 countries for large-scale, multicomponent flow simulations in environmental remediation, nuclear waste isolation, and geothermal reservoir engineering.

NERSC's Scientific Computing Group has developed a parallel implementation of TOUGH2 that enables it to run on high performance systems. This will benefit researchers such as the Yucca Mountain nuclear waste isolation project. Currently, the Yucca Mountain modeling group runs their flow model on about a dozen workstations 24 hours a day, 7 days a week. But they need to study grid blocks of 100,000 to 1 million, which is impossible on even the fastest workstations. NERSC's MPP systems will allow the model resolution to be increased significantly, and will provide a complete flow picture in a timely fashion.

TOUGH2 uses a finite-volume method to solve the mass-energy balance equation. The most computationally demanding part is to solve a large, unsymmetric, non-positive, linear equation. NERSC staff are developing a parallel implementation of the package and integrating two key software components, the domain partitioner and the linear solver. To optimize the code, they will study both parallel computing related issues such as efficiency, scalability, etc., and numerical issues such as the stiffness of the Jacobian matrix involved in solving the highly non-linear equations. Typically these equations are very stiff and difficult to solve. The effectiveness of the preconditioner and iterative methods when applied to such large-scale problems will be investigated.



Esmond Ng is head of NERSC's Scientific Computing Group, which engages in long-term research and development projects to develop state-of-the-art methodologies, algorithms, and software tools for computational sciences. The group is currently involved in major collaborations in materials science, environmental and earth sciences, astrophysics, and numerical linear algebra, and has plans to expand its efforts in several other fields. Esmond also coordinated the establishment of NERSC's new Luis W. Alvarez Postdoctoral Fellowship in Computational Science to help educate the next generation of computational scientists (http://www.nersc.gov/research/alvarez.html).

Results to date look promising. The codes have been restructured, domain decomposition is completed, and the Aztec solver from the ACTS Toolkit has been integrated into the package. On a real application of 17,584 grid blocks with 3 components (52,752 equations), the parallel codes solved the problem 60 times faster on the T3E than the original sequential codes did on workstations.

Materials Science

The electronic, optical, transport, and structural properties of semiconductor nanostructures (films, quantum

User Satisfaction Continues to Grow

"I have found the consulting services to be quite responsive, friendly, and helpful. At times they went beyond the scope of my request, which resulted in making my job easier."

"Provides reliable machines, which are well-maintained and have scheduling policies that allow for careful performance and scaling studies."

"Provides a stable, user-friendly, interactive environment for code development and testing on both MP machines and vector machines."

"NERSC provides a well-run supercomputer environment that is critically important to my research in nuclear physics."

In this year's NERSC User Survey, our clients gave us an overall satisfaction grade of 6.25 on a 7-point scale, a 0.8-point increase over last year. The biggest increases in satisfaction were with the allocations process, the HPSS system and the T3E. The average scores ranged from a high of 6.6 for timely response to consulting questions, to 4.0 for PVP batch wait time.

The areas users are happiest with this year are consulting services, HPSS reliability and uptime, as well as PVP and T3E uptime. Areas of concern are batch wait times for both PVP and T3E systems, visualization services, the availability of training classes, and PVP resources in general.

In their verbal comments, users focused on NERSC's excellent support staff and its well-run center with good access to cycles, hardware and software support, and reliable service. When asked what NERSC should do differently, the most common response was "provide even more cycles."

Of the 52 users who compared NERSC to other computing centers, half said NERSC is the best or better than other centers, 23% simply gave NERSC a favorable evaluation or said they only used NERSC, 19% said NERSC is the same as other centers or provided a mixed evaluation, and only 4 said that NERSC is not as good a other centers.

For complete survey results, see http://hpcf.nersc.gov/about/survey/99/.

dots, and quantum wires) have recently been under intense study. This interest arises because of the novel physical properties of these systems and their potential application to a whole new set of nanoscale devices such as lasers, sensors, and photovoltaics.

Before scientists and engineers can begin to design nanoscale devices with custom-made electronic and optical properties, they must have a detailed understanding of the underlying physical phenomena. In nanoscale systems whose sizes vary from 1 to 50 nanometers, these phenomena are controlled by quantum mechanical effects and can only be understood by solving Schrödinger's equation. Performing quantum mechanical calculations on systems containing thousands or millions of atoms requires state-of-the-art numerical techniques and computing resources.

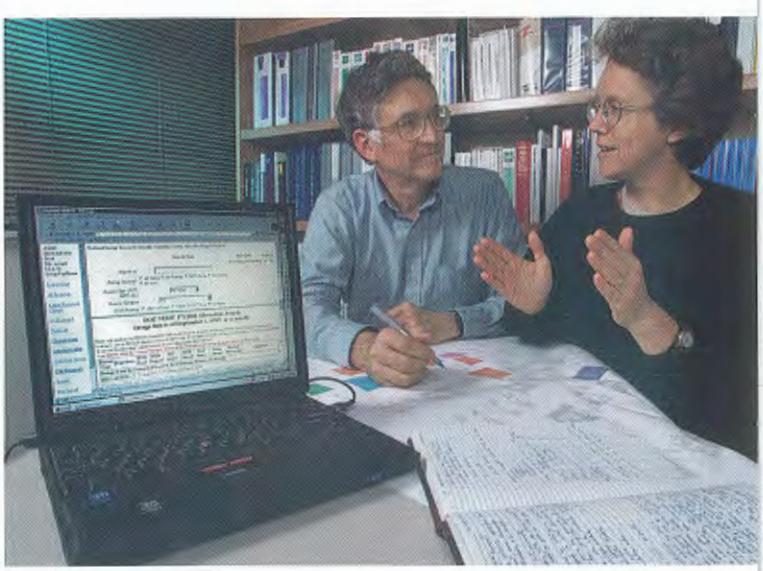
Lin-Wang Wang and Andrew Canning of NERSC's Scientific Computing group, in collaboration with Alex Zunger's research group at the National Renewable Energy Laboratory, have developed a Parallel Empirical Pseudopotential method for electronic structure calculations. This code allows the calculation of the electronic structure (for a small number of electronic states) of systems of up to 1 million atoms on the T3E at NERSC. It uses pseudopotentials for the single-electron Hamiltonians, which are commonly used for accurate *ab initio* total energy calculations. It expands the wavefunctions in planewaves, thus requiring fast Fourier transforms to convert the wavefunction from reciprocal space to real space. The number of basis functions in such a million-atom system is about 50 million. A "folded spectrum" algorithm developed by Lin-Wang Wang is used to calculate a few physically interesting states in the middle of the energy spectrum without the calculation of all the other states.

Previous methods were not able to give accurate information on the electronic structure of systems larger than 1000 atoms. The Parallel Empirical Pseudopotential program opens a new approach in this field by enabling accurate atomistic calculations

for million-atom nanosystems. This parallel code is now used by many materials science research groups and has resulted in publications in the areas of quantum dots, quantum wells, superlattices, alloys, composition modulations, ordering, and defect states.

New Peer Review Process

In February 1999, the Department of Energy announced a new policy of broader scientific peer review for use of NERSC's resources. The allocations process for FY 2000 was reorganized to accommodate and balance two major needs of the Office of Science: the need for an open competition to allocate resources to the most important, challenging, and timely scientific opportunities, and the need to direct computing resources to collaborations or individuals in order to fulfill specific mission requirements of the DOE programs.



Allocations of computer time and archival storage at NERSC are awarded by DOE to research groups based on an annual review of hundreds of proposals submitted through the Energy Research Computing Allocations Process (ERCAP). The Web-based ERCAP process is managed by Francesca Verdier, head of NERSC's User Services Group, and John McCarthy.

The new policy will help ensure that NERSC continues to be a national leader in using high performance computing as a tool for scientific discovery, just as DOE's light sources and particle accelerators are national and international leaders in their areas. As proposals are submitted, they will be subjected to peer review to evaluate the quality of the science, how well the proposed research is aligned with the mission of DOE's Office of Science, and the readiness of the specific application and applicant to fully utilize the computing resources being requested.

Beginning in FY 2000, three groups are advising the Director of Lawrence Berkeley National Laboratory and the Director of NERSC:

1. The NERSC Policy Board advises the Laboratory Director on policies that determine the impact and performance of the NERSC Center.
2. The NERSC Program Advisory Committee manages the peer review process for the allocation of NERSC resources and advises the NERSC Director.
3. The NERSC Users Group advises the NERSC director and provides feedback from the user community.

The NERSC Policy Board meets at least annually and provides scientific and executive-level advice to the LBNL Director regarding the overall NERSC program and, specifically, on such issues as resource utilization to maximize the present and future scientific impact of NERSC, and long-range planning for the program, including the research and development necessary for future capabilities. Policy Board members are widely respected leaders in science, computing technology, or the management of scientific research and/or facilities (see Appendix A).

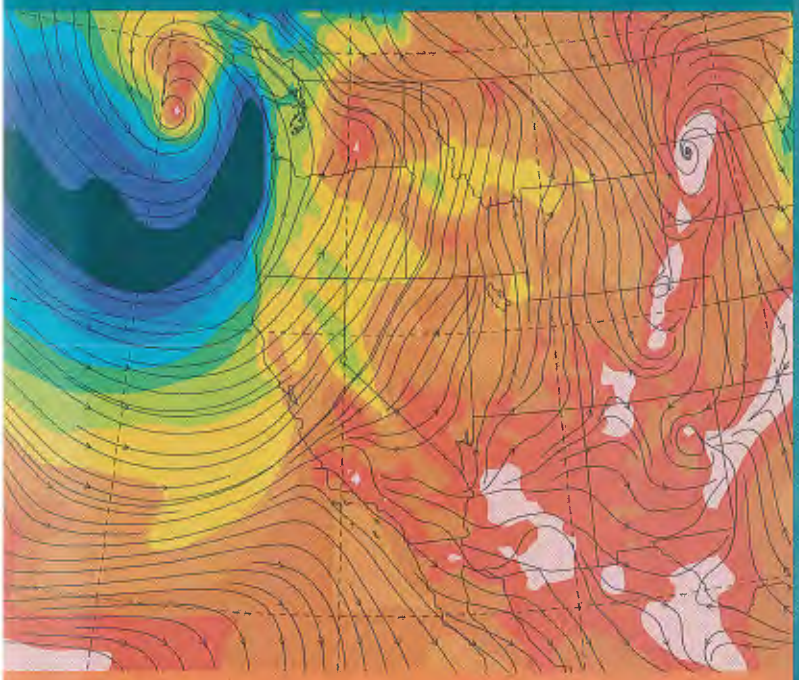
The NERSC Program Advisory Committee (PAC) is responsible for the new scientific peer review process. PAC members are broadly recognized, active scientists who are knowledgeable about the current computational challenges and opportunities in their fields (see Appendix B). This new process is being used to allocate 40 percent of NERSC's computing resources. The peer review and resource allocation process for the remaining 60 percent will be managed directly by the programs in the Office of Science, reflecting their mission priorities.

Because DOE is a mission agency charged with carrying out specific programs related to national needs, the majority of NERSC's resources will continue to be focused on large-scale computational science programs. However, the new policy is also expected to foster start-up projects that show promise, with a goal of applying for more time on NERSC's computers the following fiscal year.

New Computing

YEAR IN REVIEW

Technologies



This wind speed and direction forecast was produced by the Regional Climate System Model (RCSM), which NERSC staff are helping convert to a high performance parallel code. See page 84 for details.

In the 1990s, supercomputer centers went through two fundamental transitions which required rethinking their operation and their role in high performance computing.

The first transition in the early to mid-1990s resulted from a technology change in high performance computing architecture. Highly parallel distributed memory machines built from commodity parts increased the operational complexity of the supercomputer center, and required the introduction of intellectual services as equally important components of the center.

The second transition happened in the late 1990s as centers introduced loosely coupled clusters of shared-memory multiprocessor systems (SMPs) as their premier high performance computing platforms, while dealing with an ever-increasing volume of data. In addition, increasing network bandwidth enabled new modes of use of a supercomputer center, in particular, computational grid applications. At NERSC we call this second transition the "teraflops/petabytes production supercomputing center."[1]

This section of the Annual Report outlines what NERSC is doing to stay at the leading edge of supercomputing centers.

Optimizing the Productivity of New Architectures

In 1999, NERSC continued its tradition of making pioneering contributions to bring the newest computer architectures into a full production environment and to maximize their productivity. We installed the first phase of our new IBM SP system, developed a new flexible benchmark to assess system performance under realistic workloads, boosted our Cray T3E utilization above 90%, developed new cluster software for high performance computing, researched the comparative performance of several architectures and programming paradigms on a challenging real-life problem, and worked with Berkeley Lab to begin construction of a new facility to meet the increasing demand for floor space and electrical power.

Phase I IBM SP System

In April 1999, NERSC announced that it had selected an IBM RS/6000 SP system as the center's next-generation supercomputer. The IBM system was chosen based on its ability to handle actual scientific codes and tests designed to ensure the computer's capability as a full-production computing system at NERSC. These tests indicated that the system, when fully installed, will provide four to five times more computational power than NERSC's current systems combined. This agreement, a fixed-price, five-year contract for $33 million, is the largest single procurement in the 68-year history of Berkeley Lab.

Phase I of the RS/6000 SP system, which was installed in June 1999, uses IBM's new 64-bit, two-CPU POWER3 SMP nodes. Phase I has 256 nodes (512 processors) dedicated to large-scale scientific computing, with a peak performance of 410 gigaflops, 256 gigabytes of memory, and 10 terabytes of disk storage. The entire system, including service, file system, networking, and interactive nodes, has 608 processors and a peak performance of 486 gigaflops.

Phase II, slated for installation no later than December 2000, will be based on 16-CPU POWER3+ SMP nodes, utilizing an enhanced POWER3 microprocessor. The system will have 2,048 processors dedicated to scientific computing, with a peak performance of 2.7 teraflops, 1 terabyte of memory, and 15 terabytes of disk storage. The entire system will have 2,432 processors (in 152 nodes) and a peak performance of 3.2 teraflops.

Effective System Performance Benchmark

As part of the RS/6000 SP purchase contract, NERSC will work with IBM to develop computer-utilization

1. Horst D. Simon, William T. C. Kramer, and Robert F. Lucas, "Building the Teraflops/Petabytes Production Supercomputing Center," in *Proceedings of EuroPar '99* (Toulouse, France, September 1999). http://www.nersc.gov/aboutnersc/pubs/BuildingTeraflops.pdf

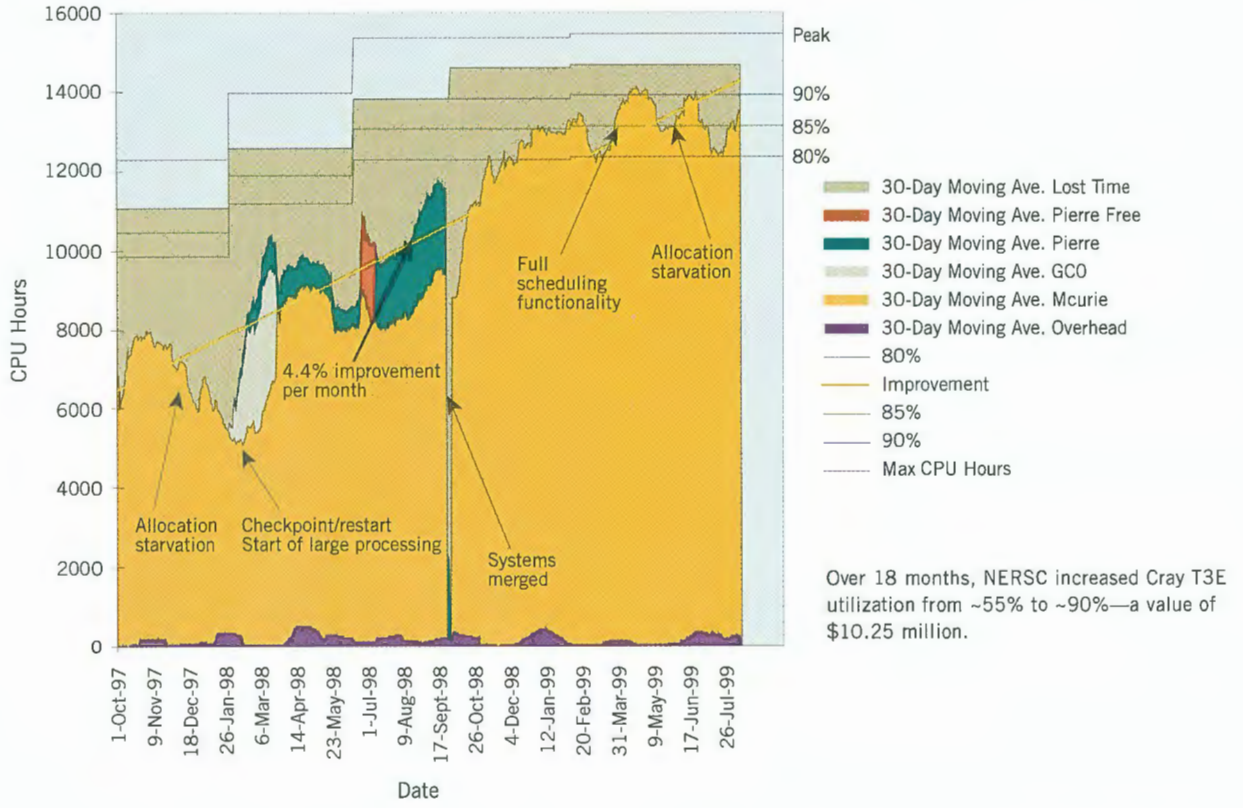
NERSC-3 Procurement Team Recognized for Successful Effort

Led by Bill Kramer (foreground), the NERSC-3 procurement team included (from left front) Bill Saphir, Norma Early, Eric Essman, Lynn Rippe, Sherry Li, Adrian Wong, Richard Arri, Nick Cardo, Tammy Welcome; (back) David Bailey, Chris Ding, Jed Donnelley; (not shown) Andrew Canning, Mike Declerck, Frank Hale, and Julie Jones.

Installation of the new IBM SP system was the culmination of an often grueling year-long effort by the NERSC-3 procurement team, led by NERSC's Deputy Director, Bill Kramer. Their achievements included assessing NERSC's near-term computational needs, developing and publishing a request for proposals, developing a test suite of scientific applications, reviewing proposals and selecting a vendor, negotiating a contract, and overseeing the delivery, installation, and testing of the Phase I system.

The procurement team accomplished these crucial and complicated tasks on schedule and maintained strict confidentiality throughout the process. The team received Berkeley Lab Outstanding Performance Awards for their contribution to NERSC's future.

Phase 1 of the NERSC-3 procurement rolled into Berkeley Lab on Saturday, June 26, 1999. Nearly filling three big-rig trailers, the system consisted of 60 cabinets, cartons, and crates with a total weight of 35,603 pounds. A crew of moving company, IBM, and NERSC staffers unloaded the equipment in about three hours, then moved it from the loading area to the machine room. There, another group of workers positioned the 23 cabinets and connected them to seismic restraints laid out under the raised flooring. All the components were cabled together during the following week.



Over 18 months, NERSC increased Cray T3E utilization from ~55% to ~90%—a value of $10.25 million.

benchmarks and methods to assess and improve the effectiveness of the SP system in a production environment. When the contract was announced, NERSC's Deputy Director, Bill Kramer, offered this explanation: "Theoretical computer speed is comparable to the top end of a car's speedometer, and while your car might be able to do 150 mph on the open road, you're really more interested in how it will carry out your day-to-day driving chores. While we anticipate that most of our users will appreciate the new machine's high-speed capability, our main concern is that they have the computing resources they need, when they need them. This contract ensures the system will live up to NERSC's standards for performance and reliability."

To that end, NERSC has already developed and tested a new prototype benchmark that measures Effective System Performance (ESP) in a real-world operational environment.[2] ESP is designed to evaluate systems for overall effectiveness, independent of processor performance. Results take into account both hardware (PE, memory, disk) and system software performance. The ESP test suite simulates "a day in the life of an MPP" by measuring total system utilization, using a suite of real scientific applications that run in a random order, testing standard system scheduling. There are also full-configuration codes, I/O tests, and typical system administration activities.

T3E Utilization Tops 90%

Continued collaboration with SGI/Cray led to the first installation of the complete Psched scheduling software system on NERSC's T3E in the spring of 1999. Psched's load-balancing features, along with queue and job control scripts written by NERSC staff, enabled us to achieve a new milestone in MPP effectiveness—a sustained T3E utilization rate of more than 93% in April 1999. This is remarkable considering that the NERSC operating environment includes a wide range of jobs, ranging from interactive and debugging jobs to 512-processor Grand Challenge runs of up to 12 hours. The increase in T3E utilization over 18 months from

2. Adrian T. Wong, Leonid Oliker, William T. C. Kramer, Teresa L. Kaltz, and David H. Bailey, "Evaluating System Effectiveness in High Performance Computing Systems," (draft, 1999). http://www.nersc.gov/aboutnersc/pubs/esp.pdf

Oakland Scientific Facility Under Construction

The transition from NERSC-2 to NERSC-3 presented the challenge of a threefold increase in the machine's footprint and a twofold increase in its power requirements. In response to this requirement, Berkeley Lab announced in August 1999 that it had selected a site in downtown Oakland for the Laboratory's new computing center, which will house NERSC's high performance systems as well as other Berkeley Lab scientific and administrative computer systems.

A request for proposals drew eight qualified responses, from which the Oakland site emerged as the favorite. The former bank building is being seismically reinforced and completely redesigned to meet or exceed all current codes and standards, with additional improvements in the electrical supply capability. The new center is scheduled to open by fall of 2000. It will be connected to Berkeley Lab and other national laboratories via a high-speed network connection provided by ESnet.

Dave Tudor, Facilities Project Manager for Berkeley Lab's new Oakland Scientific Facility, and Howard Walter, NERSC's Future Infrastructure Project Lead, have been responsible for the site search, planning, and coordination of design and construction.

Architect's rendering of renovated building.

around 55% to more than 90% is equivalent to adding more than $10 million in additional hardware.

PC Cluster Project

On a smaller scale, NERSC's PC Cluster Project is making it easier for scientists to turn a collection of PCs into a usable cluster. They are developing software to make clusters more robust and scalable, as well as providing features usually found only in high-end systems, such as accounting, quotas, and security. The Berkeley Lab Distribution (BLD) will provide the key tools for configuring, managing, and running jobs on a cluster, and will support both "task farm" and "parallel" clusters. BLD will allow small research groups to put together their own clusters, and will contribute basic infrastructure for very large clusters that provide capability computing (see http://www.nersc.gov/research/FTG/bld/).

The two primary design goals of BLD are plug-and-play ease of use, allowing computer-literate non-specialists to more easily build and manage a cluster, and scalability to a very large size. The scalability problem is being addressed in the larger context of the Tribble Project, a collaboration with Argonne and Los Alamos national laboratories. The first components of BLD are available now, and others will be released early in 2000. The first product of the Tribble Project was a tutorial at SC99 (the annual conference on high performance computing and networking) on building production Linux clusters.

Alternative Architectures

In addition to our work optimizing mainstream architectures, NERSC continues to investigate alternatives. In a collaborative agreement with DOE, the National Science Foundation, and another government agency, NERSC helped to assess the performance of the multithreaded architecture of the Tera MTA at the San Diego Supercomputer Center. One result of this work was the "Best Paper of SC99" award for Leonid "Lenny" Oliker, a post-doctoral fellow in NERSC's Scientific Computing Group, and Rupak Biswas, an employee of MRJ Technology Solutions who works in the Numerical Aerospace Simulation Division at NASA's Ames Research Center.[3] Their paper presents the parallelization of a mesh adaptation algorithm using three popular programming paradigms on three leading supercomputers, and concludes that multithreaded systems offer tremendous potential for quickly and efficiently solving some of the most challenging real-life problems on parallel computers.

Lenny Oliker, winner of the "Best Paper of SC99" award.

The Petabyte Data Challenge

In the past, increases in archival storage needs were comparable to increases in computational capability, because the amount of data generated by computer simulations was usually limited by the available computational technology. Today this is no longer the case. Increasingly-massive sets of experimental data are being generated by new technologies in fields such as genomics, climatology, high energy physics, and astrophysics. Computer centers are being called on to move, store, and analyze these datasets. NERSC is working in two directions to respond to this challenge, one dealing with storage and other with data management.

Mass Storage

NERSC's Mass Storage Group continues to provide the storage media and baseline technology for large amounts of data. This group has increased the tertiary storage capacity at NERSC at an exponential rate, and so far has done an outstanding job of keeping our available storage capacity ahead of the demand. While increasing raw capacity, NERSC transitioned its storage management system completely to the R&D 100 award-winning High Performance Storage System (HPSS) in early 1999. As a developer site, NERSC is able to influence the HPSS consortium to provide tools to meet the requirements of

3. Leonid Oliker and Rupak Biswas, "Parallelization of a Dynamic Unstructured Application Using Three Leading Paradigms," in *Proceedings of SC99* (Portland, Oregon, 1999); LBNL-43190. http://www.nersc.gov/~oliker/papers/sc99.pdf

our data intensive applications. Given the flood of future data, this will be a significant advantage for NERSC clients.

NERSC has also teamed up with Oak Ridge National Laboratory to establish Probe, a distributed testbed for storage-intensive applications. Probe has its foundation in the HPSS installations at ORNL and NERSC, with high-speed networking from ESnet providing access to researchers around the country.

The Probe testbed is available for researchers to perform comparative evaluations of the latest technologies in storage hardware and software. By linking the two testbed systems together over the network, researchers will be able to evaluate the effects of network latency in remote storage access and develop new protocols for effectively using distributed storage systems. The testbed will also provide a platform for the developers of new storage and networking hardware and software to test their devices in high-demand facilities.

Probe will be used to study strategies for exploiting wide-area, high-bandwidth networks connecting data archives across the country. Researchers can modify or augment the configuration of Probe as needed, for example, to perform comparative evaluations of equipment from various vendors or to test the throughput of a proposed configuration. With a variety of network technologies installed, Probe can be used to explore new methods for high-speed transfers from storage to remote visualization systems and other applications.

Data Management

The second thrust in meeting the petabyte data challenge is to provide tools for scientists to manage their data more effectively. There are two groups at NERSC that work in this area, the Center for Bioinformatics and Computational Genomics and the Scientific Data Management Group.

The Center for Bioinformatics and Computational Genomics (CBCG) provides tools for the analysis of biological sequences, protein structure and function prediction, and large-scale genome annotation, as well as tools for access to biological information (database integration, data mining). A new tool that went online in 1999 is the Alternative Splicing Data Base (ASDB), which identifies clusters of proteins arising from alternative gene splicing. Alternative splicing allows as many as 64 different proteins to be created from a single gene sequence, and by recent estimates, at least 30% of human genes are spliced alternatively.

The ASDB, developed by CBCG in collaboration with the Institute of Protein Research at the Russian Academy of Sciences, can be searched to find out how many known proteins can be derived from a single gene sequence, or to find all known products of alternative splicing in a given organism, such as a fruit fly, mouse, or human, or in a particular tissue such as muscle, heart, or brain (see http://cbcg.nersc.gov/asdb). In its first half year of operation, the database received more than 35,000 queries from researchers in genetics and cell and developmental biology around the world.

The Scientific Data Management Group (SDM) is involved in various projects including tertiary storage management for high energy and nuclear physics (HENP) applications, data management tools, and efficient access to mass storage data. One of their recent accomplishments is the Storage Access Coordination System (STACS), which was developed to support the Mock Data Challenge tests of the Grand Challenge Application on HENP Data.

STACS coordinates file caching from tape to a shared disk for a large number of concurrent HENP applications. The software supports simultaneous scheduling of multiple files, incorporates the NetLogger file tracking system developed at Berkeley Lab, and produces online dynamic resources usage profiles, such as disk cache in use, file transfers pending, etc. Despite its complexity, STACS is robust, with clean interfaces and efficient functionality. It performed so well in tests that the STAR and PHENIX projects at Brookhaven National Laboratory plan to use STACS in their data analysis framework, CERN is adopting the STACS index method, and several Next Generation Internet projects are considering using concepts developed in the STACS project.

NERSC staff who received Outstanding Performance Awards in 1999 for their contributions on a variety of projects included: (back row) David Turner, Martin Stoufer, Tom DeBoni, Greg Butler, Brent Draney, Terry Ligocki, Wayne Hurlburt, Majdi Baddourah, William Harris, Jed Donnelley, Alex Sim, Brian Tierney, Wes Bethel, David Robertson; (front row) Mary Thompson, Francesca Verdier, Harsh Anand, Antal Herz, Tina Butler, Nancy Meyer, John Hules, Cheri Lawrence, Lissa Prince, Lynn Rippe, Gizella Kapus, Cindy Rogers, Deb Agarwal; (not shown) Luis Bernardo, Kevin Campbell, Andrew Canning, Jonathan Carter, Phil Colella, Jim Craw, Jim Daveler, Tina Declerck, Keith Fitzgerald, Richard Gerber, Susan Green, Mark Heer, Nancy Johnston, Steve Lau, Henrik Nordberg, Ken Okikawa, R. K. Owen, Bill Saphir, Jackie Scoggins, Arie Shoshani, Mike Welcome.

The work of the SDM group is unique among supercomputing centers, and we are not aware of a comparable research effort elsewhere. Together, NERSC's research efforts in data storage and management will result in efficient new tools that our clients can use to extract scientifically significant information from their petabyte datasets.

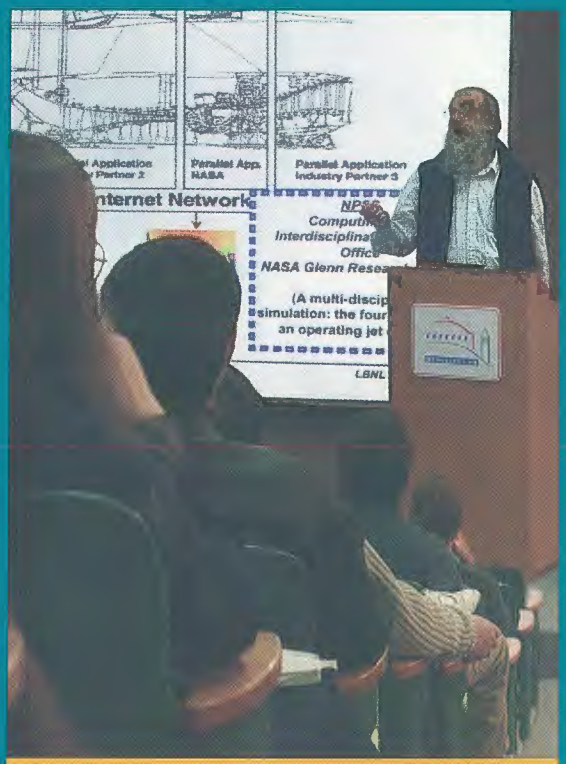
Preparing for the Computational Grid

In the last two years, the vision of a computational grid has gained broad acceptance. The grid is envisioned as a unified collection of geographically dispersed supercomputers, storage devices, scientific instruments, workstations, and advanced user interfaces. The recent book *The Grid: Blueprint for a New Computing Infrastructure*, edited by Ian Foster and Carl Kesselman, is an excellent summary of the current status of efforts to build such a grid.

Bob Lucas, head of the High Performance Computing Research Department, has played a major role in expanding grid research and development at NERSC. And early in 2000, Berkeley Lab's highly respected Data Intensive Distributed Computing Research Group, led by Bill Johnston, joined the NERSC Division as our Distributed Systems Department (see sidebar on page 22). NERSC's broad-based expertise positions us at the forefront of grid research and development, and ensures that our clients will be among the first to reap its benefits.

One significant aspect of the grid is the data grid, enabling transparent access to data by scientists widely distributed across the United States. The petabyte datasets discussed in the previous section are community resources, which will be shared by researchers who are geographically distributed yet participating in collaborative projects. We do not expect these data to reside exclusively at one site, nor do we expect access to be restricted to a local set of users. Therefore, NERSC is collaborating with other DOE laboratories and

Towards a DOE Science Grid



Bill Johnston, one of the nation's leading developers of widely distributed systems, is head of NERSC's new Distributed Systems Department.

Expanding the capabilities of the DOE Science Grid Testbed will be the focus of NERSC's new Distributed Systems Department, which joined the NERSC Division in early 2000 as part of the reorganization of Berkeley Lab's Computing Sciences Directorate.

The Science Grid will provide significant new capabilities to scientists and engineers, allowing them to address complex and large-scale computing and data analysis problems beyond what is possible today. The Distributed Systems Department will conduct research and development into various components of the Science Grid infrastructure, including collaboratory tools, computer security, distributed data intensive computing, and networking.

university researchers on a variety of projects related to large datasets distributed over a wide-area network.

The grid projects involve computer scientists working with applications specialists to tackle the real problems faced by the scientific community. Many of these projects and collaborations are interrelated, so new developments will be shared quickly throughout the community. The projects fall into three categories: research, technology development, and prototype applications.

1. NERSC's grid research projects include:

   - *Real-Time Grid Monitoring Infrastructure:* Combining network, host, and application-level monitoring to provide real-time perfomance data on the entire distributed system, and to archive the data to a central location. This research is an extension of the NetLogger methodology developed at Berkeley Lab.
   - *ENABLE:* An automated query service to improve the performance of applications over the grid by providing them with optimal network tuning parameters, based on real-time network latency and bandwidth data obtained by NetLogger.
   - *Akenti Distributed Access Control:* A security model and architecture for scalable security services in highly distributed network environments. Akenti provides a way to implement and enforce an access control policy without requiring a central enforcer and administrative authority.
   - *Advanced Visualization Communication Toolkit:* Allowing visualization applications to adapt to the dynamics of the network infrastructure by directly accessing network status information and controlling communication protocols and network behavior. The toolkit will also allow multiple sites with different network characteristics to view data simultaneously.

2. Grid technology development projects include:

   - *DOE Science Grid Testbed:* Providing a quality of service (QoS) technology development environ-

ment driven by application requirements, and exploring the issues involved in building a nationwide, multi-domain QoS testbed.

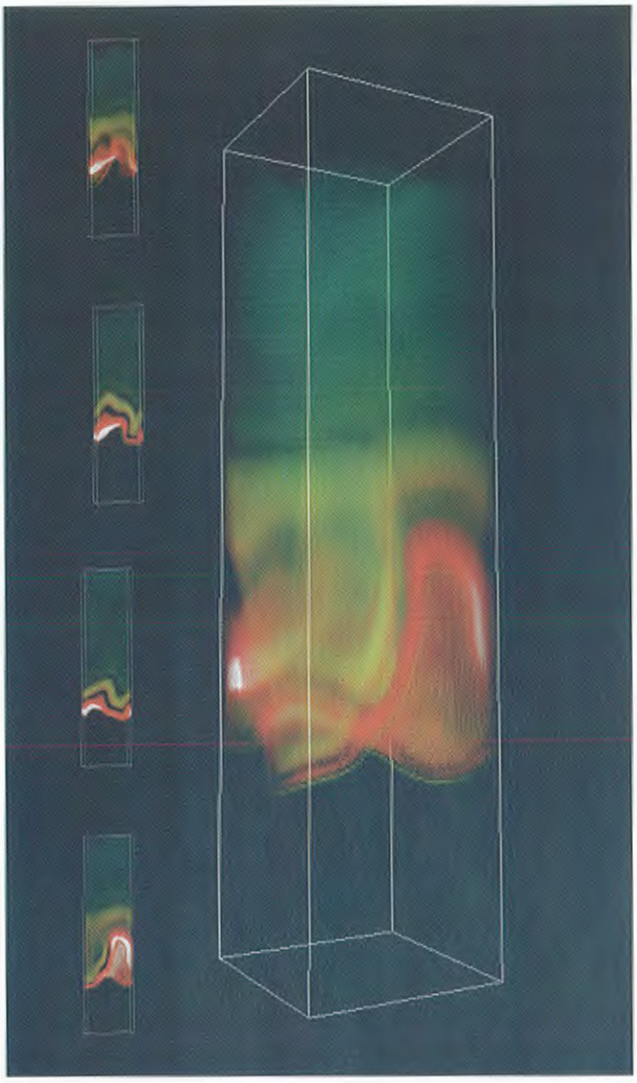
- *Distributed Parallel Storage System (DPSS):* A distributed disk cache which provides economical, high-performance, widely distributed data handling as well as a highly scalable architecture for building high-performance storage systems from low-cost commodity hardware components.

3. NERSC is also involved in several collaborative projects developing grid applications:

- *Combustion Corridor:* Real-time interactive volume visualization of combustion data sets.
- *Corridor One*: An integrated distance visualization environment for a variety of advanced simulation applications.
- *Earth Systems Grid:* High-speed data transport between climate research centers and flexible remote access for distributed scientific analysis.
- *Particle Physics Data Grid:* An infrastructure for widely distributed data analysis at multi-petabyte scales by thousands of physicists.

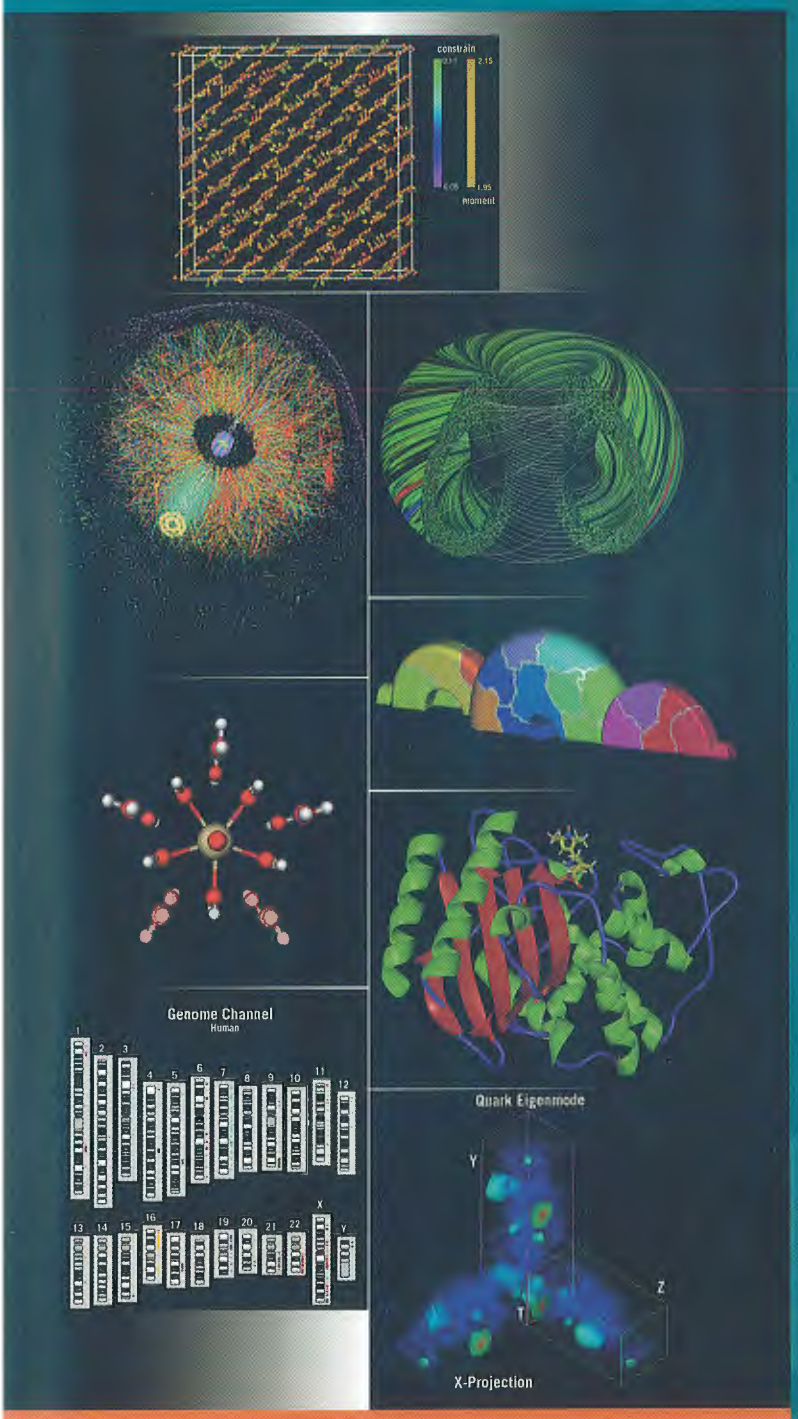
One product that has already emerged from the Combustion Corridor project is Image Based Rendering Assisted Volume Rendering, or IBRAVR. With software developed by Wes Bethel of the NERSC Visualization Group, IBRAVR enables distributed visualization of large data volumes, such as two gases mixing in a turbulent environment, on remote workstations. The fundamental idea behind IBRAVR is that large data are partially prerendered on a large computational engine close to the data, then final rendering is performed on a local workstation. Sharing the workload between a remote multiprocessor machine and the local workstation allows for some degree of interactivity on the local workstation without the need to recompute an entirely new image from all the data when the object is rotated by a small amount.

IBRAVR was demonstrated at SC99 using data from two simulations, one involving a combustion modeling code and a second one from a cosmology model. Data for the two simulations were stored on various data sources, including NERSC's Cray T3E, DPSS systems at Berkeley Lab and at the Argonne National Laboratory exhibit at SC99, and a Linux cluster at Berkeley Lab's exhibit. The composite engines for the demonstration were the NERSC T3E, the Berkeley Lab cluster, and the Cplant Linux cluster at Sandia National Laboratories in California. The data were visualized on the ImmersaDesk at the Berkeley Lab exhibit as well as at the Accelerated Strategic Computing Initiative (ASCI) exhibit.



IBRAVR sends the rendering engine 2D images from the remote data compositing engine. These images are assembled into a 3D representation that may be interactively transformed by a viewer.

Grand Challenge Retrospective



Grand Challenge applications address computation-intensive fundamental problems in science and engineering whose solutions can be advanced by applying high performance computing and communications technologies and resources. For the past three years, NERSC has been a partner in eight Grand Challenges sponsored by DOE. In this section we look back at the progress that has been made with the support of this program.

Computational Accelerator Physics

The advanced modeling tools developed in the Computational Accelerator Physics Grand Challenge are allowing particle accelerators to be designed with reduced cost and risk as well as improved reliability and efficiency. Three parallel application codes—IMPACT, Omega3P, and Tau3P—have been developed under the Grand Challenge.

These three codes have already made a significant impact on several important DOE projects such as the Next Linear Collider (NLC), Accelerator Production of Tritium (APT), and Spallation Neutron Source (SNS). The IMPACT simulation of a 500-million-particle beam helped to predict the maximum particle amplitude, and hence the required beam pipe aperture, in the SNS linac. IMPACT was also used in the first systematic study of halo formation due to longitudinal/transverse coupling in charged particle beams. Omega3P and Tau3P simulations were pivotal in realizing an improved NLC structure design with higher acceleration gradient that results in a $100 million savings in the cost of constructing the linac.

Computational Chemistry of Nuclear Waste Characterization and Processing

In this 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 have been parallelized for the T3E and extended to enable calculations on larger molecules at higher levels of accuracy.

In order to determine 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 (CI) calculations upon various actinide ions. Much effort has been devoted to developing and understanding accurate descriptions of the electronic spectra of various actinide and lanthanide ions. This is very challenging and has required development of new relativistic effective core potentials. The theoretical and computational methodology being 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.

Grand Challenge Application on High Energy and Nuclear Physics Data

The purpose of the Grand Challenge Application on HENP Data is to develop techniques and tools that will enable efficient access to the massive datasets generated by the Relativistic Heavy Ion Collider (RHIC) experiments in their search for the quark-gluon plasma. This project had several notable accomplishments. First, they 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. Second, 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.

Most importantly, over the past two years the project has generated a large set of simulated heavy ion collision data to be used as a testbed for developing data management and analysis tools and algorithms. In FY 1999 alone, approximately 250,000 PE-hours were used and over 6 terabytes of simulated data produced. These data were essential as input for two large-scale Mock Data

Challenges at the RHIC Computing Facility at Brookhaven, where the primary RHIC data will be stored and first analyzed. Mechanisms were developed to efficiently transport large volumes of data over the network between computing facilities spread across the country, a capability that will be crucial for the distribution of real RHIC data. As a result of these efforts, the RHIC physicists are now confident that the first data can be reliably handled and efficiently processed to extract the physics.

High Performance Computational Engine for the Analysis of Genomes

Interpretation of the human genome represents the next grand challenge at the interface of computing and biology. The many genome sequencing projects soon will be producing 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. The overall objective of this Grand Challenge has been to design and implement a distributed computational framework for the genome community that provides users with services, tools, and infrastructure for high-quality analysis and annotation of large amounts of genomic sequence data.

This collaboration has developed a web-based framework, The Genome Channel (now in its second version), 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, and developing specialized software and databases for genome analysis, such as the previously discussed Alternative Splicing Data Base (page 20).

Materials, Methods, Microstructure and Magnetism

This Grand Challenge collaboration earned international acclaim in 1998 when their 1024-atom first-principles simulation of metallic magnetism in iron won the Gordon Bell Prize and was the first complete scientific application to break the teraflops barrier. Using their locally self-consistent multiple scattering (LSMS) code, 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. This theory applies a separate magnetic field to each atom in a unit cell.

Developing a microscopic understanding of the dynamics of metallic magnets has been an abiding scientific challenge. An understanding of the relationship between magnetism and microstructure based on fundamental physical principles 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.

This project uses a number of different first-principles techniques, including LSMS, tight-binding molecular dynamics (TMBD), and an iterative pseudopotential (IP) method, 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 1500 atoms). In addition, they 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.

Numerical Tokamak Turbulence Project

Researchers in the Numerical Tokamak Turbulence Project (NTTP) reported a major advance in the computer modeling of fusion plasmas in the September 18, 1998 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 (an offshoot of NTTP), which compared various models for core transport in tokamaks, was also discussed in both *Science* and *Nature* in 1998.

The NTTP simulations are being used to produce linear and nonlinear calculations of drift-type instabilities in realistic tokamak equilibria, 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.

Particle Physics Phenomenology from Lattice QCD

Detailed simulations of the Standard Model of particle physics, developed in this Grand Challenge, will help determine some of the fundamental constants of nature. As a field, lattice quantum chromodynamics (QCD) provides theoretical calculations of quantities which can be measured experimentally. This provides both cross-checks of the Standard Model of particle physics, and a determination of several of its fundamental parameters.

This research team successfully computed the decay amplitudes of kaons for the first time, and successfully reproduced the observed $\Delta I = \frac{1}{2}$ effect. This is a long-standing puzzle of weak kaon decays, in which two seemingly similar decay processes ($I = 0$ and $I = 2$) proceed at very different rates. They recently computed the weak matrix elements which are responsible for the $\Delta I = \frac{1}{2}$ rule, and are working to help refine the theoretical calculation of the recently measured quantity ϵ'/ϵ. They also established a publicly available Gauge Connection archive (http://qcd.nersc.gov), which provides unquenched lattice QCD configurations that include virtual quarks.

Protein Dynamics and Biocatalysis

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 will eventually 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.

The focus of this research has been the development of a detailed understanding of the reaction mechanisms employed by beta-lactamases to hydrolyze b-lactam antibiotics. Researchers performed molecular dynamics simulations of the TEM-1 enzyme with a penicillin substrate to gain insights into accessible conformations of the enzyme/substrate (Michaelis) complex. They were interested in defining the roles of various active-site residues in binding and orienting the substrate into a conformation suitable for the catalytic reactions to proceed. The results of the simulations were consistent with two of three proposed mechanisms for the acylation step of the reaction. These simulations provide insights into the roles of several residues in binding and orienting the substrate in the active site. These insights may prove useful for the development of new antibacterial agents.

Science Highlights

Outer magnetic flux isosurface and filamentary magnet coils for a compact stellarator. Color contours indicate the magnetic field strength. See page 62 for details.

Atomic and Electronic Structure of Ceramic/Metal Interfaces

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L. H. Yang, Lawrence Livermore National Laboratory
A. Alavi, Queen's University, Belfast

RESEARCH OBJECTIVES

This simulation project is part of an effort to characterize on an atomic scale the structure and physical properties of ceramic/metal interfaces; it complements the experimental program of Prof. D. N. Seidman. A primary focus of our work is the development of a realistic model potential suitable for molecular dynamics and Monte Carlo simulation of ceramic/metal interfaces, with misfit included.

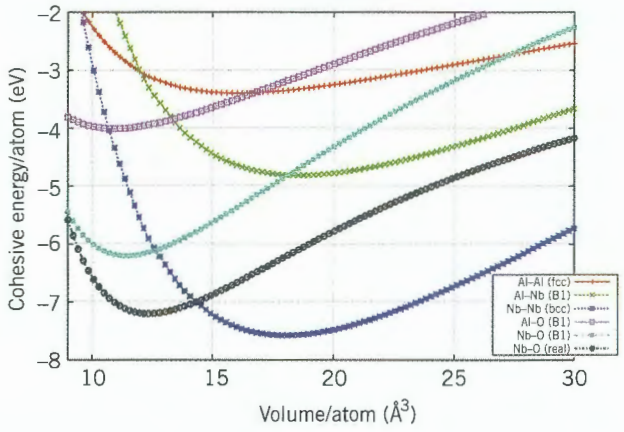
COMPUTATIONAL APPROACH

Most of our calculations are based on the plane wave pseudopotential implementation of local density functional theory (LDFT). We apply first-principles LDFT calculations to generate a database that, in conjunction with experimental information, enables parameters for a realistic interface interatomic potential to be determined. When our model ceramic/metal interface potential is validated, this potential will be embedded in a multiscale (quasicontinuum) code to enable the simulation of mechanical properties.

ACCOMPLISHMENTS

Calculations were performed of the layer-by-layer density of electronic states for coherent {222}MgO/Cu interfaces with three different parallel translations: (i) hollow site, (ii) bridge site, and (iii) on-top sites of the interface Cu layer relative to the terminating oxygen layer. The actual semicoherent interface may be viewed as a kind of composite with local regions that approximate each of these three high-symmetry configurations. The interface electronic states within the MgO gap are found shifted to higher energy for the on-top configuration relative to the hollow site, whereas a small density of states in the MgO gap are found for the bridge site configuration.

A classical modified embedded atom method (MEAM) interatomic potential has been developed for the well-studied model interface Nb/alumina. First-principles LDFT calculations were performed to generate a database for determining the potential parameters. To supplement those results, calculations of the equation of state have been performed for cubic NbO, rock salt NbAl, and rutile NbO_2.



A MEAM potential for the Nb/alumina interface has been developed using input data from first-principles total-energy calculations. The figure shows energy-volume equations of states obtained by Birch-Murnaghan fits to LDFT calculations. Each curve represents a monatomic or binary system in a cubic structure. The thermomechanical properties derived for pure Al, pure Nb and Nb-O are in excellent agreement with experimental values. Results for the hypothetical structures (i.e., oxides with B1-structure), which do not occur experimentally, are also employed in the fitting procedure.

SIGNIFICANCE

Ceramic-metal interfaces are prominent in many advanced materials, including high-temperature alloys, sensors, electronic components, and medical prostheses. But the simulation of properties of real ceramic/metal interfaces has been hampered by the lack of realistic interatomic potentials as well as the disparate length and time scales involved. Our aim is to start at the atomic scale and work towards continuum-length scales.

PUBLICATIONS

R. Benedek, D. N. Seidman, M. Minkoff, L. H. Yang, and A. Alavi, "Atomic and electronic structure and interatomic potentials at a polar ceramic/metal interface: {222}MgO/Cu," Phys. Rev. B **60**, 16094 (1999).

D. A. Muller, D. A. Shashkov, R. Benedek, L. H. Yang, J. Silcox, and D. N. Seidman, "Atomic-scale studies of the electronic structure of ceramic/metal interfaces: {222}MgO/Cu," Materials Science Forum **99**, 294 (1999).

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 (1998).

Molecular-Based Simulation of Complex Fluids

Peter Cummings, University of Tennessee

RESEARCH OBJECTIVES

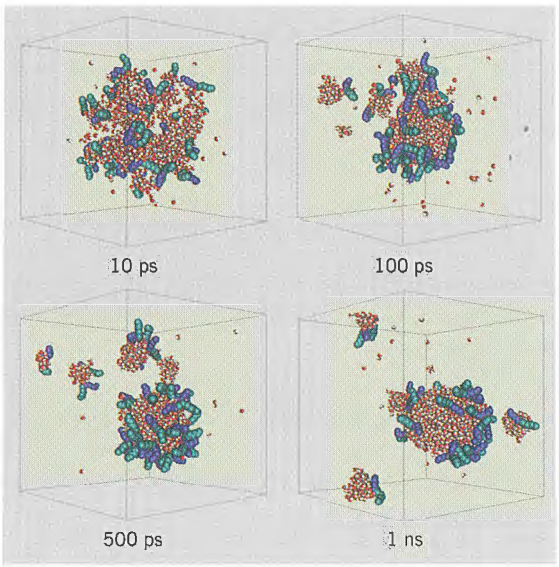
Our research is aimed at elucidating the molecular basis for the properties of complex materials and liquid systems, such as lubricants, self-assembling micellar systems, polymers, and high-temperature aqueous solutions. A common thread in all of our research is to develop and use the most accurate and 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.

ACCOMPLISHMENTS

In the past year, we performed the first atomistically detailed molecular dynamics simulation of micellization. We simulated the formation of water-containing reversed micelles in supercritical carbon dioxide. Remarkably, the reversed micelles form over a 1–2 nanosecond time scale.



Snapshots of simulation showing formation of reversed-micelle-like aggregates in water/surfactant/carbon dioxide mixtures over a period of 1 nanosecond. The color scheme of the various species is as follows: light blue for perfluoroalkane tail, dark blue for alkane tail, yellow for sulfur, red for oxygen, grey for sodium ion, and white for hydrogen. Carbon dioxide molecules are not shown for clarity. The number of atomic units in the simulation is 42,618.

We performed simulations of lubricants (particularly dodecane) confined to nanoscale (3–4 nm) gaps between mica-like surfaces to attempt to understand the extraordinarily large changes in the relaxation times associated with such confinement. We have made progress in demonstrating 1–2 order of magnitude increases. We continue this work in close collaboration with the experimental group of Steve Granick at the University of Illinois.

We performed molecular dynamics simulations of strontium chloride in supercritical water and made the first successful duplication of experimental EXAFS (extended X-ray absorption fine structure) measurements indicating changes in the solvation shell in this mixture.

We performed molecular dynamics simulations of "short" polyethylene (a C_{100} alkane) and particularly simulated the start-up of homogeneous shear in this system. This has led to new insights into the Doi-Edwards theory for the rheology of polymers. In fact, we have shown that the Doi-Edwards reptation theory explains the behavior of this polymer well, despite the fact that the molecules in a C_{100} melt are, in principle, too short to exhibit reptation dynamics.

SIGNIFICANCE

This research will lead to better understanding of the basis for the viscous properties of lubricant, leading to the design of improved lubricants in automobile engines, which will, in turn, result in better energy efficiency. We also have significant efforts under way studying the effect of nanoscale confinement on the rheology of lubricants, which has relevance to hard disk drive lubrication. Another focus of our research is aimed at finding new candidates for replacing organic solvents in chemical processes with more environmentally benign alternatives, such as supercritical carbon dioxide. Finally, we perform simulations of supercritical water and aqueous solutions which have relevance to high-temperature supercritical water oxidation.

PUBLICATIONS

S. Salaniwal, S. T. Cui, P. T. Cummings, and H. D. Cochran, "Self-assembly of reverse micelles in water/surfactant/carbon dioxide systems by molecular simulation," Langmuir **15**, 5188 (1999).

S. T. Cui, P. T. Cummings, and H. D. Cochran, "Molecular dynamics simulation of the rheological properties of a model alkane fluid under confinement," J. Chem. Phys. **111**, 1273 (1999).

J. D. Moore, S. T. Cui, P. T. Cummings, and H. D. Cochran, "The transient rheology of a polyethylene melt under shear," Phys. Rev. E (in press).

http://flory.engr.utk.edu

Benchmarking Computational Chemistry Methods for Combustion and Process Modeling Needs

David Dixon, David Feller, and Giovanni Sandrone,
Pacific Northwest National Laboratory
Douglas McLemore and Steven Strauss, Colorado State University
Karl O. Christe, Air Force Research Laboratory
Ricky Kendall, Ames Laboratory/Iowa State University and
Pacific Northwest National Laboratory

RESEARCH OBJECTIVES

We are developing a series of benchmark calculations based on solving the electronic Schrödinger equation in order to reliably predict the energetics and kinetics of chemical processes involved in the combustion of hydrocarbon fuels as well as in nuclear waste remediation. Our goal is to develop a composite theoretical approach that reliably predicts a variety of thermodynamic quantities, including heats of formation, without recourse to empirical parameters, so as to minimize the number of expensive experimental measurements needed to model complex systems and to extend limited experimental results.

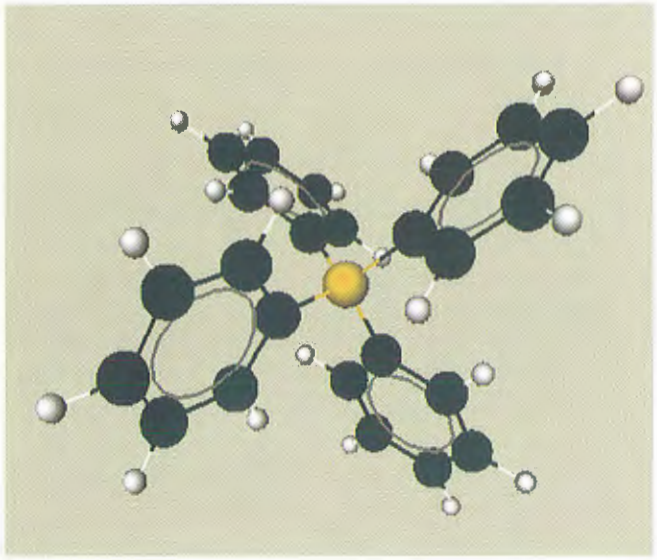
COMPUTATIONAL APPROACH

Our approach is to use coupled cluster theory with single and double excitations and a perturbative correction for the triples (CCSD(T)) to treat the n-particle problem in conjunction with extrapolations to the complete basis set limit of correlation-consistent basis sets to treat the 1-particle problem. We include additional corrections to account for core/valence, atomic spin-orbit, and molecular scalar relativistic effects as well as for higher order excitations. We are planning to predict kinetic parameters by using transition state theory (TST) including variational TST. We are completing the development of an interface between our computational chemistry code, NWChem, and the POLYRATE program, which combines variational TST and multidimensional semiclassical calculations of quantum tunneling effects.

ACCOMPLISHMENTS

Extensive calculations have been done on the fluoride anion and fluorocation affinities of more than 100 main group compounds. This has led to the development of the first quantitative Lewis acidity scale. Work on developing a generalized acid/base scale is under way.

Heats of formation were obtained from *ab initio* calculations for seven small silicon-containing molecules; for fluorinated compounds including CF_3 and its cation and anion, CF_4, C_2F_4, and $CFCF_3$; for benzene and six other small hydrocarbons; and for a number of phenyl/OH substituted boron compounds (neutrals and anions). We have improved our calculations of the heats of formation of CH, CH_2, CH_3, CH_4, HCO, and CH_2O.



Local density functional theory optimized structure of the anion tetraphenylborate, $(B(C_6H_5)_4)^-$, which was used in the In Tank Precipitation process at the Savannah River Site.

Design and implementation of an interface based on the Extensible Computational Chemistry Environment (Ecce) for calculating reaction energies and thermodynamic properties is continuing.

SIGNIFICANCE

Developments in computational chemistry over the next few years are likely to result in a major increase in our ability to compute the thermochemical properties of molecules as well as the kinetics of chemical reactions involved in combustion and atmospheric oxidation processes. In addition, the thermodynamic and kinetic properties of materials play a critical role in the design of most chemical processes, so improved modeling and simulation methodologies will help make U.S. industry more competitive globally and more responsive to environmental concerns.

PUBLICATIONS

D. A. Dixon, D. Feller, and G. Sandrone, "The heats of formation of simple perfluorinated carbon compounds," J. Phys. Chem. A **103**, 4744 (1999).

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Photonic Band Gap Materials

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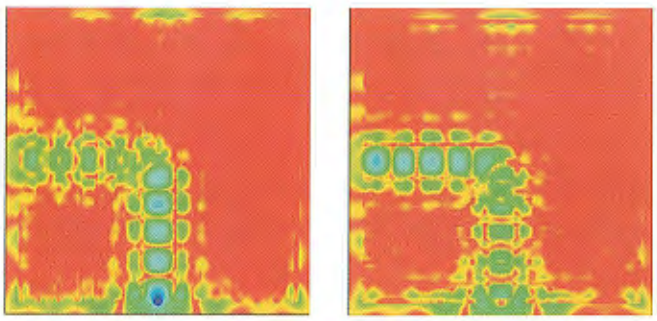
RESEARCH OBJECTIVES

This research project has two thrusts: (1) The design and development of novel structures and photonic devices in the infrared and optical regimes with full three-dimensional band gaps. These include unusual colloidal crystals being fabricated by our collaborators at Ames Laboratory, for photonic gaps at optical wavelengths. (2) Development of applications in the microwave and millimeter wave regime for existing 3D photonic band gap (PBG) crystals, especially those fabricated at Ames Laboratory. These include novel waveguides that can bend electromagnetic waves with bending radii of the order of a single wavelength.

COMPUTATIONAL APPROACH

The Transfer Matrix Method (TMM) is used to design and study PBG filters. Maxwell's equations are solved to determine the reflection and transmission of electromagnetic waves from a finite thickness PBG material. The method can incorporate realistic absorption- and frequency-dependent dielectric functions. The TMM code has been run on a variety of MPP systems including the Intel Paragon and Cray T3E. Added power and memory will enable us to study disordered systems and defect states in large cavities.

In the Finite Difference Time Domain (FDTD) method, Maxwell's equations are discretized on a real-space grid. The time evolution of the electromagnetic fields is calculated by solving the time-dependent Maxwell's equations. This code can simulate the radiation properties of antennas or the bending of light in a photonic crystal. A parallel version of this code has been developed for the Intel Paragon and workstation clusters. Some simple optimizations will allow it to run efficiently on the Cray T3E, where larger and more realistic systems can be simulated.



These figures are snapshots of the electromagnetic fields in two adjacent layers in a periodic dielectric system. Defects have been introduced so that the electromagnetic waves propagate around a corner, producing a waveguide with near perfect efficiency.

ACCOMPLISHMENTS

We have designed new photonic lattices, fabricated at Sandia National Laboratories, that can for the first time manipulate 1.5 micron wavelengths used for optical fibers. In joint work with the Sandia group, we designed an ultra-small optical cavity, with dimensions smaller than the wavelength of light. This single mode cavity has been fabricated at Sandia and is likely to be the smallest cavity ever at infrared wavelengths. We have utilized our FDTD method to calculate radiation patterns of antennas on and inside PBG crystals. We have found optimal configurations with improved radiation patterns that cannot be achieved by conventional materials.

SIGNIFICANCE

PBG structures have immense potential to develop novel materials and devices with desired electromagnetic signatures. Applications include suppression of optical radiation modes, higher-efficiency lasers, and new microwave and millimeter wave devices. The computational design of PBG structures has always been the first step in developing new photonic crystals. Computational simulation can rapidly test the electromagnetic behavior of new structures and then select the best-performing ones for fabrication. This research will open up new ways to manipulate light within these PBG structures, including the bending of light by waveguides and the ability to control emission of light within microcavities. These capabilities are essential in developing photonic devices that promise to be much faster than present-day electronic devices.

PUBLICATIONS

S. Y. Lin, J. Fleming, R. Biswas, M. M. Sigalas, K. M. Ho, B. K. Smith, D. L. Hetherington, W. Zubrzycki, S. R. Kurtz, and J. Bur, "A three dimensional photonic crystal in the infrared wavelengths," Nature **394**, 251 (1998).

S. Lin, J. Fleming, M. M. Sigalas, R. Biswas, and K.-M. Ho, "Photonic band gap microcavities in three dimensions," Phys. Rev. B **59**, 15579 (1999).

G. Subramania, K. Constant, R. Biswas, M. M. Sigalas, and K.-M. Ho, "Optical photonic crystals fabricated from colloidal systems," Appl. Phys. Lett. **74**, 3933 (1999).

http://cmp.ameslab.gov/ercap/pbg2000.html

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

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Environmental Molecular Sciences Laboratory,
Pacific Northwest National Laboratory
R. Shepard, A. F. Wagner, R. Stevens, J. L. Tilson, and M. Minkoff,
Argonne National Laboratory
C. W. McCurdy and A. T. Wong, NERSC,
Lawrence Berkeley National Laboratory
R. M. Pitzer, The Ohio State University
D. E. Bernholdt, Syracuse University
W. Ermler, Stevens Institute of Technology
K. G. Dyall, Eloret, NASA Ames Research Center

RESEARCH OBJECTIVES

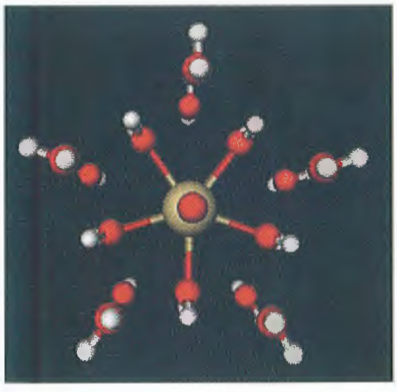
We aim to develop and apply the methods of relativistic quantum chemistry to assist in the understanding and prediction of the chemistry of actinide and lanthanide compounds.

COMPUTATIONAL APPROACH

The work involves determination of the electronic structure of molecules including relativistic effects necessary for heavy elements. 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 Cray J90s and the T3E.

Application work: Among many topics, we are studying the speciation of aqueous uranium (VI) with various ligands, 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.



A model for uranyl in aqueous solution: $(UO_2)^{2+}$ $(H_2O)_{15}$.

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.

ACCOMPLISHMENTS

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 (CI) calculations upon various actinide ions. Much effort has been devoted to developing and understanding accurate descriptions of the electronic spectra of various actinide and lanthanide ions. This is very challenging and has required development of new relativistic effective core potentials. New all-electron relativistic approximations that have been incorporated into NWChem are being tested by comparison with all-electron Dirac-Fock calculations. These new methods also require development of multiple new basis sets (up to three per atom).

SIGNIFICANCE

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

PUBLICATIONS

K. G. Dyall and E. van Lenthe, "Relativistic regular approximations revisited: An infinite-order regular approximation," J. Chem. Phys. **111**, 1366 (1999).

S. Yabushita, Z. Zhang, and R. M. Pitzer, "Spin-orbit configuration interaction using the graphical unitary group approach and relativistic core potential and spin-orbit operators," J. Phys. Chem. A **103**, 5791 (1999).

Z. Zhang and R. M. Pitzer, "Application of relativistic quantum chemistry to the electronic energy levels of the uranyl ion," J. Phys. Chem. A **103**, 6880 (1999).

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

Electronic Structure and Simulation Calculations of Reactive Chemical Systems

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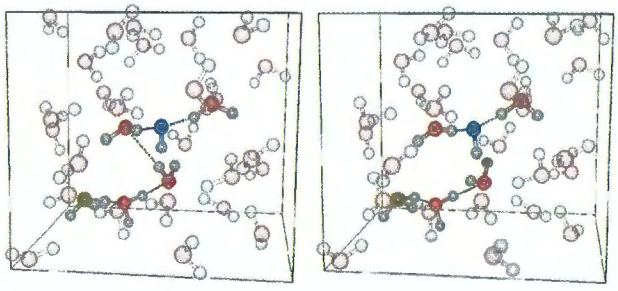
RESEARCH OBJECTIVES

(1) Exploration of density functional theory for simulation of ground and excited states of radicals. (2) Computational studies of unsaturated hydrocarbon radicals and ions. (3) Parallel electronic structure software code development. (4) Application of transition path sampling to weak acid dissociation in an aqueous environment. (5) Test of Car-Parrinello *ab initio* molecular dynamics (CPMD) force field for physically relevant nuclear configurations. (6) Development of large time step algorithms for transition path sampling.

COMPUTATIONAL APPROACH

(1) We are exploring whether ground states and low-lying excited states of radicals can be adequately described using time-dependent density functional theory (TDDFT) with existing functionals. (2) We are applying TDDFT to the problem of the excited states of unsaturated hydrocarbon radicals and ions. (3) We have pioneered a new method we call the Energy Renormalization Group (ERG) for obtaining a small number of judiciously chosen collective variables for describing long-range density matrix correlations in small-gap systems. (4) We use transition path sampling along with CPMD to simulate representative trajectories of H_2O dissociation. (5) We have created a formulation of transition path sampling that can be interfaced with any trajectory algorithm, and have used this formulation to combine transition path sampling with CPMD. (6) We apply coarse-grained methods that are consistent with principles of detailed balance and microscopic reversibility.



Transition states for water auto-dissociation involve the coincidence of two events. First, there must be a solvent fluctuation in local potential energy propelling the proton away from a nascent hydroxide ion. Second, this fluctuation must be accompanied by breaking of a hydrogen bond along the proton wire connecting the hydroxide and hydronium ions. The two illustrations show 32 water molecules shortly before (left) and after (right) crossing the auto-dissociation transition state surface. The oxygen atoms colored yellow and blue highlight the hydronium and hydroxide ions, respectively. The dotted lines show hydrogen bonding proton wires along which ionic species move relatively quickly.

ACCOMPLISHMENTS

(1) We have formulated and implemented a quasidegenerate single-reference second-order perturbation theory of electronic excitation energies. We have applied this method to evaluate excited states in large unsaturated organic species. (2) We have nearly completed a joint theoretical and experimental study of the reaction of H_2S with atomic carbon. (3) For several one- and two-dimensional model problems involving tight-binding Hamiltonians, we have been able to demonstrate near-linear scaling for the first time, using a parallel code on the Cray T3E. (4) We have demonstrated the applicability of transition path sampling to weak acid dissociation in an aqueous environment through preliminary studies of water dissociation in water, the basic kinetic step of pH. (5) We have shown that the CPMD force field for dynamically accessed configurations for proton transfer in the protonated water trimer is in excellent agreement with that predicted by higher level *ab initio* techniques. (6) We have devised a set of statistical methods for interpreting the behavior of transition paths in complex systems.

SIGNIFICANCE

Developing techniques that can reliably treat excited states, reliably break chemical bonds, and feasibly simulate molecules containing very large numbers of electrons will permit better simulations of mechanisms relevant to combustion chemistry and soot formation, structural biology, and nanocluster technology.

PUBLICATIONS

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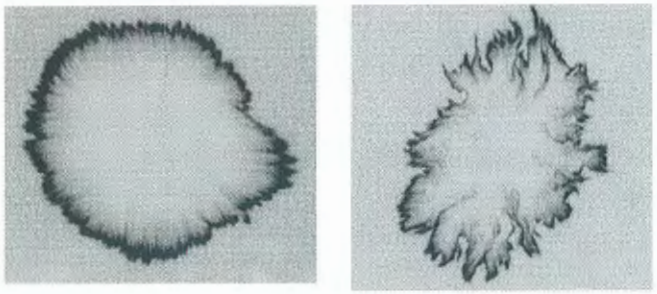
P. L. Geissler, C. Dellago, and D. Chandler, "Kinetic pathways of ion dissociation in water," J. Phys. Chem. **103**, 3706 (1999).

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

Particulate Dynamics in Filtration and Granular Flow

Joel Koplik and German Drazer,
City College of the City University of New York
Jean Pierre Hulin, Laboratoire FAST, Orsay, France
Jysoo Lee, Korea University, Seoul



Examples of flow in a self-affine fracture. A granite rock is fractured to produce a self-affine surface which is used as a mold for a transparent plastic copy. The rock and its copy are placed in register and then separated vertically to give a self-affine fracture. Fluid is injected through the center and flows out to the boundaries, and images of the front at two successive times are taken from above. The difference in the images indicates the location of the moving front. In Figure 1, the surfaces are simply separated vertically, producing a roughly circular outgoing fluid front. In Figure 2, however, the surfaces are shifted laterally, leading to a surprisingly strong anisotropic flow. (Figures provided by Harold Auradou and Jean Pierre Hulin, Laboratoire FAST.)

RESEARCH OBJECTIVES

We are concerned with two related topics involving the motion of particulate matter in porous media formations of relevance to transport in industrial and geological porous media: (1) A quantitative study of the dynamics of deep bed filtration—filtering suspended particles from a solvent when the mixture passes through a porous medium. We aim to determine how the parameters of the process such as flow rate, filtrate concentration, and porous medium structure control the efficiency of filtration, the time scales for the process, and the spatial distribution of the deposit. (2) A study of flow, passive tracer dispersion, and depositional processes in the self-affine fractures often observed in naturally fractured rock. In such systems the rock surfaces have long-range correlations which have been shown to significantly enhance and modify the dynamics of passive tracers used as diagnostic tools. We further wish to examine the motion of rock suspended in flowing fluid in fractured geological formations, and in particular study the evolution of the fractured pore space as deposition occurs.

COMPUTATIONAL APPROACH

In statistically isotropic and homogeneous porous media, transport properties are readily obtained from an equivalent network description in which the pore space is modeled as a "ball and stick" network with appropriately sized elements and connection topology. The relevant network-scale simulations of particle deposition may then be formulated as a time-sequence of analog resistor network problems, and amount to averaging over solutions of large sets of linear algebraic equations. The problem of flow and particle deposition in self-affine fractures occurs at a different scale, and the problem here is to efficiently solve for the flow in a highly irregular and evolving geometry. This case is treated using the lattice Boltzmann method, which is optimal for flow problems in complicated regions because only a geometrical specification of the solid region is needed.

ACCOMPLISHMENTS

We have completed and published the initial work needed for both problems. In porous medium filtration, we have determined the junction rules for particle motion around grains in a porous medium, and can now abstract the local geometry into a suitable random network. In fracture flow, we have performed the initial (approximate) simulations showing that self-affine fractures lead to enhanced dispersion, and have modified a borrowed lattice Boltzmann code for the purpose of systematically studying passive tracer dispersion as well as the behavior of suspended particles large enough to modify the flow field.

SIGNIFICANCE

The efficient extraction of water and hydrocarbon resources from underground reservoirs, as well as the use of underground formations as waste disposal sites, requires a full understanding of the dynamics of the flow of fluids and various suspended matter in the disordered porous media which comprise geological formations and reservoirs. This research studies the transport and deposition of solid particulates which may clog or perhaps break open new flow channels in these systems, and the effects of subtle correlations resulting from fracture processes on tracer tests. In addition, some of the results are relevant to commercial filtration processes used in purification and manufacturing.

PUBLICATIONS

J. Lee and J. Koplik, "Microscopic motion of particles passing through a porous medium," Phys. Fluids **11**, 76 (1999).

F. Plouraboue, J. Koplik, J. P. Hulin, and S. Roux, "Numerical study of geometrical dispersion in self-affine rough fractures," Phys. Rev. E **58**, 3334 (1998).

S. Rojas and J. Koplik, "Nonlinear flow in porous media," Phys. Rev. E **58**, 4776 (1998).

Quantum and Classical Simulations of Clusters, Nanostructural Manipulations, and Nanotribology

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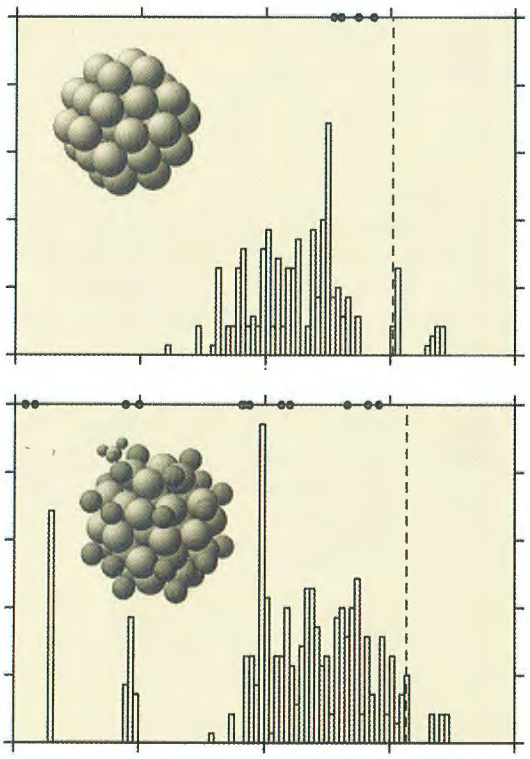
RESEARCH OBJECTIVES

This project is investigating the microscopic physical and chemical processes underlying the properties of novel materials. These investigations aim at discovering and elucidating size-dependent evolutionary patterns of materials properties, bridging the molecular, cluster, and condensed-phase regimes.

COMPUTATIONAL APPROACH

Our computational approaches include large-scale classical molecular dynamics, employing tested many-body interactions, and *ab initio* quantum molecular dynamics (in conjunction with norm-conserving non-local pseudopotentials and a plane-wave basis) based on local-spin density functional theory (LSD) with the inclusion of generalized exchange-correlation gradient corrections. In these *ab initio* simulations, the dynamics of the ions evolve on the concurrently calculated electronic ground state (Born-Oppenheimer, BO) potential energy surface, using the BO-LSD-MD method. We also employ various structural optimization methods (conjugate-gradient and variants thereof, simulated annealing and genetic algorithms), as well as an arsenal of analysis techniques, including animation.



Density of Kohn-Sham states (DOS) of the (a) Au_{38} cluster and (b) passivated $Au_{38}(SCH_3)_{24}$ cluster. The dots on the upper axes denote the eigenenergies of (a) Au atomic valence states, and (b) SCH_3 molecular valence states. The dashed line denotes the Fermi energy. The width of the energy bins is 0.2 eV. The insets show the optimized structures of the bare gold and the passivated clusters, respectively. In (b) the sulfur atoms are depicted as darker spheres and only one CH_3 group is shown.

ACCOMPLISHMENTS

Ab initio investigations of the electronic structures and optimal configurations of gold nanocrystals (Au_{38}) passivated by methylthiols showed that the electronic states of the bare cluster are modified upon passivation by an organic monolayer, and that added charges are delocalized on the passivating layer. Such clusters serve as quantum dots, capable of accepting charge and transporting electrons between source and drain electrodes. Our study demonstrated the first *ab initio* calculation of the capacitance of such passivated nanocrystals. Investigations of the electronic structure and addition-energy spectrum in two-dimensional quantum dots led to the discovery of spontaneous symmetry-breaking at zero and low magnetic fields in single dots and dot molecules. The discovery of Wigner molecules whose formation can be controlled via voltage gates suggests new strategies for information coding and logic gates using quantum dots. Investigations of the mechanisms of the low-temperature combustion of CO catalyzed by small gold clusters adsorbed on the surface of magnesium oxide elucidated the origins of the clusters' surprising catalytic activity. These results are significant for the development of novel catalytic systems.

SIGNIFICANCE

Understanding the microscopic origins of the properties of materials with reduced physical dimensions is essential for the utilization of such materials in advanced technologies. *Small is different*—new and often unexpected behavior emerges whenever the physical size of the materials system approaches a length-scale characteristic to the phenomenon under study.

PUBLICATIONS

H. Häkkinen, R. N. Barnett, and U. Landman, "Electronic structure of passivated $Au_{38}(SCH_3)_{24}$ nanocrystal," Phys. Rev. Lett. **82**, 3264 (1999).

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W. D. Luedtke and U. Landman, "Structure and thermodynamics of self-assembled monolayers on gold nanocrystallites," J. Phys. Chem. B **102**, 6566 (1998).

Quantum Monte Carlo for Electronic Structure of Combustion Systems

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Xenophon Krokidis, Lawrence Berkeley National Laboratory
Nigel W. Moriarty, University of California, Berkeley

RESEARCH OBJECTIVES

This research will accomplish the accurate specification of important reaction pathways in the postulated mechanism of soot formation.

COMPUTATIONAL APPROACH

The version of diffusion Monte Carlo (DMC) that is used employs effective core potentials to minimize computational effort. Variational Monte Carlo computations are carried out to test trial functions for DMC constructed as products of independent particle wave functions, e.g., HF, MCHF, and CI, and correlation functions that depend on interparticle distances.

ACCOMPLISHMENTS

We have quantitatively characterized the important pathways leading to the formation of cyclopentadienyl radical from the reaction of propargyl radical with acetylene to order 1 kcal/mol. Further, we have determined the heat of formation of the radical to 1 kcal/mol—essential information in understanding the mechanism of reaction. We have also been able to resolve uncertainty connected with the ground state of cyclopentadienyl radical and to establish it firmly as a doublet A2 state. We have unambiguously characterized bonding in propargyl radical using the electron localization function (ELF) method (see figure). We have determined the atomization energy of propargyl radical to an accuracy of 1 kcal/mol using the DMC method and have obtained a result in excellent agreement with experiment.

SIGNIFICANCE

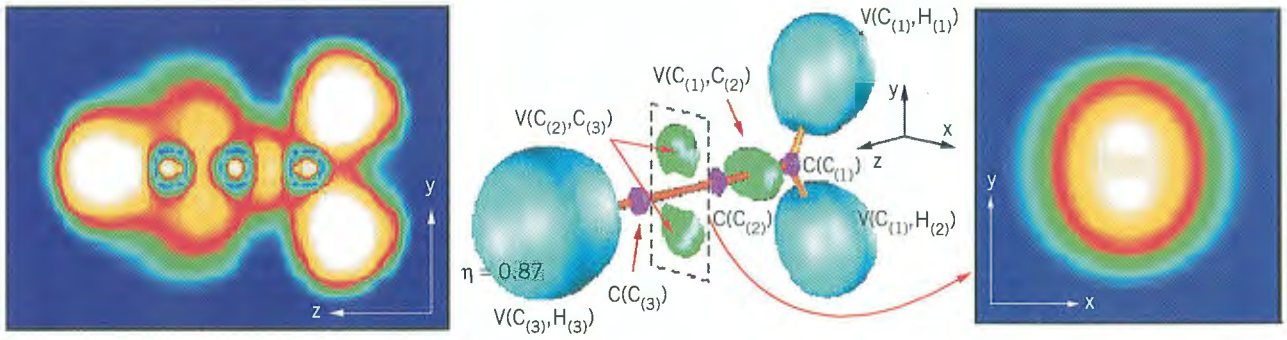
With elementary steps determined to 1 kcal/mol, uncertainties in reaction paths can be resolved, removing ambiguity in mechanisms for the formation of successively larger precursors to soot formation. The ultimate goal is full characterization of the mechanism of soot formation, which will provide valuable insight on how to reduce a major pollution source.

PUBLICATIONS

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. (in press).

J. C. Grossman, W. A. Lester, Jr., and S. G. Louie, "Cyclopentadiene stability: Quantum Monte Carlo, coupled cluster, and density functional theory determinations," Mol. Phys. **96**, 629 (1999).

X. Krokidis, N. W. Moriarty, W. A. Lester, Jr., and M. Frenklach, "Propargyl radical: An electron localization function study," Chem. Phys. Letters (in press).



The figure shows domains of localization (or "basins" in topological terms) of pairs of electrons in C_3H_3 as they are reproduced by ELF. These domains are distinguished as core (C) or valence (V), and correspond to regions in real space where pairs of electrons are likely to be localized. The valence localization domains may correspond to bonds or regions where lone pairs or single electrons (in the case of radicals) may be found. Within this approach multicenter bonds are possible.

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

The objective is 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 and magnetism independently.

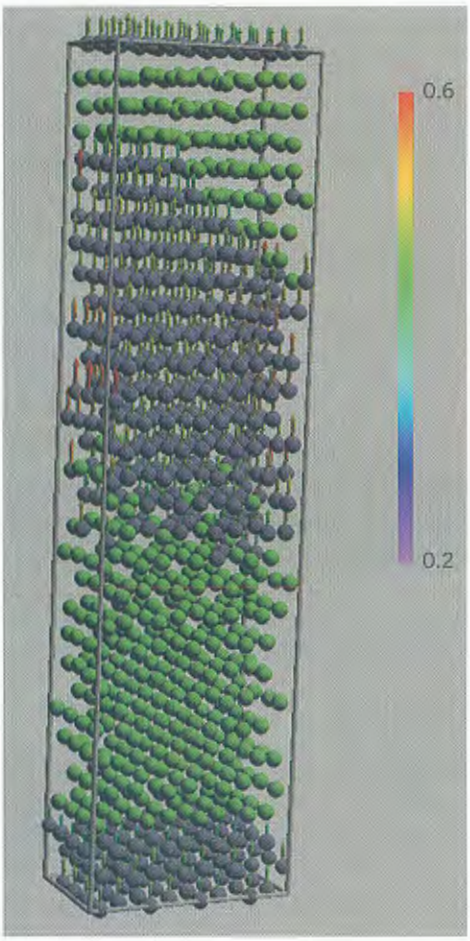
COMPUTATIONAL APPROACH

A number of first-principles techniques are used to perform fundamental studies of the atomistic, electronic, and magnetic structure of metals, alloys, and semiconductors. The goal is to understand the influence on properties of microstructural defects and inhomogeneities. First principles methods include an iterative pseudopotential (IP) method, locally self-consistent multiple scattering (LSMS) and layer Korringa-Kohn-Rostoker (LKKR) methods, and tight-binding molecular dynamics (TBMD). In addition, first principles spin dynamics is being developed as a fundamental theory of the magnetic properties of metals and alloys.

ACCOMPLISHMENTS

Non-collinear magnetic structure at interfaces: The LSMS method was used to calculate the magnetic structure at interfaces between Cu and permalloy (Py). Multiple non-collinear metastable magnetic configurations with similar energies were found. The non-collinearity deduced from these calculations explains the observed trend in saturation magnetization as a function of permalloy layer thickness. The same method was used to study the magnetic structure of Cu-Ni interfaces using very large cell models (883 atoms) obtained from independent deposition modeling. Taken together, the work on Cu-Py and Cu-Ni interfaces demonstrates that the constrained local moment theory implemented in the LSMS can provide accurate descriptions of the magnetic structure at technologically important magnetic interfaces.

Atomistic simulations of martensitic transformations: Large-scale simulations of both the high-temperature body-centered-cubic (bcc) phase of Zr, as well as the transformation from bcc to hexagonal-closest-packed (hcp) have been performed. These simulations allow for a full calculation of the dynamic structure factor and how the scattering evolves as the system transforms from the bcc to the hcp phase. The actual atomic arrangements are observed during the transformation process, in order to learn about the nucleation and growth processes. The calculated X-ray scattering of the high-temperature phase shows the characteristic streaking of the Bragg peaks observed in experiments. By examining the scattering as a function of time, it has been shown that the streaking in the high temperature phase mimics the coherent movement of Bragg peaks that occurs during the transformation. This demonstrates that the observed anomalous scattering is caused by coherent fluctuations towards the hcp phase. The development of microstructure has also been observed as the transition progresses.

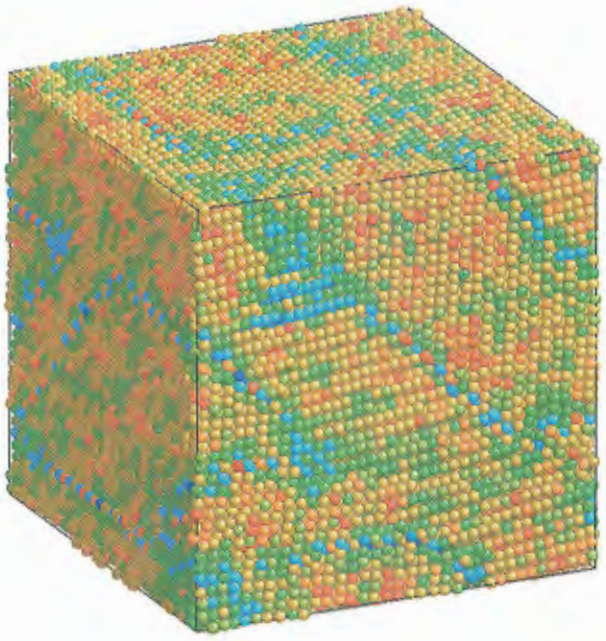


Magnetic structure at interfaces: Distribution of magnetic moments in a Cu-Ni multilayer calculated using the first-principles LSMS method. Ni atoms are coded blue and Cu atoms green. The size of the magnetic moments is color-coded onto the arrows. Red arrows indicate Ni atoms whose magnetic moment is near the Ni bulk value. The magnetic moment is suppressed on atoms at the Ni-Cu interface. The atomic positions were obtained from Monte Carlo modeling of the deposition process. The structural model contains 883 atoms per unit cell.

Dislocation-nucleated twin boundaries in hcp metals: One of the fundamental questions in materials science is to understand the nucleation and growth of twin boundaries, and the competition between twinning and slip deformation modes. These issues can play an important role in the ductility of materials and are cur-

rently being studied in hcp metals, where the ability to twin makes Zr and Ti very ductile even at low temperatures. Conversely, materials such as Mg and Be do not twin, and are brittle. Large-scale atomistic simulations have shown that twin boundaries may be nucleated via dislocation cores. One such observation was of a dislocation in an hcp metal that had dissociated into a large twin nucleus, with a small partial dislocation at the bottom of the simulation cell. These two dislocations are connected by a stacking fault, making the arrangement difficult to move. Instead, tension along the c-axis has the effect of causing the twinned region to grow. This arrangement has not been seen in previous simulations, due to the small simulation sizes used previously. This provides a microscopic explanation for the observed fact that systems that twin under c-axis compression also twin under tension.

First-principles calculations of Mo_5Si_3 and Ti_5Si_3: Intermetallic M_5Si_3-type silicides have been of great interest as potential candidates for high-temperature materials operating above 1500 C. First-principles calculations for the phase stability, bonding mechanism and elastic properties of this material have been performed. Results are in good agreement with experimental measurements. An extensive study of the lattice parameters of C, B, N, and O-doped D_{88}-Ti_5Si_3 has been made. In collaboration with the experimental group of M. Akinc at Ames Lab, it was demonstrated that the calculated heats of formation and the variation of lattice constants and interatomic distances compare well with experimental data.



Atomistic simulations of martensitic transformations: Final simulation cell obtained during a simulation of a transformation of Zr from the high-temperature bcc phase to the low-temperature hcp phase. The atoms are colored according to potential energy (with blue being the highest). The domain walls are evident. The system develops long domains along the [111] direction as the transition progresses. This allows three different hcp domains to form.

Core level shifts in metallic alloys: Experimentally, core level binding energy shifts can be measured using electron spectroscopy for chemical analysis (ESCA). Chemical shifts and their distribution about their mean have been calculated for three alloy systems, CuPd, CuZu, and AgPd. The calculations were based on large supercell models of the disordered phase that contain hundreds of atoms and were performed using first principles order-N LSMS method. Results were compared with predictions based on the commonly used ESCA potential model that relates the core shifts to charge transfer. Since the charge transfer is also obtained in the first principles calculations, this allows detailed testing of the ESCA model. While first principles calculations provide reliable predictions for the chemical shifts in the alloys, the relationship between chemical shifts and the charge transfer do not agree with the ESCA potential model.

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.

PUBLICATIONS

G. M. Stocks, B. Ujfalussy, X. Wang, D. M. C. Nicholson, W. A. Shelton, Y. Wang, and B. L. Gyorffy, "Towards a constrained local moment model for first principles spin dynamics," Phil. Mag. B **78**, 665 (1998).

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

Semiclassical Initial Value Representation Methods for Reaction Dynamics

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RESEARCH OBJECTIVES

This research aims to develop accurate simulation methods to investigate quantum processes and spectroscopy associated with realistic chemical reactions.

COMPUTATIONAL APPROACH

The algorithms are based on efficient semiclassical initial value representation (SC-IVR) strategies that generalize classical molecular dynamics techniques to include quantum interference and even tunneling to some extent within the description. We evaluate a high dimensional integral over initial conditions for semiclassical trajectories that evolve according to classical equations of motion. Trajectories are integrated independently of each other and are computed in parallel.

ACCOMPLISHMENTS

Accomplishments achieved during FY 1999 include:

1. The development of adiabatic SC-IVR methods for simulations of the photo-excited double proton transfer reaction in a model DNA base pair.
2. The development of forward-backward SC-IVR methods for simulations of ultrafast pump-probe photoelectron spectroscopy.
3. Simulations of electronic nonadiabatic effects in both the photofragment rotational distributions and the photoabsorption cross section associated with the photodissociation dynamics of ICN in the A continuum.
4. The development of a full dimensional excited state potential energy surface, obtained according to a reaction surface approach, and the simulation of the excited-state intramolecular proton transfer reaction in 2-(2'-hydroxyphenyl)-oxazole using SC-IVR.
5. The development of an efficient algorithm for time slicing the SC-IVR.

SIGNIFICANCE

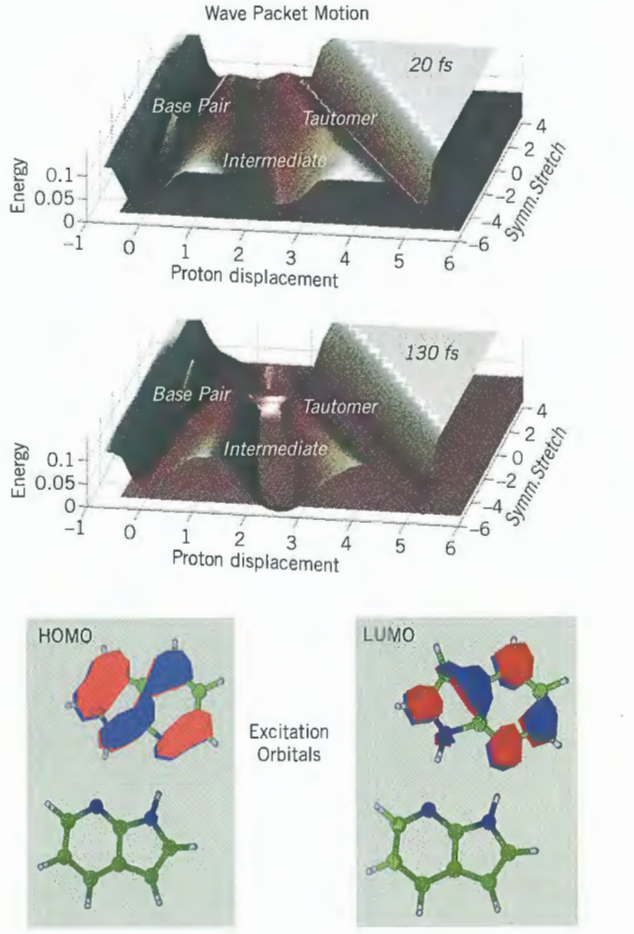
Incorporating quantum mechanical effects into simulations of chemical reaction dynamics, including modeling of biological systems, could have a major impact on research and technology development.

PUBLICATIONS

V. S. Batista, M. T. Zanni, B. J. Greenblatt, D. M. Neumark, and W. H. Miller, "Femtosecond photoelectron spectroscopy of the I2– anion: A semiclassical molecular dynamics simulation method," J. Chem. Phys. **110**, 3736 (1999).

V. Guallar, V. S. Batista, and W. H. Miller, "Semiclassical molecular dynamics simulations of excited state double proton transfer in 7-azaindole dimers," J. Chem. Phys. **110**, 9922 (1999).

X. Sun and W. H. Miller, "Forward-backward initial value representation for semiclassical time correlation functions," J. Chem. Phys. **110**, 6635 (1999).



The ultrafast excited state double proton transfer in the tautomerization reaction of photo-excited 7-azaindole dimers is visualized in terms of the nuclear wave packet motion on the S1 CIS electronic excited state potential energy surface. Proton transfer usually occurs during the first intermonomer symmetric-stretch vibration, about 100 fs after photoexcitation of the system, and produces an initial 15% population decay of the reactant base-pair, which is significantly reduced by isotopic substitution. The S1 electronic excited state is found to have predominant (HOMO)→(LUMO) MO excitation, and the largest oscillator strength constant in the FC region.

Advanced Computation for Geophysical Inverse Problems

Don Vasco, Lawrence Berkeley National Laboratory
Osni Marques, NERSC, Lawrence Berkeley National Laboratory
Lane Johnson, University of California, Berkeley

RESEARCH OBJECTIVES

The Center for Computational Seismology is developing computational methods for solving geophysical inverse problems. Inverse methods image the Earth by taking observations gathered at the Earth's surface and inferring the internal structure of our planet. Our prototype problem uses several million seismic arrival times to estimate the full three-dimensional velocity structure of the Earth. In addition to producing images of Earth structure, we seek to estimate the reliability of the images by computing our resolution of Earth structure and the associated uncertainties of our estimates.

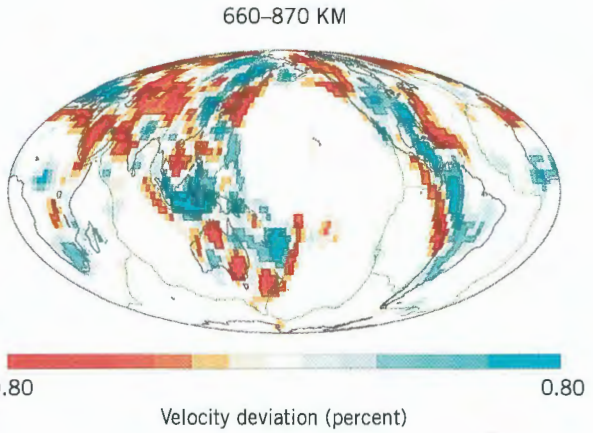
COMPUTATIONAL APPROACH

The estimation of structure and the model assessment can be reduced to large-scale problems in linear algebra. Ideally we would invert the matrix relating the seismic travel times to the Earth's structure. However, the matrix is approximately 1 million rows by 300,000 columns, precluding a formal inversion. We use an iterative block Lanczos code to estimate successive singular values and singular vectors associated with our data matrix.

ACCOMPLISHMENTS

In the past year we were successful in imaging the Earth on a 6° by 6° scale (the lateral dimension of a typical cell). We were able to image subducting tectonic plates, ocean ridges, and velocity anomalies at the base of the Earth's liquid core. We ported the block Lanczos code to the T3E and applied it to assess the resolution of the 6° by 6° grid, some 1 million equations by 100,000 unknowns. We were able to calculate up to 9,000 Lanczos values and vectors. Our estimates of the full three-dimensional Earth velocity structure are the first ever, and our model assessment is the first complete analysis of resolution and uncertainty.

Recently, two research groups have produced models of mantle structure (velocity variations in only the mantle) on a finer scale of 1°–3°. Such small cells are necessary for imaging features like the thin subducting slabs. We are now extending our work to the finer 3° by 3° grid in the mantle while retaining our current 6° grid in the Earth's core. Thus, we will be able to estimate velocity structure and assess its reliability on a finer scale. The new finer grid will have almost 4 times the number of parameters. In order to estimate resolution and uncertainty, we must calculate between 10,000 and 30,000 Lanczos values and vectors.



An image of the compressional velocity variation within the Earth's mantle, that is, the velocity at which seismic waves propagate through the mantle. Cold colors signify higher average velocities, while warm colors signify lower velocities. The high velocities circling the Pacific are thought to represent subducting crust associated with plate tectonics.

SIGNIFICANCE

To date, seismic research has focused on specific regions of the Earth, such as the mantle, using only data most sensitive to these regions. Ours is the first study to attempt to utilize all seismic arrival times to solve for the structure of the entire Earth—crust, mantle, and core. We are also the first to conduct a thorough assessment of our model by calculating model parameter resolution and uncertainty. No one to date has adequately characterized the reliability of the finer-scale models, so, it is not clear if the seismic data actually allow us to image such fine details. Our work will provide the first definitive answer to this question.

The Lanczos code being used here has other applications such as structural engineering, web search engines, and numerical applications.

PUBLICATIONS

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D. W. Vasco, J. E. Peterson, and E. L. Majer, "Resolving seismic anisotropy: Sparse matrix methods for geophysical inverse problems," Geophysics **63**, 970 (1998).

Chemical Scaling Studies in Combustion

Albert F. Wagner, Larry A. Curtiss, Peter Zapol, and Michael Minkoff,
Argonne National Laboratory

RESEARCH OBJECTIVES

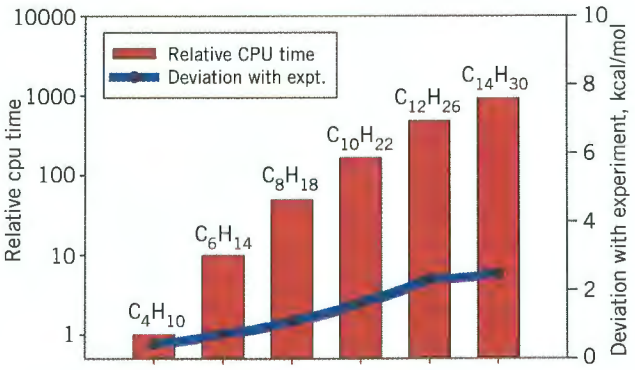
High fidelity simulations of combustion devices will require the application of (1) electronic structure methods to the thermochemistry of hydrocarbons with up to 16 carbon atoms, (2) electronic structure methods to account for local and bulk environmental effects at active molecular sites in catalytic converters, and (3) theoretical kinetics approaches to much larger combustion chemistry problems than are currently examined. Our objective is to carry out scaling studies of code performance using existing or emerging algorithms in both the kinetics and electronic structure areas.

COMPUTATIONAL APPROACH

Most of this work utilizes the NWChem package and PETSc software. The applications codes themselves are written in Fortran.

ACCOMPLISHMENTS

In our thermochemistry effort, the most expensive step in the G3(MP2,CCSD) method, namely a single-point CCSD(T) calculation, was carried out on linear alkane hydrocarbons up to $C_{14}H_{30}$. These results were used in the G3(MP2,CCSD) method to obtain enthalpies of formation that agree well with experiment. It was found that the CCSD CPU time is proportional to the number of Gaussian basis functions to the power of 5.8. The relative times and accuracies for a series of alkanes are shown in the figure. The atomic basis set for the largest molecules, $C_{14}H_{30}$, had 270 basis functions, giving a CPU time of almost 11 hours using 256 PEs, or 2850 hours of serial time. Besides establishing the scaling dependencies for computer resources, these calculations test G3 theory accuracy for much larger molecules than those included in the usual test sets and provide a solid basis for accurate chemical calculations of large hydrocarbon reaction energetics.



Relative total CPU times and deviations with experimental enthalpies of formation for quantum chemical energy calculations on C_nH_{2n+2} linear alkanes containing up to 14 carbons.

In our catalytic effort, we have used NWChem on the T3E to study with Hartree-Fock theory the effect on reaction energies of including up to 112 tetrahedral atoms of the zeolite framework about the active site. Time-to-solution scales as the 2.1 power of the number of Gaussian basis functions. The largest system completed (58 tetrahedral atoms) takes about 160 PE hours. The environmental effects track with size such that by 112 tetrahedral atoms, we believe for even polarizable reactants the environmental effects will be converged.

In our kinetic effort, we completed a successful port and initial scaling studies of our cumulative reaction probability code with the PETSc linear solver.

SIGNIFICANCE

We hope to provide baseline information that will motivate either new method development or define the scale of applications studies that would be required in high fidelity combustion simulations. Besides establishing the scaling dependencies for computer resources, these calculations have the following benefits: (1) for the thermochemistry studies, extending tests of G3 theory accuracy to much larger molecules than those included in the usual test sets, providing a solid basis for accurate calculations of large hydrocarbon reaction energetics; (2) for the catalysis studies, determining the sphere of influence of chemical and electrostatic forces around a catalytic site and thus contributing to more approximate but efficient theoretical methods; (3) for the kinetics studies, shedding light on how many degrees of freedom in a reaction need to be explicitly treated with quantum dynamics and how many are just spectators to the reaction and need be only approximately and implicitly included.

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L. A. Curtiss, K. Raghavachari, P. C. Redfern, A. G. Baboul, and J. A. Pople, "Gaussian-3 theory using coupled cluster energies," Chem. Phys. Lett. **314**, 101 (1999).

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L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolov, and J. A. Pople, "Gaussian-3 (G3) theory for molecules containing first and second-row atoms," J. Chem. Phys. **109**, 7764 (1998).

Application of Electronic Structure Methods to Large Semiconductor Quantum Nanostructures

Alex Zunger, National Renewable Energy Laboratory

RESEARCH OBJECTIVES

We are studying the electronic and optical structure of a range of semiconductor quantum dots at the atomistic level. The study focuses on both one-body electronic structure and many-body (configuration interaction) treatments.

COMPUTATIONAL APPROACH

We have developed a parallel Folded Spectrum Method (FSM) code that allows us to find the exact near-edge eigenenergies and eigenfunctions of million-atom systems using an accurate, pseudopotential plane-wave description. We are using this code to study the electronic structure of million-atom quantum dots.

We have developed a set of codes to calculate the Coulomb, exchange, and polarization integrals associated with the near band edge levels calculated by the FSM. We are using this code to predict quantities such as singlet-triplet exchange splittings of excitons in quantum dots.

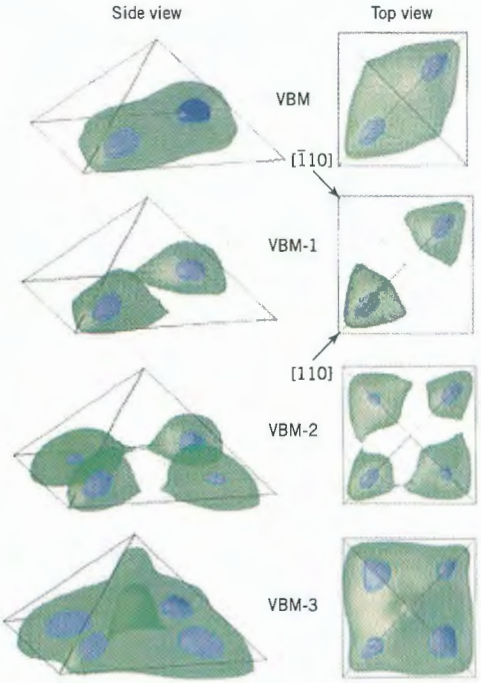
We have developed the first of a new generation of local-density approximation codes which feature many algorithmic advances over the standard parallel Car-Parinello or conjugate gradient codes currently in use.

ACCOMPLISHMENTS

We have calculated the electronic structure of self-assembled InAs quantum dots embedded in GaAs. We have investigated the dependence of the optical properties on the different shapes, sizes, and composition profiles in the dots. Using these results to analyze measured optical spectra has enabled us to distinguish between several proposed models for the shape and composition profile of these quantum dots.

We have studied the difference between embedded (in GaAs) and freestanding InAs quantum dots. We found much larger quantum confinement effects in the freestanding quantum dots and big wavefunction spillage outside the quantum dot for the embedded quantum dot. We also found one unusual X-derived state bound outside the surface of the InAs quantum dot, induced by the compressive strain on the GaAs matrix. When pressure is applied to the system, this X state will cross through the internal Gamma derived states and quench the quantum dot photoluminescence. This finding has been confirmed by experiment.

The electronic structure of arrays of vertically stacked quantum dots has also been calculated. The dot-dot interactions have been analyzed in terms of the interaction between the strain profiles of the quantum dots and the coupling of their wavefunctions.



Isosurface plots of the charge densities of the valence-band states for the b=20a pyramids. The charge density equals the wave-function square, including the spin-up and -down components. The level values of the green and blue isosurfaces equal 0.25 and 0.75 of the maximum charge density, respectively.

This analysis has been used to interpret the optical spectra of quantum dot samples grown to contain multiple levels.

SIGNIFICANCE

The electronic, optical, transport, and structural properties of semiconductor nanostructures (films, quantum dots, and quantum wires) have potential applications in a whole new set of nanoscale devices such as lasers, sensors, and photovoltaics.

PUBLICATIONS

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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).

http://www.sst.nrel.gov

Modeling 3D Decaying Turbulence on the Sphere with SEAM

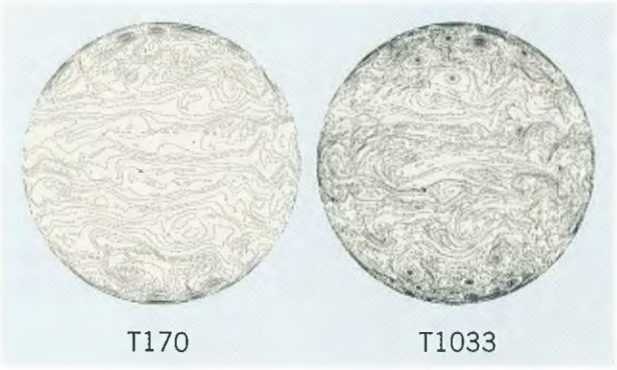
Ferdinand Baer, University of Maryland
Joseph J. Tribbia, National Center for Atmospheric Research
Mark Taylor, Los Alamos National Laboratory

RESEARCH OBJECTIVES

Our goal is to use the parallel efficiency of SEAM (Spectral Element Atmospheric Model) to perform simulations of three-dimensional decaying stratified turbulence on a rotating sphere. Decaying geophysical turbulence simulations have so far been carried out in spherical geometry only with two-dimensional models. In three dimensions, it has previously only been possible to carry out these types of experiments with filtered equations in periodic Cartesian domains, such as the well known quasi-geostrophic experiment carried out by McWilliams, Weiss, and Yavneh. With the SEAM model on 128 nodes of the T3E, we will be able to perform this simulation of rotating, stratified turbulence for the first time using the full primitive equations at very high resolution and in full spherical geometry.

COMPUTATIONAL APPROACH

SEAM is a spectral element atmospheric global circulation model which is ideal for MPPs such as the T3E. SEAM achieves almost perfect parallel scalability up to 256 processors. SEAM has proven to be spectrally accurate, producing results of comparable accuracy to the more conventional spherical harmonic based climate models.



The potential vorticity on Jupiter after integrating the dynamical equations on that planet using the SEAM model for 276 days. Two different truncation experiments are shown. Note how much more detail can be seen in the jet streaks using T1033, one of the highest-resolution experiments yet attempted.

ACCOMPLISHMENTS

In the past year we made many preliminary 3D decaying turbulence runs and discovered that the conventional initial conditions used for these types of runs (with simplified equations) are ill-posed for the full 3D primitive equations used in atmospheric modeling. We have addressed this issue by developing a 3D nonlinear balance procedure which creates initial data with random vorticity but with physically correct correlations between the horizontal and vertical scales. The nonlinear balance equations need to be solved only once for each resolution, and this is done efficiently with several spherical harmonic expansions. Despite this difficulty, intriguing results were obtained regarding the columnization of vortices in the primitive equations. This was heretofore only observed in quasi-geostrophic systems. Similarly, interesting coherent vortex formation was noted in simulations with planetary rotation and radius similar to Jovian values. These had previously been noted in shallow water computations.

SIGNIFICANCE

With the strong emphasis on global modeling of the climate system, substantial interest is developing on the evolution of regional climate. This requires an interface among many scales in a model and an efficient way of doing this. SEAM is ideal for this purpose because it not only allows for small-scale prediction at arbitrary locales over the globe—those regions for which the modeler has a particular interest relating to a specific climate or event—but also is optimized to do such integrations on an MPP system. Thus SEAM should be a desirable alternative to other climate models for predicting both regional and global climate events simultaneously and in a highly efficient, real-time environment.

PUBLICATIONS

M. Taylor, R. Loft and J. Tribbia, "Performance of a spectral element atmospheric model (SEAM) on the HP Exemplar SPP2000," Parallel Computing (submitted).

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Computer Simulation of Enzyme Reactions

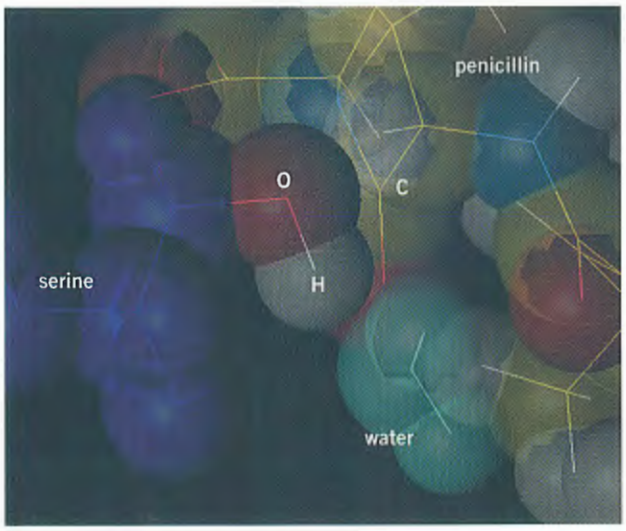
Paul Bash, Northwestern University Medical School

RESEARCH OBJECTIVES

The most successful defense bacteria have developed against antibiotics is the expression of enzymes known as b-lactamases, which hydrolyze the amide bond in the b-lactam ring of antibiotic agents such as penicillin and cephalosporin. Despite intensive experimental scrutiny, basic information about how these enzymes achieve their catalytic efficiency is still lacking. This project uses computational techniques to define the specific chemical mechanisms employed by the enzyme TEM-1, a prototypical class A b-lactamase, and AmpC, a prototypical class C enzyme. This research will provide insights into the roles of the different active-site residues in substrate recognition and binding and in the catalytic process.

COMPUTATIONAL APPROACH

Our hybrid quantum/molecular mechanics method (QM/MM) begins with structural information obtained from x-ray crystallography and uses first-principles physical and chemical numerical methods, calibrated to characterize the basic chemical interactions found in the b-lactamase system, to describe the catalytic process at an atomic level. This hybrid method utilizes a semiempirical quantum mechanics description of atoms in the active site while representing the remaining atoms with a molecular mechanics model. We use the *ab initio* quantum mechanical code Gaussian 98, the CHARMM molecular mechanics code, and the semiempirical QM code MOPAC97.



The enzyme beta-lactamase with the drug penicillin bound to its active site. A hydoxyl oxygen group (OH) of the enzyme is in position for the transfer of a proton (H) to a water molecule and for the nucleophilic attack of an oxygen (O) on the carbonyl carbon (C) of penicillin.

ACCOMPLISHMENTS

We have performed several molecular dynamics simulations of the TEM-1 enzyme with a penicillin substrate to gain insights into accessible conformations of the enzyme/substrate (Michaelis) complex. We used a molecular mechanics Hamiltonian, and we were interested in defining the roles of various active-site residues in binding and orienting the substrate into a conformation suitable for the catalytic reactions to proceed. We performed four separate simulations of the TEM-1 b-lactamase using different starting conformations to assess the sensitivity of our calculations to initial conditions. The results of the simulations are consistent with two of three proposed mechanisms for the acylation step of the reaction. These simulations provide insights into the roles of several residues in binding and orienting the substrate in the active site.

We have found that the interactions between Ser-130, Lys-234, Ser-235, and Arg-244 and the carboxylate oxygen atoms of the substrate are essential for securing the substrate in the active site. Additionally, the O8 carbonyl oxygen of the b-lactam ring interacts with the main chain nitrogen atoms from Ser-70 and Ala-237. The N14 nitrogen and O16 oxygen atoms of the carboxyamide group interact with a main chain carbonyl oxygen from Ala-237 and the side chain of Asn-132, respectively. Together, these interactions orient the substrate in the active site into a conformation suitable for the subsequent catalytic reactions to proceed.

SIGNIFICANCE

Under intense evolutionary pressure, bacteria have developed several countermeasures to antibacterial agents, posing a serious risk to public health. The most successful of these defenses is expression of enzymes known as b-lactamases, which efficiently hydrolyze the amide bond in the b-lactam ring (red) of antibiotic agents such as benzylpenicillin and cephalosporins. The focus of our research is the development of a detailed understanding of the reaction mechanisms employed by these enzymes to hydrolyze b-lactam antibiotics. Understanding these mechanisms will yield insights that may prove useful for the development of new antibacterial agents.

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 (1997).

Modeling of Scintillation Produced by Ionizing Radiation in Inorganic Crystals

Stephen E. Derenzo, Marvin J. Weber, and Mattias K. Klintenberg,
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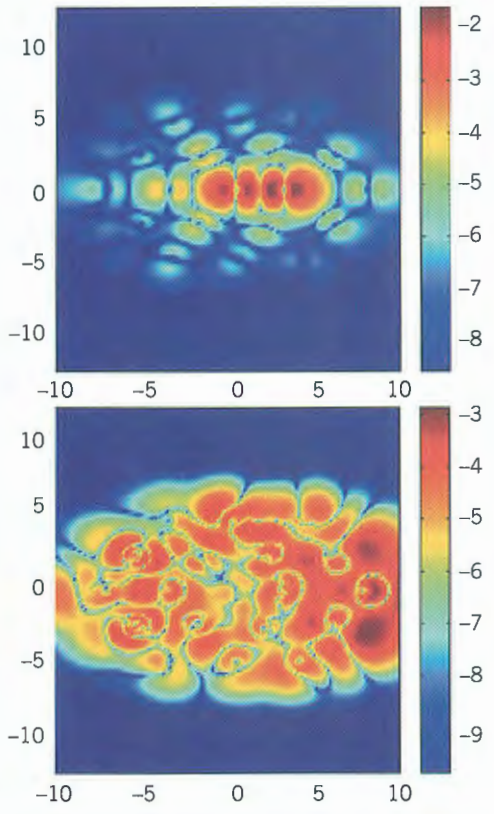
RESEARCH OBJECTIVES

The purpose of this research is to discover improved inorganic scintillator crystals for the detection of gamma rays in medical imaging, guided by computer simulations of critical processes.

COMPUTATIONAL APPROACH

The crystal is modeled as an atomic cluster of 30 to 50 atoms embedded in an array of thousands of point charges optimized to reproduce the electrostatic field of the infinite crystal. The Schrödinger equation is solved for the embedded atomic cluster using the Jaguar quantum chemistry package. This provides the molecular orbitals and energies for each of the typically 500 electrons in the system and the total energy of the system. The energies for ground, hole, electron and excited states are computed for various atomic geometries to determine the relaxed configuration, the barrier configuration for hole transport, and the configurational overlap that causes non-radiative quenching. We also compare electron, hole, and excited state energies with and without an impurity atom to determine whether the initial reaction is electron capture or hole capture, and to model the subsequent capture of the other carrier to form the excited state.



Images of the spatial distributions of the two electrons that describe an exciton (excited state) in the cesium iodide crystal, determined by solving the Schrödinger equation for a system of 520 electrons, 65 nuclei, and 8127 point charges. Top panel shows the charge distribution of the lower energy electron, which appears as two dumbbells, each concentrated on an iodine ion. Bottom panel shows the charge distribution of the higher energy electron, which is spread out over all 65 ions. Horizontal and vertical coordinates are in Ångstroms, and the color scale is the power of ten of the electron density.

ACCOMPLISHMENTS

(1) The first development of a general method for determining optimized point charge arrays that accurately reproduce the electrostatic field of the infinite crystal for any crystal whose structure is known. (2) Development of methods for computing the energy barrier for hole transport and their application to CsI, PbF2, PbF4, and CaF2. (3) Modeling of the ultra-fast (<100 ps) hole transport that occurs in CaF2:Eu and CdS:Te. (4) Modeling the impurity conduction bands in ZnO:Ga and CdS:In in support of the valence-conduction recombination theory that explains their fast, bright optical emissions and their electrical conductivity.

SIGNIFICANCE

The fields of medical imaging, high energy physics, nuclear physics, and astrophysics would greatly benefit from a scintillator with high density and improved light output and response time.

PUBLICATIONS

S. E. Derenzo and M. J. Weber, "Prospects for first principle calculations of scintillator properties," Nucl. Instr. Meth. A **422**, 111 (1999).

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http://cfi.lbl.gov/instrumentation

High-Resolution Sensitivity Studies of Southern Ocean Eddies Using Two Ocean Models

Robert Hallberg, Stephen M. Griffies, Bonita Samuels, and
J. Robert Toggweiler, NOAA Geophysical Fluid Dynamics Laboratory
Thierry Huck and Geoffrey Vallis, Princeton University

RESEARCH OBJECTIVES

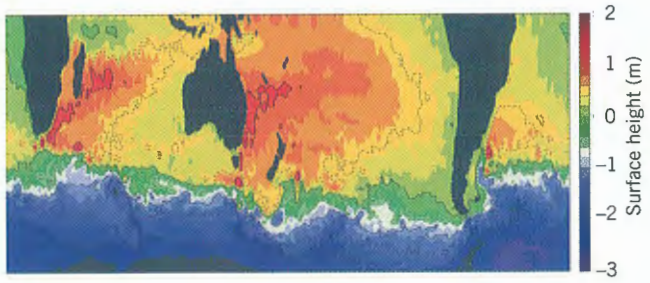
The Ocean Group at GFDL is embarking on an ambitious, multi-year effort to model the Southern Ocean with sufficient horizontal and vertical resolution to resolve the ubiquitous energetic mesoscale eddies. We are using a series of numerical simulations to determine the role of the Southern Ocean eddy dynamics in setting the structure and magnitude of the Antarctic Circumpolar Current and in determining the global mean density structure of the ocean.

COMPUTATIONAL APPROACH

We have begun a sequence of experiments using two different primitive equation ocean models. At each resolution we spin up from a climatological state for 20 years using climatological wind stresses. At that point, we start three separate simulations with wind stresses that are stronger, weaker, and the same as the winds used in the spinup phase. These experiments will test the sensitivity to changing surface forcing of the mean circulation and the balance between diabatic flows and eddy fluxes. Comparison between the various runs will provide a prognostic estimate of the sensitivity of the various terms in the momentum, potential vorticity, and heat and salt balances, in addition to the diagnostic description available from the Fine Resolution Antarctic Model (FRAM). The comparison will also directly test the hypothesis that the principal response to the changing wind stress is in the vigor of the eddy field, and not in the mean density structure.

ACCOMPLISHMENTS

We have run a 20-year spinup simulation with the hybrid isopycnal model (HIM) at 1/2° resolution at NERSC. This run identified certain problems with the experimental setup, and we are refining it in shorter runs at GFDL. We have also performed the entire suite of experiments at 1° resolution with GFDL's Modular Ocean Model (MOM). While these preliminary experiments are not capable of exploring the extent to which eddies control the dynamics of the Southern Ocean, they are the necessary preliminary exercise to the higher resolution, eddy permitting and eddy resolving experiments.



The instantaneous sea surface height in a 1/2° resolution simulation of the Southern Hemisphere ocean circulation using an isopycnal coordinate ocean model. The near-surface flow is very nearly along contours of sea surface height. The mean path of the Antarctic Circumpolar Current is roughly given by the large-scale zonal contours in the Southern Ocean, while the small-small wiggles and extrema are caused by the rich transient eddy field.

SIGNIFICANCE

The dynamical balance of the Southern Ocean may be the key to predicting the changes in the density structure of the deep ocean. Heretofore there have been no experiments which directly address this hypothesis. Our proposed experiments will test it directly. Understanding the response of the abyssal ocean to changing atmospheric forcing will be critical in determining the rate, extent, and satial distribution of climate change due to changing greenhouse gas concentrations. It is also anticipated that these experiments will lead to superior parameterizations of the effects of mesoscale eddies on the large-scale ocean circulation, thereby improving the reliability of predictions from coarse-resolution climate simulations.

PUBLICATIONS

A. Gnanadesikan, "A simple predictive model for the structure of the oceanic pycnocline," Science **283**, 2077 (1999).

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Protein Dynamics and Enzyme Function

Martin Karplus, Ioan Andricioaei, Guo Hong, Fabrice Leclerc,
Paul Lyne, and Cui Qiang, Harvard University
Paul Bash, Northwestern University Medical School

RESEARCH OBJECTIVES

The goal of this project is to develop a greater understanding of the mechanisms involved in enzyme catalysis and related protein functions. We are studying two types of enzymes: nucleic acids (specifically hammerhead ribozyme) and proteins.

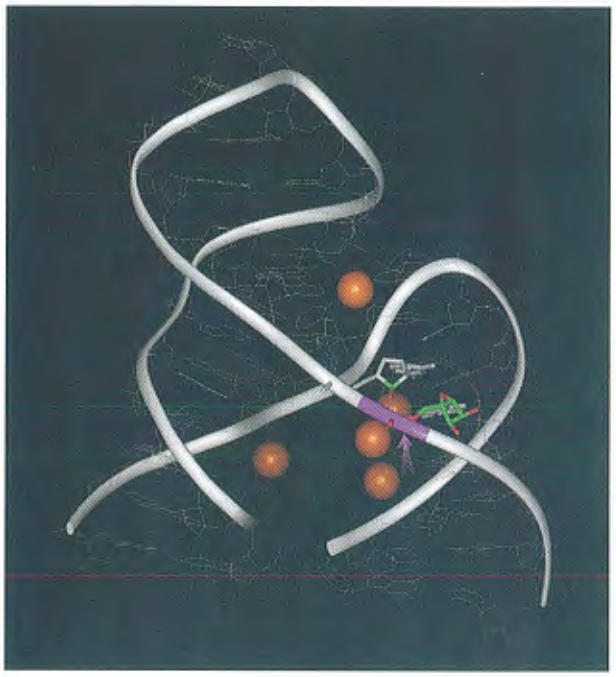
COMPUTATIONAL APPROACH

Our methods are based on the physical and chemical principles of statistical mechanics and quantum mechanics, implemented in computational form using techniques from computational chemistry. For example, we use the structural data as inputs for molecular dynamics simulations to determine the structural and dynamics properties of enzyme systems. Given the reactive conformation, the chemical steps involved in the reaction mechanism are studied using *ab initio* QM on model systems in the gas phase and the hybrid semiempirical and *ab initio* quantum-classical methods (QM/MM) implemented in the CHARMM program.

ACCOMPLISHMENTS

Simulations of the hammerhead ribozyme several nanoseconds in length have been performed for a system consisting of the hammerhead plus counterions to neutralize the backbone phosphate charges, all solvated with explicit water molecules. The simulation system is stable but some conformational changes do occur. In particular, the two arms which are constrained in the crystal structure undergo relative displacements of about two angstroms. As a result of the motion, the parts of the ribozyme involved in the catalysis undergo a conformational change. The details of the changes are being examined to provide an appropriate system for initiating the quantum and molecular mechanics (QM/MM) on the ribozyme.

Ab initio studies of the reaction path of phosphate ester hydrolysis of a model for the hammerhead ribozyme have also been completed, and the effects of thio-substitution at the pro-R site and at the leaving group have been studied. A theoretical estimate of the acid-base ionization constant (pKa) of the 2'-OH at the active site of hammerhead ribozymes was made based on quantum chemistry calculations of a phosphorylated ribose. The large value found (pKa = 14.9) has implications for the mechanism of hammerhead ribozyme catalysis and more specifically for the role played by metal ions in the reaction.



X-ray structure of the hammerhead ribozyme. The RNA backbone is represented by a white ribbon. The active site region, treated by quantum mechanics, is included in a yellow circle, and the phosphodiester bond cleaved during the reaction is indicated by a purple arrow. The metal cations (Mg^{2+}) used as cofactors are represented by CPK spheres.

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.

PUBLICATIONS

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Recognition and Classification of Protein Folds in Complete Genomes

Sung-Hou Kim and Igor Grigoriev,
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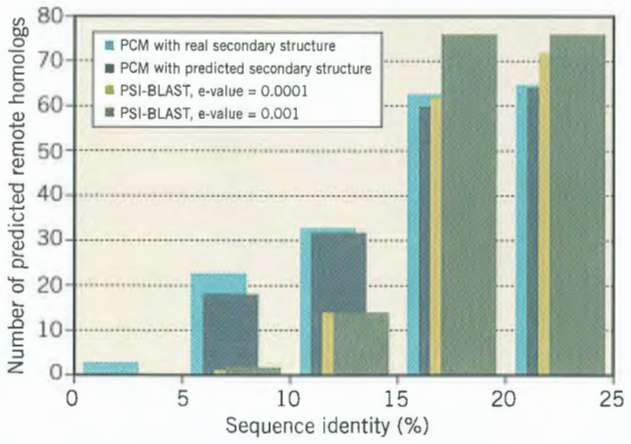
RESEARCH OBJECTIVES

(1) Further development of the proximity correlation method (PCM), which detects protein fold similarities on the basis of sequence-derived characteristics of proteins. (2) Application of PCM to fold recognition in several complete genomes. (3) Determination of new protein targets for experimental structural studies.

COMPUTATIONAL APPROACH

PCM uses the predicted secondary structure and the local correlation of the hydrophobicity of amino acid residues for alignment of two protein sequences. Dynamic programming techniques are used in the global alignment procedure (algorithm of Niddleman and Wunsch) with no terminal penalties. Statistical significance is estimated with a Z score. In contrast to classic hard cutoff, a heuristic cutoff is introduced and applied to predict protein folds reliably. The single-linkage clustering algorithm was optimized to group proteins with the same fold. For fold recognition, each gene product of a complete genome is compared with a library of known folds (a non-redundant set of known protein structures). For fold classification purposes, the sequences of gene products in a complete genome are compared in all-against-all manner, and then clustered by the single-linkage algorithm.



PCM is more successful than PSI-BLAST in predicting fold similarities of proteins with low sequence identities.

ACCOMPLISHMENTS

A pilot version of PCM was developed and tested on a data set of 64 proteins and about 400 structural homologues. The optimal physical property of amino acid residues, a method for secondary structure prediction, and alignment and scoring schemes were obtained during test experiments. The method demonstrated good performance in fold recognition on the test protein set compared with advanced sequence- and structure-based fold recognition methods. It was applied to trial fold recognition in the *Methanococcus jannaschii* genome and predicted protein folds of several hypothetical proteins. Later the method was applied to protein fold classification, or clustering proteins into groups with similar three-dimensional folds. The appropriate clustering scheme was developed, and for the test data set, it provided most of the known well-populated folds as distinct clusters.

SIGNIFICANCE

The explosion in the number of genome sequences during the past several years makes functional characterization of gene products overwhelming. Classical sequence similarity methods predict the functions of proteins with high sequence similarity to other proteins with known functions. Threading, or aligning sequence and three-dimensional structure, can detect the structural similarity of proteins with low sequence identity, but requires knowledge of structure and is limited by the number of known structures. We developed a new method, PCM, for detecting similarity of protein folds on the basis of protein sequences and sequence-based properties only. It does not require known structures for fold recognition and extends the sequence similarity boundary of sequence comparison methods. Therefore, it may predict the structure and function of many hypothetical proteins by exploring their structural relationships. In fold classification, PCM helps to identify new targets for experimental determination of new folds by detecting fold similarity in the groups of hypothetical proteins.

PUBLICATIONS

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Chao Zhang and Sung-Hou Kim, "The anatomy of protein beta-topology: I. Single beta-sheet. II. Beta-barrels and beta-sandwiches," J. Mol. Biol. (submitted).

Coupled Parallel Climate Model (PCM) Applications to Climate Change Prediction for the IPCC and the National Assessment

Warren Washington, National Center for Atmospheric Research
Albert Semtner, Naval Postgraduate School
John Weatherly, U.S. Army Cold Regions Research and Engineering Laboratory
Robert Malone, Los Alamos National Laboratory
Tim Barnett and David Pierce, Scripps Institution of Oceanography
John Drake, Oak Ridge National Laboratory
Phil Duffy, Lawrence Livermore National Laboratory
The Program for Climate Model Diagnosis and Intercomparison (PCMDI), Lawrence Livermore National Laboratory

RESEARCH OBJECTIVES

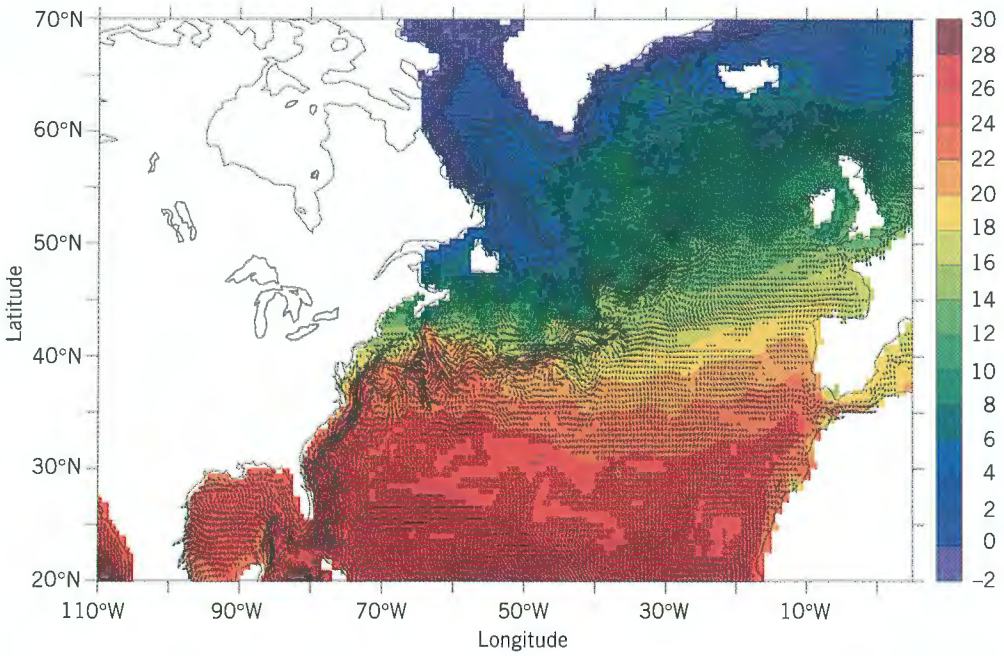
The main purpose of this research is to develop and use a new Parallel Climate Model (PCM) for studies of anthropogenically forced climate change simulations. Because it is difficult to separate anthropogenic climate change from natural climate variability, it is necessary to carry out ensembles of simulations in order to statistically find the climate change signal. Results of this research are being used by the Intergovernmental Panel on Climate Change (IPCC) and the U.S. National Assessment of the Potential Consequences of Climate Variability and Change.

COMPUTATIONAL APPROACH

We use a newly developed climate model that has state-of-the-art components for the atmosphere, land, ocean and sea ice. The PCM can execute on distributed and shared memory parallel computer systems.

We have developed an ocean component that uses the finite difference Parallel Ocean Program (POP) with a displaced north pole. The model in its present form runs at 2/3° and 1/3° resolution and yields an extraordinary simulation of the Arctic Ocean, tropical Pacific, and boundary currents, such as the Gulf Steam, with eddies. POP has recently been reformulated with improved data structures and enhanced memory and cache performance in a message passing environment. Many additional model physics options have been added to improve the model's fidelity.

The sea ice model component was developed by Yuxia Zhang of NPS and uses the Hibler ice dynamics with line relaxation for solving the equations. The viscous-plastic constitutive law is applied, and the Parkinson-Washington thermodynamics are included. The grid is transformed such that resolution is roughly linear in distance, thus avoiding the pole convergence



This simulation from the DOE-supported Parallel Climate Model (PCM) shows the upper ocean flow of the North Atlantic current system along with the ocean temperature. It demonstrates that a 2/3° horizontal resolution ocean model coupled to an atmosphere model and a sea ice model can simulate more realistic ocean eddies in the Gulf Stream and North Atlantic current systems.

problem with a latitude-longitude grid. The spatial resolution is about 27 km, which provides a highly realistic Arctic and Antarctic simulation of ocean and sea ice motion that includes the explicit effects of eddies. Recently, an option for using elastic-viscous-plastic physics has been added using the E. Hunke and J. Dukowicz approach to the solution of the ice dynamics. This latter option is being adapted for use on the IBM SP-3.

The atmospheric model component is the massively parallel version of the NCAR Community Climate Model version 3 (CCM3). This model includes the latest versions of radiation, boundary physics, and precipitation physics and runs at T42 resolution or higher. This model runs efficiently on the Cray T3E, the SGI Origin 2000, and the IBM SP.

The flux coupler ties the components together and allows the exchange of fluxes and variables. Since the component grids are different, there is an interpolation scheme for passing information between the atmosphere component grid and the ocean/sea ice grid that has been developed by P. Jones of LANL. The interpolation algorithm has been designed to run efficiently on distributed memory architectures. The component interfacing through the flux coupler is sufficiently flexible to handle a large range of resolutions, so that high-resolution models can use the same structure as lower-resolution models.

ACCOMPLISHMENTS

We now have a 300-year control experiment that is the baseline for our climate change simulations. This control run shows very little climate drift and has remarkable El Niño and La Niña events that are close to the observed levels of natural variability. Also, these events cause changes in the extratropical planetary wave patterns. After we established a control experiment, we carried out five experiments with a 1%/yr increase in atmospheric CO_2. At the doubling point of roughly 70 years, we stopped the atmospheric CO_2 increase. From the ensemble of 1%/yr runs we can better establish the geographic change in sea surface temperature and other climate variables over the entire globe.

We also have conducted two historical simulations from 1870 to the year 2000 in which the changes in greenhouse gases and sulfate aerosol distributions are provided. We plan to carry out several ensemble experiments to see how much decade-to-decade variability exists and how well the historical simulation agrees with observed changes.

Finally, we are in the process of conducting several ensemble experiments of future climate change from year 2000 to year 2100. These experiments require assumptions of future increases in greenhouse gases and sulfate aerosols.

SIGNIFICANCE

Accurate prediction of climate change on decadal and longer time scales is a major scientific objective of the DOE's Environmental Sciences Division. The DOE Climate Change Prediction Program is focused on developing, testing, and applying climate simulation and prediction models that stay at the leading edge of scientific knowledge and computational technology. A unique feature of the program is the establishment of a distributed modeling center involving DOE national laboratories, the National Center for Atmospheric Research, and the non-Federal research community. The intent is to increase dramatically both the accuracy and throughput of computer model-base predictions of future climate system response to the increased concentrations of greenhouse gases.

In the Kyoto Protocol on climate change, there are several climate change scenarios that must be completed for the U.S. National Assessment. These simulations assume emissions of greenhouse gases and sulfate aerosols. Data sets from these simulations are being used by the National Assessment and the IPCC.

PUBLICATIONS

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

Three-Dimensional Global Atmospheric Chemistry Modeling

Joyce Penner and Sanford Sillman, University of Michigan

RESEARCH OBJECTIVES

To evaluate the role of emissions of volatile organic carbon species (VOCs) and other energy-related pollutants from biomass and fossil fuel burning on the chemical climatology of the global troposphere, with an emphasis on the role of these pollutants in altering O3 photochemistry and the chemistry of CH_4, both of which are important greenhouse gases.

COMPUTATIONAL APPROACH

We have developed a global tropospheric chemical model that is capable of treating the chemistry of CO, CH_4, NO_x, and a suite of VOCs. The model is computationally fast, while providing much better chemical resolution than is available in other tropospheric chemistry models, and is configured so that it may also be run interactively with a climate model.

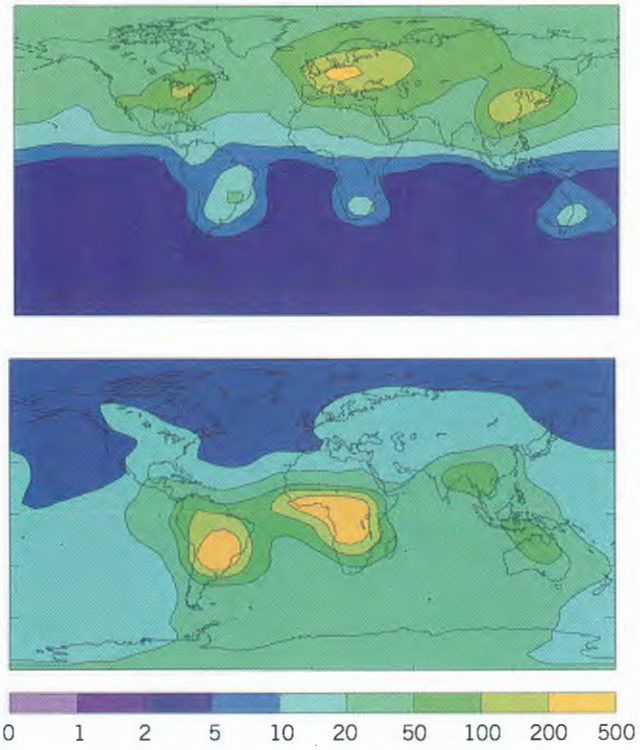
In order to study the sources of CO and CH_4 in the model, we have simplified the chemistry of the troposphere to mainly focus on the interactions between OH, CH_4, and CO. Ambient distributions of 17 species were calculated for a prescribed methane and CO distribution using the 3D chemistry-transport model GRANTOUR. Meteorology was provided for a 4.5° × 7.5° resolution every 12 hours over a yearly cycle. This simulation was used to diagnose reaction rate coefficients as a function of latitude, longitude, height, and time.

ACCOMPLISHMENTS

Comparison of the predicted CO and CH_4 concentrations with data from the NOAA Climate Monitoring and Diagnostics Laboratory indicated that our initial sources result in an underestimate of CO concentrations. Therefore, we adjusted the fossil fuel sources up by a factor of 1.7. The new sources result in a much improved comparison of predicted and observed CO concentrations. We are continuing to use the model to help refine our understanding of CO sources. In addition, we are building a version of the model with interactive isoprene chemistry. This will allow us to determine the additional effects of non-methane hydrocarbon chemistry on the concentration of OH.

SIGNIFICANCE

Our model represents a significant advance over previous models for tropospheric chemistry because it includes a full suite of VOCs with explicit chemistry represented in the model. These simulations should improve our estimates of the effects of fossil fuel and biomass burning on the global climate by better quantifying the source magnitude and distribution of both biomass and fossil fuel burning. A better definition of the source strength of CO from fossil fuels and from biomass burning will also help us to quantify the sources of aerosols (sulfates and smoke). In contrast to the greenhouse gases, aerosols tend to cool the climate. Thus, the quantification of these sources is extremely important.



Annual average surface concentrations of CO (in ppbv) from fossil fuel sources (top) and biomass burning sources (bottom).

PUBLICATIONS

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http://aoss.engin.umich.edu/Penner/

PCMDI: Coupled Atmosphere-Ocean Modeling

Michael Wehner, Lawrence Livermore National Laboratory

RESEARCH OBJECTIVES

The principal mission of the Program for Climate Model Diagnosis and Intercomparison (PCMDI) is to develop improved methods and tools for the diagnosis, validation, and intercomparison of global climate models (GCMs) and to engage in research on a wide variety of outstanding problems in climate modeling and analysis. In this project, we are using the T3E to expand a set of ensemble climate integrations of the coupled ocean-atmosphere model of the Hadley Centre in the United Kingdom. Specifically, we are investigating the linearity of the climate's response to different kinds of forcing. Previous integrations performed in Great Britain are being augmented to include integrations with only anthropogenic sulfate aerosol forcing.

COMPUTATIONAL APPROACH

Much of the previous year was spent porting the model (HADCM2) from the UK Meteorological Office T3E to the NERSC T3E. The model is extremely large, both in number of Fortran lines and K-shell scripting lines. The porting is complete and the model is currently running. The model is not highly parallel, running at only 24 processors. Model runs are extremely lengthy, requiring about 32,000 node hours per integration. However, additional parallelism is obtained by running more than a single integration at a time.

ACCOMPLISHMENTS

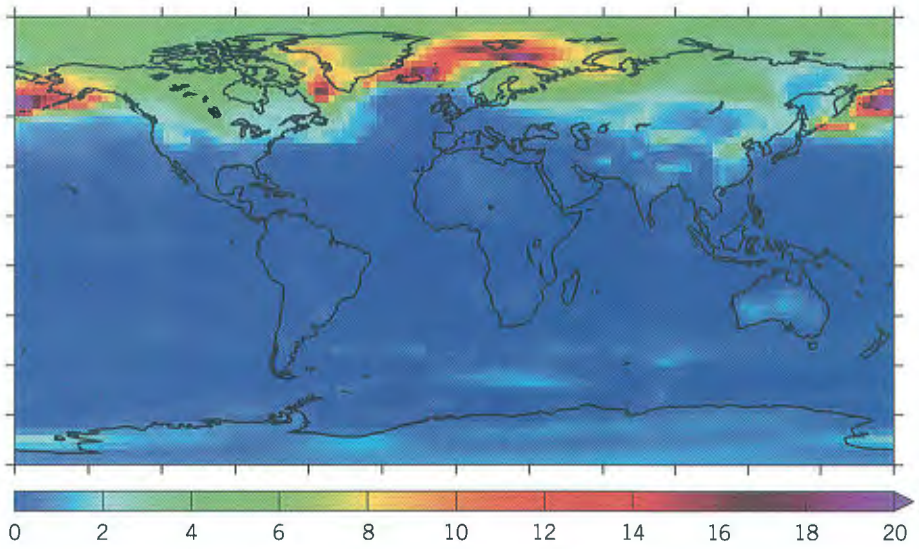
About 50 years of integration have been performed, which is about one-eighth of the requirement for this project.

SIGNIFICANCE

The coupled climate system is a complex nonlinear system. Our understanding of the climate response to different types of forcing, e.g., enhanced carbon dioxide concentrations, variations in solar forcing, sulfate aerosols, etc., comes largely from integrations of global coupled GCMs. The chaotic nature of the climate system requires us to perform ensembles of integrations to separate response signal from climatic noise. This work will complete the missing parts of the most comprehensive set of coupled model ensembles.

PUBLICATIONS

http://www-pcmdi.llnl.gov



Number of simulation runs required to determine decadal mean December through February surface air temperature within 1.0°K at 95% statistical confidence. Results are shown for temperatures obtained from the NCAR Parallel Coupled Model. Ensembles of climate simulations enable researchers to quantify climate variability and better predict the uncertainty of future climate change. Unfortunately, the high computational costs of fully coupled climate models limit the size of such ensembles. Our research has provided a means of determining how many ensemble realizations are required in advance of performing the calculations. This number is dependent on which climate variable is of interest and on the desired accuracy.

Numerical Tokamak Turbulence Project

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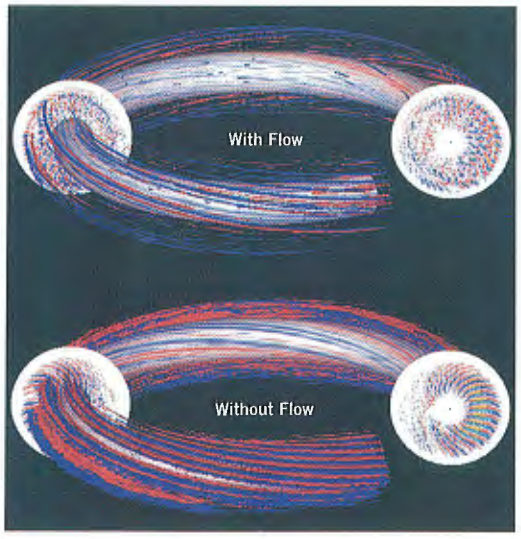
J. V. W. Reynders, Los Alamos National Laboratory
V. K. Decyk, University of California, Los Angeles
W. D. Dorland, University of Maryland
G. W. Hammett, Princeton Plasma Physics Laboratory
G. D. Kerbel, Lawrence Livermore National Laboratory
J.-N. Leboeuf, Oak Ridge National Laboratory
W. W. Lee, Princeton 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 main 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 (1) particle-in-cell (PIC) methods for the self-consistent solution of Poisson's equation (reduced to a quasi-neutrality relation), Maxwell + Poisson equations in electromagnetic extensions, and plasma equations of motion; and (2) domain decomposition methods to run efficiently in parallel on the T3E and other parallel computers. An electromagnetic, 5-D Eulerian GK code has been developed in the last year and a half that is not particle-based and is noise-free, and whose efficiency and resolution characteristics are being explored. 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 massively parallel computers, particularly the T3E at NERSC. Both flux-tube, i.e., toroidal annulus, and global toroidal GK and GLF simulations are being performed to study tokamak turbulence.



Global gyrokinetic simulation of tokamak ion temperature gradient turbulence with and without zonal flows, whose inclusion moderates the turbulent transport. (Z. Lin, PPPL)

ACCOMPLISHMENTS

Significant advances have been realized on both the gyrokinetic and the gyrofluid fronts. Gyrokinetic calculations have been extended to more than one ion species to study the influence of impurity injection on ion temperature gradient (ITG) driven turbulence. These calculations have shown a dramatic reduction in the fluctuation levels and heat conductivity upon injection and have helped elucidate experimental results on DIII-D and TEXTOR which show the same effect. Results from extensive gyrokinetic and gyrofluid calculations of ITG instability have been obtained, tabulated and prepared for publication as part of the Cyclone Project, an outgrowth of the NTTP. These predictions have been compared with tokamak plasma thermal transport models that have been widely used for predicting the performance of the proposed ITER tokamak. These comparisons provide information on effects of differences in the physics content of the various models. Many of the comparisons are undertaken for a simplified plasma model and geometry which is an idealization of the plasma conditions and geometry in a fusion-reactor-relevant experiment in DIII-D. Most of the models show good agreement in their predictions and assumptions for the linear growth rates and frequencies. There are some differences associated with different equilibria. However, there are significant differences in the transport levels between the models. The causes of some of the differences have been examined in some detail, with particular attention to numerical convergence in the turbulence simulations. The gyrokinetic results are giving guidance to other NTTP researchers in improving the closure model(s) in the gyrofluid formalism to obtain better agreement with the gyrokinetic results.

A simple fit for the dependence of the thermal flux on the temperature gradient has been discovered which takes into account

the nonlinear upshift of the effective marginal temperature gradient found in FY98, and suggests a considerable simplification in the theoretical picture of toroidal ITG turbulence. The gyrokinetic simulations demonstrated good agreement with the analytical theory of Hinton and Rosenbluth in the role of neoclassical physics in relaxing zonal shear flows. Such shear flows have a profound influence on the steady-state turbulence level. Gyrokinetic simulations with collisions showed how collisions further relax the zonal flows, which in turn leads to a higher level of turbulence, in qualitative agreement with experiments. Gyrokinetic simulations addressing the influence of the scale size of equilibrium temperature and density gradients demonstrated how the results of radially local flux-tube simulations can be approached in the results of simulations in which the length scale of the profile variations is increased, and that profile variations reduce the transport below the local expectation at the radius at which the temperature gradient has its maximum. However, because of the nonlocal character of the turbulence in such cases, the transport at other minor radii can increase relative to the local value.

A new global gyrofluid code was developed and results were obtained for ITG-driven turbulence in cylindrical and toroidal geometry. An electromagnetic, five-dimensional gyrokinetic code was brought on line in parallel mode, and first simulations of ITG and electron temperature gradient (ETG) turbulence were undertaken (separately). Encouraging agreement with the gyrokinetic flux-tube particle code results have been seen so far for ITG turbulence. Gyrofluid results for toroidal ETG modes have also been confirmed with this code.

Steady progress was made in adding non-adiabatic electron physics and electromagnetic effects to more codes in the NTTP suite. Part of our team has taken a direct approach to comparing turbulence-based theories with experiment. The ITG code (Gryffin) is run to saturation using experimentally measured plasma profiles as input, and the results are compared with both the measured turbulence characteristics and the transport fluxes.

Massively parallel gyrokinetic particle simulations show that the ion thermal transport from electrostatic ITG turbulence depends on ion-ion collisions for representative tokamak core H-mode plasma parameters. The collisionality-dependence of the turbulent transport comes from the neoclassical damping of self-generated zonal flows which regulate the turbulence. The results from our full torus gyrokinetic simulations are consistent with the experimental observation that the collisional dependence of transport is much more pronounced in the enhanced confinement regime where turbulence is expected to be weaker than that of typical L-mode plasmas. Furthermore, the fluctuations and heat transport in these simulations exhibit bursting behavior with a period corresponding to the collisional damping time of poloidal flows. This is consistent with the observation in TFTR core plasmas of a density fluctuation bursting with a period close to the collisional flow damping time calculated from experimental plasma parameters. The extension of field-line following coordinates for global simulations enables full-torus nonlinear simulations with realistic plasma parameters.

A significant accomplishment during the past year was the development of a practical formulation for real tokamak geometry which could be simply incorporated into both gyrokinetic and gyrofluid linear and nonlinear codes. We used the Miller local equilibrium developed at General Atomics, which generalizes the conventional s–α infinite aspect ratio circle to a finite aspect ratio, shifted, elongated and triangulated ellipse. The formulation resembles circular geometry with an effective magnetic field when the minor midplane radius is used as a flux surface label.

With our reformulated flux tube gyrofluid code, we mapped out the dependence of ITG turbulent transport and E × B shear stabilization on elongation. Considerable effort has been devoted to the major development of a continuum full radius gyrokinetic code. The code has real geometry, full electron physics with electromagnetism. As computers become larger, the low-n magnetohydrodynamics limit will be spanned with a full torus mode of operation.

SIGNIFICANCE

The NTTP simulations are being used to produce linear and nonlinear calculations of drift-type instabilities in realistic tokamak equilibria, 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

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T. S. Hahm, M. A. Beer, Z. Lin, G. W. Hammett, W. W. Lee, and W. M. Tang, "Shearing rate of time-dependent E × B flow," Phys. Plasmas **6**, 922 (1999).

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

Numerical Study of Global Stability of Field-Reversed Configurations

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Princeton Plasma Physics Laboratory

RESEARCH OBJECTIVES

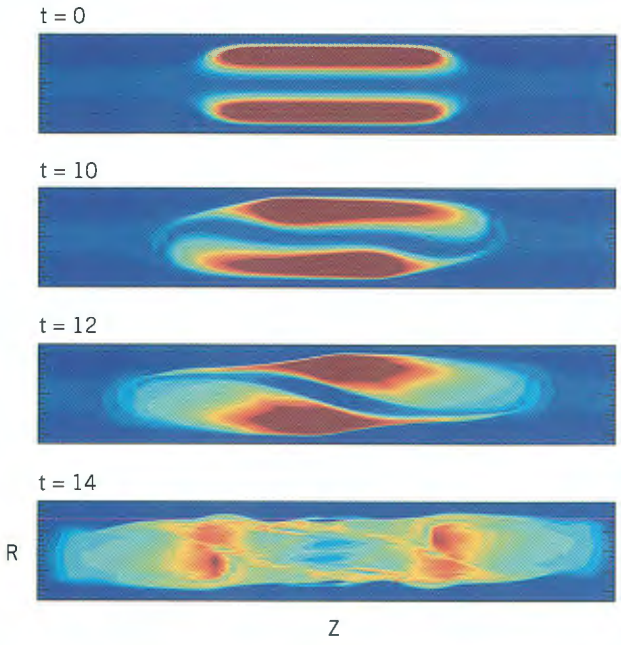
The objective is to determine the gross stability of the field-reversed configuration (FRC). This is a plasma confinement configuration that is relatively simple to make and has some desirable features from a fusion reactor perspective. These configurations have been made in the laboratory and show some signs of stability for short times. However, analysis of the configuration with fluid equations, i.e., in the magnetohydrodynamic (MHD) approximation, shows that they should be unstable to a number of different modes. Our objective is to use a more accurate description of the plasma by including particle orbit effects and to see if this would improve the theoretical predictions of stability.

COMPUTATIONAL APPROACH

The approach is to use a hybrid MHD code that treats the electrons as a cold fluid and the ions as particles. The particle ion motion is described by the Lorenz force equations with the standard leapfrog scheme used for the time advance. The electric field is calculated from the electron momentum equation neglecting the inertial term. The fluid equations are advanced on a finite-difference mesh in a cylindrical coordinate system, while the particle pushing is done on a Cartesian grid. In contrast to previous work, the δf method is utilized to reduce numerical noise in the simulations.

ACCOMPLISHMENTS

The potentially unstable modes can be categorized by their dominant Fourier component about the symmetry axis. The $n = 1$ mode is normally the most unstable. The mode has a tilt-like structure. Elongated FRC with $E > 1$ are called prolate, and those with $E < 1$ are called oblate. We have found that the tilt mode is mostly internal to the configuration for prolate until it has grown to large amplitude, and then it suddenly acts to destroy the configuration. For the oblate configuration, the mode is external from the beginning and involves substantial distortion of the plasma boundary. We find that the effects of particle orbits are especially important for the prolate configuration, and that they can reduce the growth rate of the tilt mode by an order of magnitude or more. Also, the tilt mode in the prolate configuration is very difficult to measure experimentally because of its largely internal nature.



Snapshots showing a 2D slice of the constant pressure contours during the evolution of a tilt-instability in a field-reversed configuration. This was a 3D MHD simulation of an $E = 3.7$ prolate configuration with elongation of 3.7. Times are normalized to the Alfven-wave transit time. Including particle orbit effects was found to slow down but not completely stabilize this mode.

SIGNIFICANCE

This research has done much to explain the previously apparent discrepancy between experimental observations and theoretical calculations using MHD. Not only have we found a substantial growth rate reduction, but we have also illustrated the signature of the mode and thus helped in developing suitable diagnostics for detecting this mode experimentally.

PUBLICATIONS

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Turbulent and MHD Behavior of Free Liquid Jets and Films and Magnetically Confined Plasmas

J. M. Dawson, V. K. Decyk, M. W. Kissick, J. N. Leboeuf, and
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R. D. Sydora, University of Alberta, Edmonton

RESEARCH OBJECTIVES

(1) Investigate the possible application of free surface liquid magnetohydrodynamic (MHD) flows for liquid walls to both magnetic and inertial fusion plasma chambers. This involves the modeling of turbulent liquid free surface flows in the presence of strong magnetic fields in some cases. (2) Extend the capabilities of the three-dimensional global toroidal gyrokinetic particle model of ion temperature gradient driven turbulence in magnetically confined plasmas beyond adiabatic electrons and in the longer term beyond electrostatics.

COMPUTATIONAL APPROACH

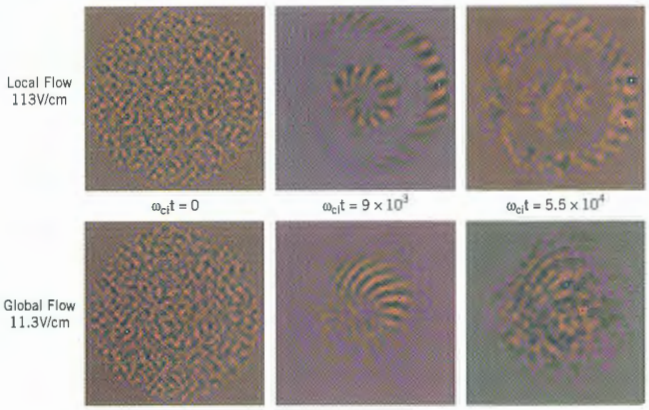
(1) The standard formulation for incompressible liquid flow is the so-called projection or fractional step method. This solution methodology can be applied to the magnetic vector potential equations as well. Message passing will be used to partition this among multiple processors in the massively parallel implementation. (2) Gyrokinetic particle code techniques currently applied to the ions will be duplicated for the now mobile electrons by calling the particle manager routines in the PLIB library once for each mobile species. This simplifies the coding enormously and insures symmetry in the massively parallel treatment of the multi-particle species.

ACCOMPLISHMENTS

(1) The parallel work is still in the developmental stages. (2) Production calculations have enabled us to investigate the effects of impurities and externally imposed poloidal flows on ion temperature gradient driven turbulence. Both of these additions to the standard description of ion temperature gradient driven instabilities have a stabilizing influence on the growth rates, and lead to a reduction of the saturation level and of the heat flux.

SIGNIFICANCE

(1) The interaction of turbulence with both free surface interfaces and magnetic fields is of interest in many scientific disciplines, including atmospheric sciences (missing CO_2 sink in oceans) and metallurgy (casting of metal components). We are interested in the application to free liquid walls in fusion reactors as a possible new paradigm for plasma containment structures. (2) Including



Turbulence mitigation by externally imposed local and global flows in UCLA's Electric Tokamak, as simulated by massively parallel 3D full torus gyrokinetic particle-in-cell calculations. Localized flow suppresses fluctuations where flow shear is largest.

electrons in the gyrokinetic description of ion temperature gradient driven instabilities extends the applicability of the model to describe particle transport as well as heat transport. It also provides a more relevant description of the physics of ion temperature gradient driven modes, since trapped electrons are known to enhance the growth rate of the underlying instability.

PUBLICATIONS

R. D. Sydora, V. K. Decyk, J. M. Dawson, J. Ongena, A. Messiaen, P. E. Vandenplas, and J. Boedo, "3D global gyrokinetic particle simulation study of turbulence suppression in neon impurity-seeded tokamak plasmas," Bull. Am. Phys. Soc. **44**, 357 (1999).

A. Ying, N. Morley, M. Abdou, and M. Youssef, "Description and thermalhydraulic analysis of liquid surface FW/blankets concepts for high power density reactors," Fusion Technology **34**, 1035 (1998).

A. M. Dimits, M. A. Beer, G. W. Hammett, C. Kim, S. E. Parker, D. E. Shumaker, R. Sydora, A. J. Redd, J. Weiland, M. T. Kotschenreuther, W. M. Nevins, G. Bateman, C. Bolton, B. I. Cohen, W. D. Dorland, A. H. Kritz, J. E. Kinsey, L. L. Lao, and J. Mandrekas, "Comparisons and physics basis of tokamak transport models and turbulence simulations," Phys. Plasmas (submitted).

http://exodus.physics.ucla.edu
http://www.fusion.ucla.edu/apex

Microstructure Evolution in Irradiated Materials

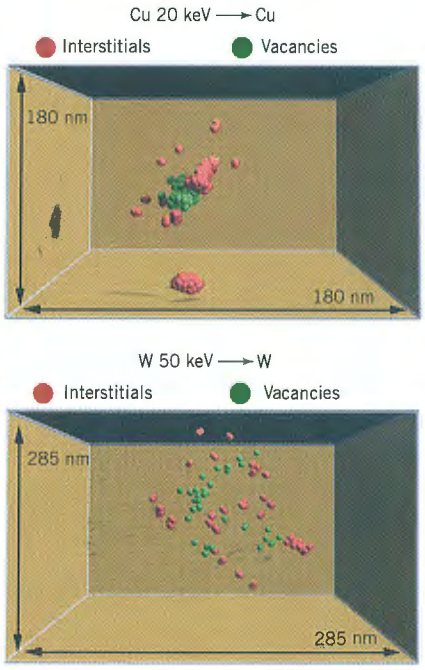
Tomas Diaz de la Rubia, Brian Wirth, and Eduardo Alonso,
Lawrence Livermore National Laboratory

RESEARCH OBJECTIVES

We are studying the interaction of defects produced during irradiation or deformation of a metal with the microstructure of that particular material, such as dislocations and grain boundaries. In particular we are studying the interaction of dislocations with interstitial loops and stacking fault tetrahedra, and the production of displacement cascades close to dislocations and grain boundaries. The data obtained from these simulations will be used as input to diffusion models and dislocation dynamics models.

COMPUTATIONAL APPROACH

Mostly we employ molecular dynamics simulations using empirical interatomic potentials. Parinello-Rahman boundary conditions are used to apply stress to study dislocation motion. The link cell method is used to efficiently calculate the neighbors of the atoms in the computational box. The partition into link cells is also used to distribute the atoms across the nodes in the parallel machine. Defect diffusion is studied using kinetic Monte Carlo models. The reaction rates for defect interaction and defect dissolution are input for this method, as well as the defect distribution, obtained from molecular dynamics simulations.



Damage produced by a 20 keV recoil atom in copper. Red spheres represent the location of interstitial atoms; green spheres represent vacancy sites. The damage produced in this face-centred cubic material due to irradiation results in large clusters of interstitials and vacancies. The production of a large interstitial cluster that migrates along a <110> direction is observed in this simulation.

ACCOMPLISHMENTS

We have simulated the formation of stacking fault tetrahedra (SFT) in copper both from the collapse of a vacancy plane and directly during irradiation. The presence of SFT after irradiation of copper has been observed experimentally for many years; however, molecular dynamics simulations have failed until now to reproduce this observation. We were able to simulate the production of SFT during irradiation of copper by using high energy irradiation and long relaxation times.

We have also simulated the damage produced by self-irradiation of copper, for energies between 200 eV and 20 keV. Several cascades were obtained for each energy (maximum 12 and minimum 5). The defect production as a function of energy was compared to that obtained from the Kinchin-Pease model. The production rate is comparable to the Kinchin-Pease only for low energies, reaching a constant value of 0.2 × Kinchin-Pease at energies ~5 keV. The database extracted from these simulations was used to study defect accumulation and diffusion using kinetic Monte Carlo. One of the cascades was followed for 100 picoseconds. An interstitial cluster containing 38 defects was produced in this cascade. This interstitial is highly mobile, and its migration is followed in this simulation. The next step in our simulations is to study the interaction of these types of clusters with dislocations.

SIGNIFICANCE

The interaction of the microstructure with defects produced during irradiation is responsible for material degradation under irradiation. Fundamental studies of the interaction of defects with dislocations and grain boundaries are necessary to develop predictive models for materials performance under irradiation and deformation, important issues in the development of materials for fusion reactors and other applications.

PUBLICATIONS

M.-J. Caturla, N. Soneda, E. Alonso, B. D. Wirth, T. Diaz de la Rubia, and J. M. Perlado, "Comparative study of radiation damage accumulation in Cu and Fe," J. Nucl. Mater. (submitted).

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Modeling of Intense Beams for Heavy-Ion Fusion

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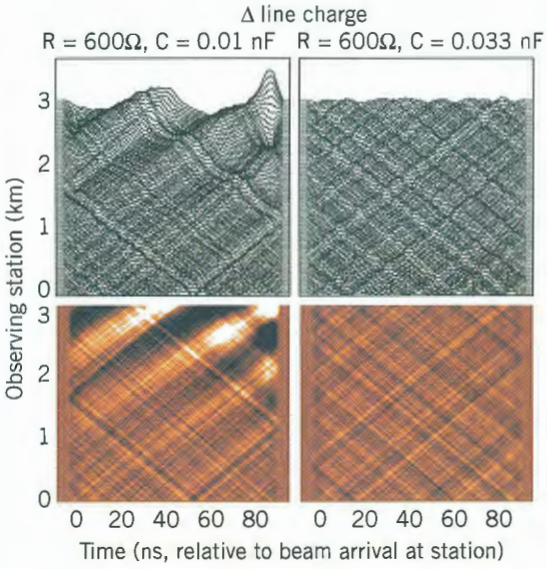
RESEARCH OBJECTIVES

This project entails the numerical simulation of beam dynamics for heavy-ion fusion (HIF) in the accelerator and in the fusion chamber. Current activities include the exploration of basic accelerator physics questions, such as emittance growth and halo formation, the analysis of ongoing experiments, and the design and optimization of planned experiments.

COMPUTATIONAL APPROACH

A hierarchy of codes is used for numerical simulation of HIF beam dynamics. A fast-running truncated-moment code, CIRCE, is used for design and optimization of accelerators, for generating fields for beam acceleration, compression, and longitudinal control, and for testing algorithms for pulse steering, shaping, and final focus. Detailed accelerator simulations are done mainly with the 2D and 3D electrostatic particle-in-cell (PIC) code WARP. A 2D semi-Lagrangian Vlasov code is being developed to study halo questions and to corroborate the PIC modeling. Beam transport in the fusion chamber is modeled with electromagnetic codes such as BICrz or BPIC. A 1D Lagrangian-fluid code, CYCLOPS, is being used to study a z-pinch for possible beam focusing.



Behavior of longitudinal waves on an intense ion beam in a heavy-ion fusion driver accelerator, as simulated using the WARP3d PIC code. A random initial perturbation to the beam velocity is applied, launching waves which propagate in both directions. The plots depict the change in line charge density (relative to its initial value) for two cases. In each, the upper frame is an overlay of traces at a number of observing stations, with a vertical offset corresponding to the separation between stations. The lower frame is a "cell array" wherein "peaks" appear in light color, "valleys" in dark. In the left column, the waves moving toward the tail of the beam are seen to be unstable; in the right column, the accelerating module capacitance has been increased, and the instability is effectively suppressed.

ACCOMPLISHMENTS

Evaluation of possible layouts and acceleration schedules for the Integrated Research Experiment (IRE) included studies of multiple-beam injection, emittance growth due to misalignments and quadrupole rotations, the effects of applied-field non-linearities (anharmonicities), and beam dynamics during final focus. Separate studies were carried out to investigate a kinetic instability driven by a temperature anisotropy, to determine equilibrium distribution functions of beams in curved lattices, and, in collaboration with the HIF group at GSI in Germany, to investigate bunch compression in storage rings.

Numerical support was provided to several ongoing experiments, and simulations were made to assist the design of planned experiments.

SIGNIFICANCE

Beam physics in a heavy-ion driver cannot be adequately modeled by analytic means due to the spatially varying focusing fields and the intense, anharmonic space-charge field of the beams, so that simulations are needed to model and understand the underlying phase-space dynamics.

PUBLICATIONS

S. M. Lund, et al., "Numerical simulation of intense-beam experiments at LLNL and LBNL," Nuclear Instruments and Methods A **415**, 345 (1998).

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A. Friedman, et al., "Beam dynamics studies for heavy ion fusion drivers," in *Proceedings of the 1999 Particle Accelerator Conference*, edited by A. Luccio and W. MacKay, (IEEE Service Center, Piscataway, NJ, 1999), p. 1830.

http://www-hifar.lbl.gov/HIFhomepage/hifhome.html

Large-Scale Gyrokinetic Simulation of Electromagnetic Plasma Turbulence

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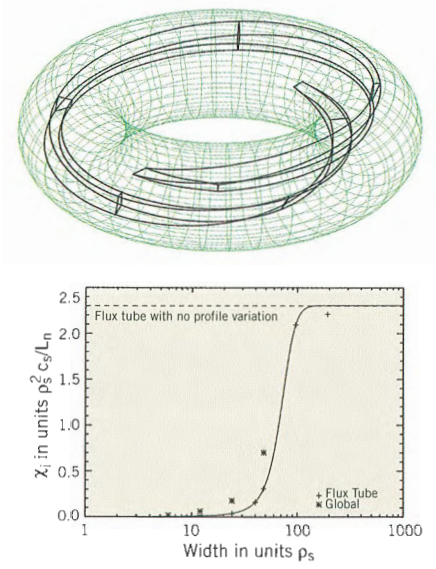
RESEARCH OBJECTIVES

We are currently studying the role of electromagnetic fluctuations in tokamak plasma turbulence; equilibrium and self-generated zonal flows and related techniques for controlling transport; and techniques for long-time meso and macro simulation. Current δf methods fail at long times, and we are studying an evolving equilibrium approach with an appropriate collision operator which attracts the distribution function back towards the evolving equilibrium distribution.

COMPUTATIONAL APPROACH

We have developed a drift-fluid-electron gyrokinetic-ion simulation to study electromagnetic turbulence. This is a fully parallel 3D toroidal simulation. We use a 1D domain decomposition in the direction along the magnetic field line. We are also utilizing a domain-cloning technique, in which the grid is replicated on a second set of processors. This is useful when there are more processors then grid cells in the decomposed direction, or for optimal performance on SMP clusters. The drift-fluid electron model uses finite-difference for solving the hyperbolic partial differential equations. The particle-ion part uses δf particle-in-cell methods. Poisson solvers are used in the direction perpendicular to the magnetic field, and these are done spectrally.



Explanation of the apparent anomaly between the two common approaches used to simulate tokamak plasma turbulence. Top: Views of both flux-tube and global computational domains. Bottom: Plot of heat transport versus the derivative of the temperature gradient showing a transition from low-level global-like transport to the larger flux-tube-like transport.

ACCOMPLISHMENTS

We have carefully benchmarked the model in the shearless slab limit to numerical solution of the dispersion relation including full kinetic and finite gyro-radius effects. Recently we have developed a fully toroidal model. We observe finite-β stabilization at low ratios of the plasma pressure to the magnetic pressure, then strong destabilization at higher values along with a large increase in transport levels.

We have put a significant effort into identifying the differences between global and flux-tube simulations. We have shown theoretically that the behavior of the purely radial mode can be predicted from the perpendicular flux-surface-averaged ion temperature. With significant profile variation, the heat flux flattens the equilibrium temperature, leading to the generation of the global purely radial mode. On the other hand, when the temperature gradient is constant, there is no preferred location of profile flattening, and the radial mode is then more turbulent, which is observed in constant temperature gradient flux-tube simulations.

Using the knowledge of how the self-generated flows are produced, we did a simple numerical demonstration of a new scheme to reduce the heat transport by slightly rippling the temperature profile. A slight ripple in the equilibrium temperature profile ripples the transport, causing the generation of short-scale zonal flows. This, in turn, reduces the heat transport.

SIGNIFICANCE

We are developing tools which provide better understanding of turbulent transport in magnetic fusion plasmas. Better understanding, in turn, may lead to control of transport.

PUBLICATIONS

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S. E. Parker, C. C. Kim, and Y. Chen, "Large-scale gyrokinetic turbulence simulations: Effects of profile variation," Physics of Plasmas **6**, 1709 (1999).

A. M. Dimits, B. I. Cohen, N. Mattor, W. M. Nevins, D. E. Shumaker, S. E. Parker, and C. Kim, "Simulation of ion-temperature-gradient turbulence in tokamaks," in *Proceedings of the 17th IAEA Fusion Energy Conference* (paper IAEA-F1-CN-69/TH1/1); Nuclear Fusion (in press).

http://fluid.colorado.edu/

NIMROD Code Development

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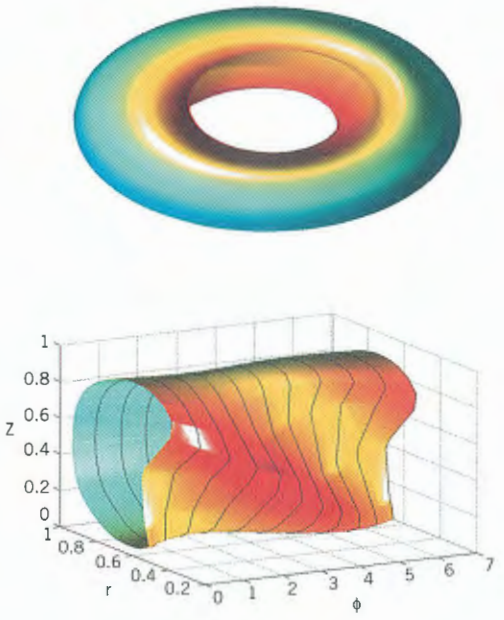
RESEARCH OBJECTIVES

The goal is to develop a fusion plasma simulation code which provides both flexibility in the physics—by using two-fluid or magnetohydrodynamic (MHD) models with analytic or gyrokinetic closures—and flexibility in the geometry—allowing studies of any axisymmetric fusion concept, no matter how complicated the cross-section. NIMROD is designed to be user-friendly (but not simple), and is available to the entire fusion community. Because NIMROD was designed to include massively parallel constructs, the code can take advantage of the most powerful MPP machines to tackle the largest problems in fusion.



Closed flux surfaces generated in NIMROD simulations of spheromaks. NIMROD computations of z-pinches with embedded axial magnetic field produce sustained spheromaks as the nonlinear saturation of an MHD instability. Weakly driven cases yield flux surfaces threaded by a helical current column. Two views of a surface, with color indicating radial position, illustrate the helical distortion on the inboard side. (Carl Sovinec, John Finn, and Diego del Castillo Negrete, LANL)

COMPUTATIONAL APPROACH

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

ACCOMPLISHMENTS

The NIMROD code, currently at version 2.3.2, is maturing rapidly. The code performance has more than doubled in the past year, and we are actively working on further improvements. The physics models are being extended, with two analytic closure schemes implemented in the past year, as well as further use of the two-fluid equations. The code is broadening its user base, with simulations done for General Atomics, UCLA, the University of Washington, and the University of Wisconsin. In the past year the team has continued its extensive validation campaign, including the numerically challenging kink-ballooning case. In addition, challenging first-of-a-kind problems have exercised the code: neoclassical tearing modes in DIII-D geometry, spheromak sustainment and production, field-reverse configurations, and toroidal reversed field pinch (RFP) simulations. The breadth of these simulations testifies to the flexibility of the code.

SIGNIFICANCE

NIMROD is designed to do nonlinear, initial-value simulations of long-wavelength phenomena in fusion-relevant plasmas. These types of motions severely constrain the operating regime of fusion experiments. By applying modern computational techniques to the solution of extended MHD equations, NIMROD can lead to improved understanding of these types of motions. This understanding should help overcome the operating limits of fusion devices, providing better approaches to producing fusion energy.

PUBLICATIONS

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http://nimrod.saic.com/

Theoretical Calculations of Plasma Turbulence, RF Heating, and Stellarator Physics

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RESEARCH OBJECTIVES

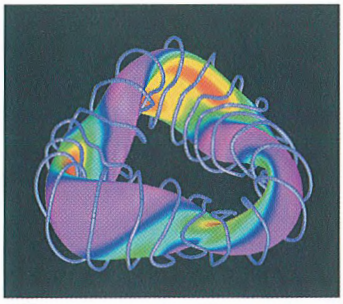
The ORNL Fusion Theory Group is pursuing computational research in three areas that encompass understanding plasma behavior in existing devices and the design of future experiments. These topics are: stellarator optimization and physics, toroidal plasma turbulence and its effects on transport, and radio frequency (RF) heating of plasmas.

COMPUTATIONAL APPROACH

Stellarator optimizations are carried out using using a steepest-descent method to minimize a variational form for the 3D plasma equilibrium. The plasma optimization is then carried out with a Levenberg-Marquardt algorithm. Plasma turbulence models evolve coupled sets of partial differential equations for the ion density, parallel velocity, and temperature in time in the presence of a noise source (to simulate heating). Finite differences in radius and Fourier expansions in the toroidal and poloidal angles are used. The time stepping scheme is time-implicit for the linear terms and time-explicit for the nonlinear terms. Particle models are used both in the stellarator transport physics studies and the self-organized criticality sandpile calculations.

ACCOMPLISHMENTS

We have developed compact stellarator 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 during 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. Our optimization techniques and stellarator analysis codes have helped translate both of these new optimization strategies into realizable experimental designs. These developments have opened up a new niche for the U.S. within the world stellarator program. Successful completion of these designs could result in a $40–50 million investment by DOE in new experimental facilities that have been designed predominantly through the application of NERSC's high performance computing resources.



Outer magnetic flux isosurface and filamentary magnet coils for a compact three field period transport-optimized stellarator. Color contours indicate the magnetic field strength: red = high field, magenta = low field.

Self-organized criticality sandpile models are used to study the nonlinear dynamics of plasma instabilities. These have now been run in parallel using enough particles and for long enough times to collect large statistical samples. This is leading to an improved understanding of L-H transition dynamics in tokamak experiments, control of internal transport barriers in reversed shear discharges, evaluation of superdiffusive transport regimes, and better analysis of the long time correlations in plasma edge turbulence. In addition, Landau fluid calculations of ion temperature gradient-driven turbulence have been incorporated into a simple gyrofluid model that evolves equations in time for the ion density or vorticity, the parallel ion velocity, and the ion temperature.

RF calculations have been performed in support of plasma heating efforts on the NSTX device at Princeton Plasma Physics Lab. Mechanisms have been identified and analyzed by which RF can drive wave-induced plasma flows.

SIGNIFICANCE

The development of new compact stellarators is of interest for near term experiments, where it allows larger-volume plasmas to be designed at a fixed cost. Larger-volume plasmas provide better shielding of neutrals and allow better science to be carried out. Compact plasmas could lower the development costs of fusion reactor devices and allow smaller, more modular devices to be built. If successful, this could significantly improve the economics of fusion power.

PUBLICATIONS

L. A. Berry, E. F. Jaeger, and D. B. Batchelor, "Wave-induced momentum transport and flow drive in tokamak plasmas," Phys. Rev. Lett. **82**, 1871 (1999).

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L. Garcia, B. A. Carreras, and V. E. Lynch, "Spatio-temporal structure of resistive pressure-gradient-driven turbulence," Phys. Plasmas **6**, 107 (1999).

http://www.ornl.gov/fed/theory/Theory_Home_page.html

Lattice Boltzmann Simulations for Divertor Physics and Turbulence

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RESEARCH OBJECTIVES

Novel thermal lattice Boltzmann simulations (TLBM) are being investigated to consider parameter regimes appropriate for the tokamak divertor. TLBM are much better suited for MPP systems than computational fluid dynamics (CFD) codes. In the divertor region there are time varying regimes in which the neutral collisionality ranges from highly collisional (well treated by fluid equations) to weakly collisional (requiring Monte Carlo). It is numerically stiff to couple fluid and kinetic codes due to the disparate spatial and temporal scales. However, this stiffness is avoided when coupling TLBM to Monte Carlo, since both these descriptions are kinetic.

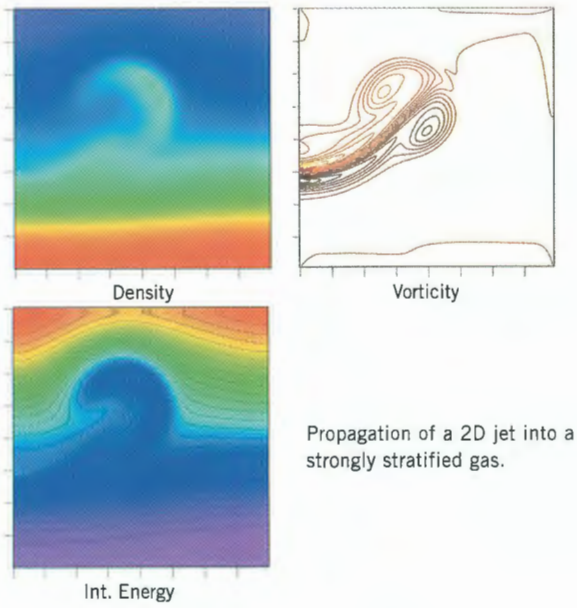
COMPUTATIONAL APPROACH

TLBM codes solve the linearized Bhatnagar-Gross-Krook (BGK) system and so involve: (a) computation of the mean density, velocity, and temperature at each spatial node; (b) collisional relaxation; and (c) Lagrangian free-streaming. Our TLBM code has two computational kernels which act only on local data, and a streaming operation that passes boundary data between PEs.

ACCOMPLISHMENTS

The simplicity of TLBM has a drawback—numerical instability. As more and more moment constraints are imposed on the distribution function, the further one must go in Taylor expansions in the mean velocity for the relaxed distribution function. To eliminate discrete lattice symmetry effects that can enter into the higher moment equations, the relaxed distribution function must not be a Maxwellian. Hence there is no H-theorem for TLBM. We have been exploring the utilization of higher isotropy phase space velocity lattices—in particular, the octagonal lattice in 2D (with its 53-bit generalization to 3D). This forces us to decouple the velocity lattice from the spatial grid, since an octagonal lattice is not space-filling. The use of second-order interpolation does not introduce measurable numerical viscosity or conductivity. These higher isotropy lattices are much more numerically stable. Further generalizations are being considered in allowing the streaming to be nodal temperature dependent. This allows simulations of flows with Mach numbers up to 0.5.

We have also extended our TLBM to multiple species in preparation for plasma divertor studies. This multi-species model will be used to solve models like the UEDGE-Navier-Stokes coupled set of equations. For 2D turbulence, we have investigated the interaction and relaxation of double vortex layers that are perpendicular to each other.



Propagation of a 2D jet into a strongly stratified gas.

SIGNIFICANCE

In the standard CFD approach to solving the nonlinear equations, one must handle the nonlinear Riemann problem, which consumes over 30% of the CPU time in accurate resolution of the nonlinear convective derivative. In TLBM, one sidesteps the Riemann problem altogether and can use Lagrangian streaming to handle the (linear) advective derivative. By embedding the nonlinear system into higher dimensional phase space (i.e., by going to a linearized kinetic description), we can choose a simplified system (e.g., a BGK collision operator) to recover the desired equations.

PUBLICATIONS

P. Pavlo, G. Vahala, and L. Vahala, "Higher order isotropic velocity grids in lattice methods," Phys. Rev. Lett. **80**, 3960 (1998).

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http://www.physics.wm.edu/~vahala/aug99.html

Monte Carlo Methods for Nuclear Structure

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RESEARCH OBJECTIVES

Quantum Monte Carlo methods for the nuclear shell model allow exact calculations in much larger model spaces than can be treated by conventional methods. The methods are applied to study various properties of medium-mass and heavy nuclei at zero and finite temperature, including level densities, collective properties, pairing, and strength functions.

COMPUTATIONAL APPROACH

We use a representation of the many-body propagator (in imaginary time) in terms of a functional integral over one-body propagators in fluctuating external fields, known as the Hubbard-Stratonovich (HS) transformation. Monte Carlo methods are used to perform the high-dimensional integration. A modification of the Metropolis algorithm, based on Gaussian quadratures, improves the efficiency of the Monte Carlo random walk. Various projection methods are implemented in the HS representation. The calculations are done in the framework of the nuclear shell model.

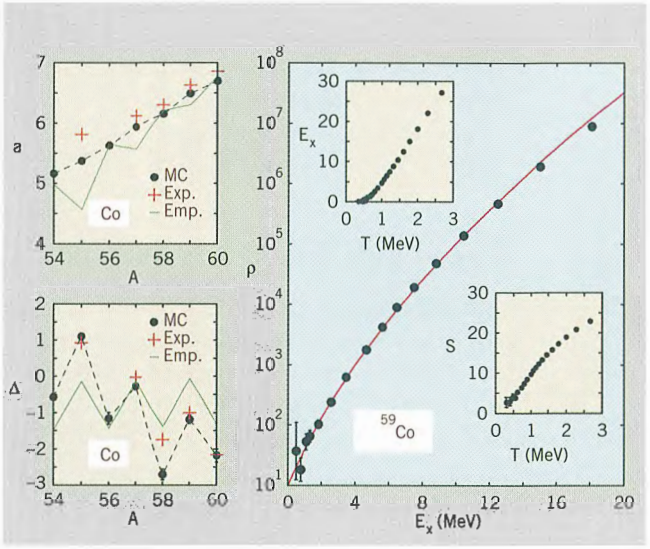
ACCOMPLISHMENTS

Using the Monte Carlo methods in the full $fpg_{9/2}$-shell, we have calculated accurate level densities of nuclei in the iron region and found excellent agreement with experiment. We extracted single-particle level density and backshift parameters by fitting the calculated densities to a backshifted Bethe formula, and found new and interesting shell effects in the systematics of these parameters.

We have used a particle-number reprojection method to calculate thermal observables (e.g., level densities) for a series of nuclei using a Monte Carlo sampling for a single nucleus. Level densities of odd-mass and odd-odd nuclei are reliably extracted despite a sign problem. Both the mass and isospin dependence of the experimental level densities are well described without any adjustable parameters. The single-particle level density parameter is found to vary smoothly with mass. The odd-even staggering observed in the calculated backshift parameter follows the experimental data more closely than do empirical formulas.

SIGNIFICANCE

The initial applications of these techniques had been severely limited by the sign problem which is generic to fermionic Monte Carlo methods and occurs for all realistic nuclear interactions. We have developed a practical solution to the sign problem in the nuclear case which opens the door to new and interesting realistic calculations in much larger configuration spaces than could be treated previously. Our approach can address a variety of problems in nuclear physics and astrophysics that could not otherwise be solved in full shell calculations. Similar methods might also be useful in other fields in physics that require a non-perturbative approach to the interacting many-body problem.



Right panel: The level density of ^{59}Co versus excitation energy E_x. The solid circles are the Monte Carlo (MC) results, and the solid line is the experiment. The two insets show the excitation energy and entropy as a function of temperature. The MC level density is well described by the backshifted Fermi gas formula, which is parametrized by the single-particle level density parameter a and the backshift parameter Δ. Left panels: a and Δ versus mass number A for cobalt isotopes. The solid circles are obtained from the MC calculations, while the pluses are the experimental values. The MC results follow the experimental data more closely than do empirical formulas (solid lines).

PUBLICATIONS

Y. Alhassid, S. Liu, and H. Nakada, "Particle-number reprojection in the shell model Monte Carlo method: Application to nuclear level densities," Phys. Rev. Lett. **83**, 4265 (1999).

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H. Nakada and Y. Alhassid, "Microscopic nuclear level densities from Fe to Ge by the shell model Monte Carlo method," Phys. Lett. B **436**, 231 (1998).

Quantum Monte Carlo for Nuclei and Nuclear/Neutron Matter

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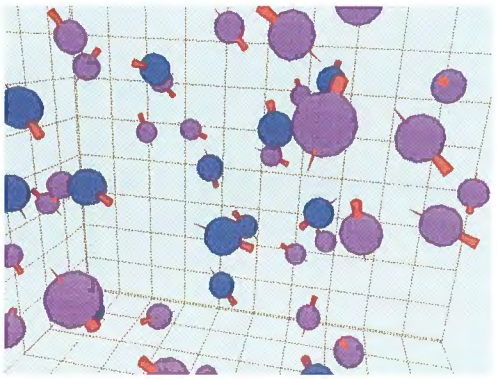
R. Schiavilla and J. Forest,
Thomas Jefferson National Accelerator Facility
V. R. Pandharipande, University of Illinois
K. E. Schmidt, Arizona State University
S. Fantoni, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy



A Quantum Monte Carlo simulation of neutron star matter; individual neutrons are shown with arrows representing each neutron's spin. Different colors represent periodic images.

RESEARCH OBJECTIVES

The goal of this project is to calculate the properties of nuclei and neutron matter with realistic interactions. This project studies the spectra of nuclei and equation of state of neutron matter, and also studies a variety of weak-interaction processes of importance in astrophysics and elsewhere.

COMPUTATIONAL APPROACH

The computational approach is based on a variety of quantum Monte Carlo algorithms. In light nuclei, variational and Green's function Monte Carlo are used to study structure and low-energy reactions. Constrained path-integral algorithms allow us to study many-fermion systems quite accurately. Methods which combine auxiliary-field and diffusion Monte Carlo should allow us to perform accurate simulations for much larger numbers of particles, including studies of finite nuclei and neutron matter.

ACCOMPLISHMENTS

We have constructed a new class of three-nucleon interactions which yield significantly improved results for the structure of light nuclei. In particular, these models reproduce the binding of neutron-rich nuclei and the LS splittings much better than previous-generation interactions. We expect these new models to play a significant role in neutron-rich nuclei generally, as well as in the structure and response of neutron-star matter.

We have also developed new codes which combine diffusion and auxiliary field methods for treating many-body nuclear physics problems. Initial tests in neutron drops and neutron matter have been extremely encouraging. The present calculations are more accurate (as tested against exact calculations of smaller systems) than previous efforts at variational calculations of neutron matter. We are continuing to develop these algorithms to be able to study possible phase transitions in neutron matter as well as neutrino scattering, an important ingredient in supernovae.

Finally, we have developed new algorithms for treating low-energy scattering within the Monte Carlo framework. These schemes work very well in determining parameters such as scattering lengths, effective ranges, and positions and widths of resonance. We have used them to explore the parity-violating spin rotation of neutrons passing through helium. This experiment is designed to help determine the weak parity-violating π-NN coupling constant, a subject of much current theoretical and experimental interest.

SIGNIFICANCE

It is now possible to computationally study nuclear systems with realistic nuclear interactions, that take into account the vast amount of nucleon-nucleon scattering data. These interactions produce large spatial, spin, and isospin correlations between the nucleons. These correlations can play an important role in a variety of intriguing processes, ranging from the reactions that produce solar neutrinos, the scattering of electrons by nuclei, and parity-violating weak interactions in the NN interaction, to the structure of neutron stars and their interactions with neutrinos.

PUBLICATIONS

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Continuing Studies of Plasma Beat Wave Accelerators

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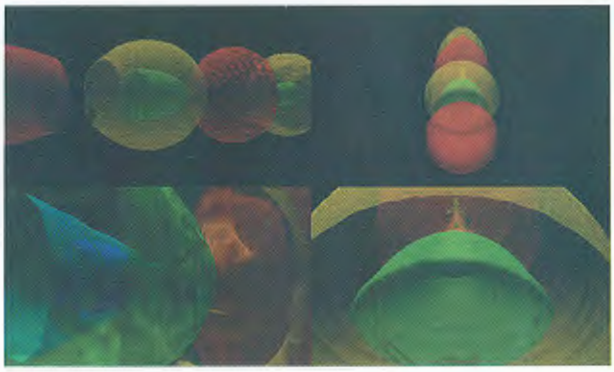
RESEARCH OBJECTIVES

This research attempts to test the feasibility of various plasma-based accelerator concepts, to model full-scale plasma-based accelerator experiments, and to help develop new advanced accelerator concepts.

COMPUTATIONAL APPROACH

We are applying particle-based models, including fully explicit particle-in-cell (PIC) codes, ponderomotive guiding center PIC codes, and new photon kinetic codes. We are integrating all these algorithms into an object-oriented framework we have developed which supports massively parallel processing.



These images are isosurface contours of the accelerating electric field from a 3D PIC simulation of a plasma wakefield accelerator. The simulation was done on 64 nodes of the T3E at NERSC. It used 14 million grid cells and 56 million particles. In the upper and lower left, the wake shown was excited by an azimuthally symmetric drive beam, while for the upper and lower right, the drive beam was asymmetric. The asymmetry leads to a lower peak amplitude in the wake and in an asymmetric transverse profile for the accelerating field. The same color maps were used for each figure. The dark blue, light blue, green, and yellow surfaces correspond to acceleration gradients of 0.5, 0.4, 0.2, and 0.1 GeV/m, while the red surfaces correspond to a decelerating gradient of 0.1 GeV/m. The simulation parameters were chosen to accurately model the E-157 plasma wakefield experiment (a collaboration of SLAC, UCLA, USC, and LBNL). The figure was rendered with the help of the Office of Academic Computing at UCLA.

ACCOMPLISHMENTS

We have developed a new fully parallel, multidimensional (2D or 3D) object-oriented PIC code which is optimized for modeling plasma-based acceleration. The object-oriented code design allowed us to implement multiple algorithms that can that be chosen at runtime. The code is also designed to be extendable to advanced features like dynamic load balancing and adaptive mesh refinement. We used this code to model 1-meter plasma wakefield stages, 2D and 3D simulations of plasma wakefield excitation, 2D and 3D simulations of the generation of single-cycle laser pulse by photon deceleration, and 3D simulations of Cerenkov radiation from plasma wakes. We also developed a new ponderomotive guiding center code for efficient modeling of laser-plasma accelerator stages.

SIGNIFICANCE

In plasma-based acceleration, electrons "surf" on relativistic space charge plasma waves. In such waves, electrons can be accelerated with gradients orders of magnitude larger than is possible with current technology. If plasma-based accelerator technology is successfully developed, then multi-GeV stages could be miniaturized to fit on a tabletop. Just as the advent of tabletop high-powered lasers have had a tremendous impact, miniature tabletop accelerators could have cross-cutting impacts in fields as diverse as high-energy physics, synchrotron radiation sources, medicine, and biology.

PUBLICATIONS

B. J. Duda, R. G. Hemker, K.-C. Tzeng, and W. B. Mori, "A new long-wavelength hosing instability for lasers propagating in plasmas," Phys. Rev. Lett. (in press).

K.-C. Tzeng and W. B. Mori, "Suppression of electron ponderomotive blowout and relativistic self-focusing by the occurrence of raman scattering and plasma heating," Phys. Rev. Lett. **81**, 104 (1998).

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Weak Matrix Elements from Lattice QCD

Gregory Kilcup and Dmitry Pekurovsky,
The Ohio State University

RESEARCH OBJECTIVES

Our objectives are computation of non-perturbative renormalization for staggered weak operators; computation of matrix elements for parameters B7 and B8; comparison of quenched and dynamical matrix element and quark mass results using QCDSP (Quantum Chromodynamics on Digital Signal Processors) configurations; and providing an archive of valuable gauge configuration data which can be used by the lattice community at large.

COMPUTATIONAL APPROACH

We use Monte Carlo methods, fast Fourier transforms, and standard linear solvers including conjugate gradients and minimal residual.

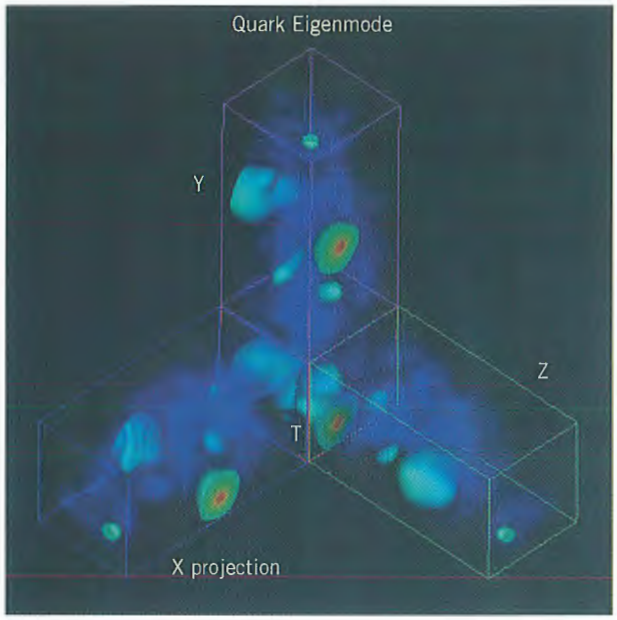
ACCOMPLISHMENTS

Using Grand Challenge resources at NERSC, we have computed the weak matrix elements which are responsible for the $\Delta I = 1/2$ rule. This is a longstanding puzzle of weak kaon decays, in which two seemingly similar decay processes ($I = 0$ and $I = 2$) proceed at very different rates. For the $I = 2$ amplitudes, we were able to run on a whole ensemble of quenched gauge configurations and extrapolate to the continuum limit. For the more difficult $I = 0$ amplitudes, we ran at two quenched lattice spacings and on one small dynamical ensemble. To compute the matrix elements for ϵ'/ϵ, we find we also need to do a nonperturbative renormalization. As a first step in this direction, we have computed the light quark mass renormalization.

As a service to the whole lattice QCD community, we have also gauge-fixed all the configurations used and archived them in the qcd.nersc.gov archive.

SIGNIFICANCE

As a field, lattice QCD provides theoretical calculations of quantities which can be measured experimentally. This provides both cross-checks of the Standard Model of particle physics, and a determination of several of its fundamental parameters. This work in particular is aimed at quark masses and certain weak



Visualization of typical fluctuations in the quark field. The underlying data are four-dimensional, and we show all four possible projections (x, y, z, t) down to 3D arranged as a tesseract.

interaction matrix elements using staggered fermions. In conjunction with results from other groups using different fermion formulations (e.g., Wilson, improved, domain wall), this research will help refine the theoretical calculation of the recently measured quantity ϵ'/ϵ.

PUBLICATIONS

D. Pekurovsky and G. Kilcup, "Lattice calculation of matrix elements relevant for $\Delta I = 1/2$ rule and ϵ'/ϵ," e-print hep-lat/9903025 (1999).

D. Pekurovsky and G. Kilcup, "Matrix elements relevant for $\Delta I = 1/2$ rule and ϵ'/ϵ from lattice QCD with staggered fermions," e-print hep-lat/9812019 (1998).

D. Chen, G. Kilcup et al., "QCDP: A status report," Nucl. Phys. Proc. Suppl. **63**, 997 (1998).

http://www.physics.ohio-state.edu/~kilcup/Lattice_QCD/
http://qcd.nersc.gov

Cosmic Microwave Background Data Analysis—The BOOMERANG Long Duration Balloon Flight

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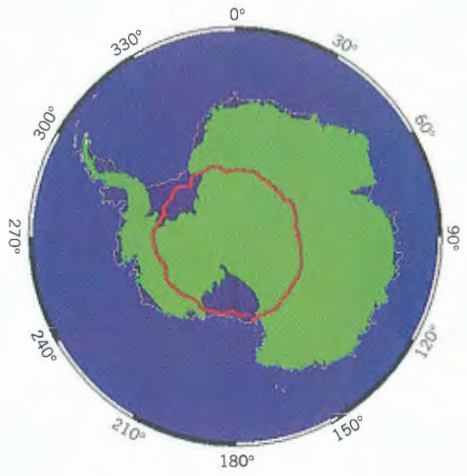
Paolo de Bernardis, Università de Sapienza, Rome
Phillip Mauskopf, University of Massachusetts
Julian Borrill, NERSC, Lawrence Berkeley National Laboratory

RESEARCH OBJECTIVES

In December 1998 and January 1999, the BOOMERANG (Balloon Observations of Millimetric Extragalactic Radiation and Geophysics) Long Duration flight spent 10.5 days in the Antarctic stratosphere measuring the temperature of the cosmic microwave background (CMB). The resulting data set is the most significant measurement of the tiny fluctuations in the microwave sky temperature since they were first detected by the COBE satellite. The data covers 2000 square degrees of the sky at 10 arcminute resolution and high signal-to-noise. This research project is devoted to analyzing the BOOMERANG LDB data set, first to produce a map of the CMB anisotropies and then to extract their angular power spectrum.

COMPUTATIONAL APPROACH

The analysis of a massive CMB data set can be recast as a problem in numerical linear algebra, and, in particular, in the solution of linear systems involving very large, dense, symmetric matrices. First we convert the time-ordered CMB data to a pixelized map, triangular-solving a linear system with a single right hand side to obtain the maximum of the map likelihood function. Then we apply a Newton-Raphson iterative method to locate the peak of the CMB power spectrum likelihood function (which has no closed-form solution) given this map. Each iteration requires triangular-solving many linear systems, each with as many right hand sides as there are pixel-pixel correlation matrix rows and columns. The entire analysis algorithm has been implemented in parallel on the T3E at NERSC as the Microwave Anisotropy Dataset Computational Analysis Package (MADCAP).



BOOMERANG was launched on December 29, 1998. For the next 10.5 days it made its way slowly around Antarctica at an altitude of 120,000 feet, collecting CMB temperature data. Finally, after a complete circle, the payload was dropped by parachute to a spot about 50 km from the launch pad for an easy recovery.

ACCOMPLISHMENTS

Over the past year we have used MADCAP to analyze the data from the 1997 BOOMERANG North America flight. Although this was primarily a test flight in preparation for the Long Duration/Antarctic flight, the data obtained was still one of the best measurements of the CMB to date. The results of this analysis, which are about to be submitted for publication, provide the first single-experiment measurement of the CMB angular power spectrum over a wide enough range of angular scales to place a significant constraint on cosmological models. Based on this work we can be confidant that (i) BOOMERANG LDB will be an extraordinarily powerful data set, capable of providing the tightest constraints yet on cosmological parameters; (ii) our current data analysis approach is capable of extracting a significant fraction of the information content of BOOMERANG LDB, whilst the promise of the full data content will be a compelling driver for further CMB data analysis research.

SIGNIFICANCE

The tiny fluctuations in the CMB temperature correspond to the very first density perturbations in the universe and contain detailed information about all the fundamental parameters of cosmology—the universe's geometry, expansion rate, number of neutrino species, ionization history, and the energy density in baryons, dark matter, and cosmological constant.

PUBLICATIONS

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P. D. Mauskopf et al., "Measurement of a peak in the cosmic microwave background power spectrum from the North American test flight of BOOMERANG," Astrophys. J. (submitted, 1999). astro-ph/9911444

A. Melchiorri et al., "A measurement of Omega from the North American test flight of BOOMERANG," Astrophys. J. (submitted, 1999). astro-ph/9911445

http://astro.caltech.edu/~lgg/boom/boom.html
http://cfpa.berkeley.edu/~borrill/madcap.html

STAR Detector Simulations and Data Analysis

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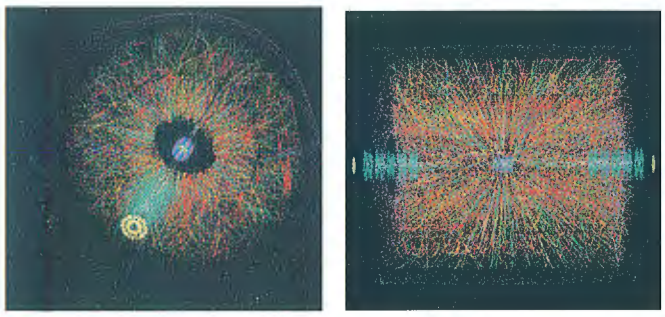
J. Yang, University of California, Los Angeles
P. Nevski, Brookhaven National Laboratory
and the STAR Collaboration

RESEARCH OBJECTIVES

The STAR detector at Brookhaven National Laboratory (BNL) is designed to study the collision of heavy nuclei at very high energy. Its goal is to investigate nuclear matter at extreme energy density and to search for evidence of the phase transition between hadronic matter and the deconfined quark-gluon plasma. STAR and the RHIC accelerator (Relativistic Heavy Ion Collider) will generate over 300 terabytes of data each year, with an additional large volume of simulated data needed for data analysis and for understanding the performance of the detector. The generation and analysis of this simulated data is the objective of this research.

COMPUTATIONAL APPROACH

Physics results from experimental relativistic heavy ion collisions are derived from statistical analysis of large numbers of events (collisions of individual atomic nuclei). The theoretical models are implemented as Monte Carlo codes that describe the final state of each of the thousands of particles that are produced in these collisions. We use a number of these theoretical codes (VENUS, HIJING, RQMD, and others) to produce large samples of events. A simulation code called GEANT is used to propagate each of these thousands of particles through the material of the STAR detector and compute the reactions and energy deposition that occurs throughout the detector. These theoretical model codes and the detector simulation code are run on the MPP system utilizing the natural parallelism of the problem, namely that each event is independent, so that different events are computed in parallel on the various processor nodes.



This simulation shows a single event, the collision of two gold ions with a center-of-mass energy of 200 AGeV. The color code indicates hits in the various subdetector components as well as indicating the momentum of particles. The image on the left is a perspective view near one end of the detector, looking roughly along the beam axis. The right image is a side view of the same event.

ACCOMPLISHMENTS

Over the past two years, STAR has generated a large set of simulated data on the Cray T3E. Approximately 250K PE-hours were used in fiscal 1999 and over 6 terabytes of simulated data produced. These data have been invaluable for understanding the detector response of STAR and developing analysis algorithms. They were essential as input for two large-scale Mock Data Challenges (MDC) at the RHIC Computing Facility at BNL, where the STAR primary data will be stored and first analyzed. Mechanisms were developed to efficiently transport large volumes of STAR data over the network between computing facilities spread across the country, a capability that will be crucial for the distribution of real STAR data. As a result of these efforts, STAR is now confident that the first data can be reliably handled and efficiently processed to extract the physics.

SIGNIFICANCE

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

PUBLICATIONS

J. W. Harris et al. (STAR Collaboration), "STAR physics in the first two years at RHIC," *Proc. 15th Winter Workshop on Nuclear Dynamics, January 1999, Park City, UT*, Advances in Nuclear Dynamics, Plenum Press (in press).

T. J. Hallman et al. (STAR Collaboration), "The STAR scientific program," *Proc. XIV Int. Symp. on High Energy Physics Problems, Relativistic Nuclear Physics, and Quantum Chromodynamics, August 1998, Dubna, Russia* (in press).

H. Caines et al. (STAR Collaboration), "The year-one physics capabilities of STAR," *Proc. APS Centennial Meeting, March 1999, Atlanta, GA*, Relativistic Heavy Ion Mini-Symposium, World Scientific (in press).

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

Computational Accelerator Physics Grand Challenge

R. Ryne, S. Habib, and J. Qiang, Los Alamos National Laboratory
K. Ko, N. Folwell, Z. Li, B. McCandless, C. Ng, and M. Wolf,
Stanford Linear Accelerator Center
G. Golub, W. Mi, M. Saparov, and Y. Sun, Stanford University
V. Decyk, University of California, Los Angeles
J. Ahrens, T. Cleland, J. Cummings, W. Humphrey, S. Karmesin,
P. McCormick, A. McPherson, J. Painter, G. Mark,
Advanced Computing Laboratory, LANL
E. Ng, W. Saphir, NERSC, Lawrence Berkeley National Laboratory

RESEARCH OBJECTIVES

The goal of this Grand Challenge is to develop a new generation of accelerator modeling tools, targeted to very large scale (tera-scale) parallel computing platforms, and to apply them to accelerator projects of national importance. The new capability will enable computations for accelerator design and analysis on a scale that is unprecedented in size, accuracy, and resolution. Specific objectives include the development of parallel beam dynamics codes aimed at simulating, from end to end, intense beams through a variety of accelerator systems, and parallel electromagnetics codes for modeling large, complex beamline components and accelerating structures.

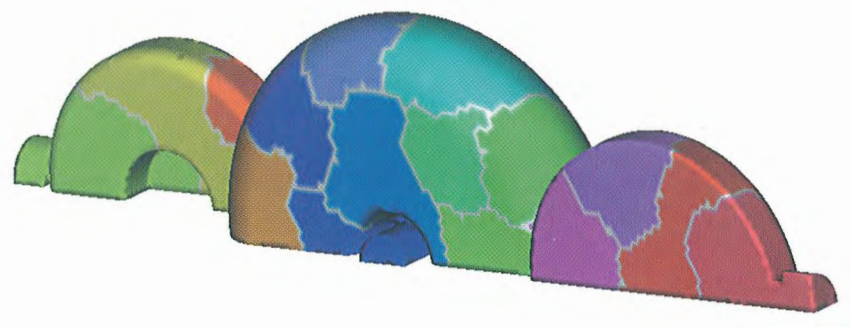
COMPUTATIONAL APPROACH

The beam dynamics component of this research uses parallel particle-in-cell (PIC) techniques, particle managers, dynamic load balancing, fast Fourier transform (FFT) based Poisson solvers, and techniques from magnetic optics. Split-operator methods are used to combine magnetic optics and parallel PIC techniques in a single framework and to establish particle advance algorithms. The electromagnetics component utilizes unstructured grid generation, domain decomposition, adaptive mesh refinement, finite element formulation for the eigenmode solver, and the modified Yee algorithm for the time-domain solver. Systems involving particles in electromagnetic structures are treated using hybrid grids, with a structured mesh in the region of the beam and an unstructured grid near the structure boundaries.

ACCOMPLISHMENTS

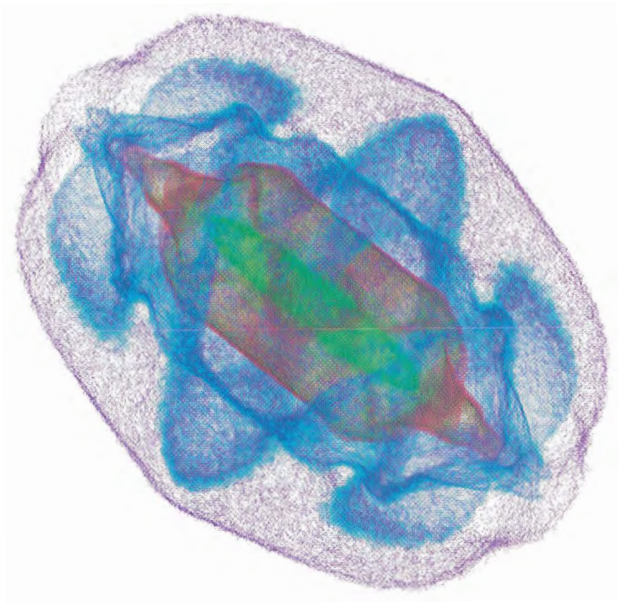
Three parallel application codes, IMPACT, Omega3P, and Tau3P, have been developed under the Grand Challenge. The following improvements made during FY99 result in significant increases in performance.

The IMPACT beam dynamics code has seen a performance improvement of a factor of 4 due to a replacement of the original charge deposition/field interpolation routines with a parallel particle manager. Other improvements for FY99 include significantly reduced memory overhead, a choice of parallel particle managers (with fixed and variable message buffers), parallel I/O, and restart capabilities. The POOMA version has been modified to improve the performance of FFTs across boxes on the SGI Origin 2000 system. IMPACT was used in the first systematic study of halo formation due to longitudinal/transverse coupling in charged particle beams. IMPACT was also used to model the Accelerator Production of Tritium (APT) and Spallation Neutron Source (SNS) linacs, including the largest simulations to date of the SNS linac, with 500 million particles. The capability to include machine imperfections was added in order to model more realistic accelerators.



Domain decomposition associated with an Omega3P calculation of the Accelerator Production of Tritium coupled cavity linac.

The accomplishments in the electromagnetics area include a new, hybrid Jacobi-Davidson algorithm that dramatically accelerates the eigensolver convergence in Omega3P, and the incorporation of a superior mesh distribution preprocessor in Tau3P that greatly improves its parallel efficiency. Using 128 processors on the T3E, Omega3P can calculate the accelerating mode in the Next Linear Collider (NLC) accelerating structure on the order of minutes for a geometry involving 1 million degrees of freedom, and the code achieves close to linear scalability. In addition, progress has been made in developing a complex solver for Omega3P to treat lossy cavities and in implementing a rigid beam in Tau3P to model wakefield effects.



Volume rendering of phase space output data from an IMPACT simulation of the Spallation Neutron Source linac.

SIGNIFICANCE

The state-of-the-art accelerator codes IMPACT, Omega3P, and Tau3P have made a significant impact on several important DOE projects such as the NLC, APT, and SNS. The IMPACT simulation helped to predict the maximum particle amplitude, and hence the required beam pipe aperture, in the SNS linac. Omega3P and Tau3P simulations were pivotal in realizing an improved NLC structure design with higher acceleration gradient that results in a $100 million savings in linac construction cost and anticipated operational cost savings as well.

PUBLICATIONS

A. V. Fedotov, R. L. Gluckstern, S. Kurennoy, and R. Ryne, "Halo formation in 3D bunches with different phase space distributions," Phys. Rev. ST Accel. Beams 2, 014201 (1999).

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http://t8web.lanl.gov/people/salman/capgca/
http://public.lanl.gov/ryne/gca.html

Optimal Photometric Reduction of Supernova Images for Cosmological Measurements

Saul Perlmutter, Robert Knop, Greg Aldering, and Peter Nugent,
Lawrence Berkeley National Laboratory
Alex Conely and Michael Wood-Vasey,
University of California, Berkeley

RESEARCH OBJECTIVES

Several supernova search and asteroid search groups formed an alliance to find a large batch of nearby supernovae. The key element of the alliance was to run all of the supernova searches simultaneously so that the follow-up resources were used in a concentrated and complementary fashion. This provided us with the well-sampled photometric (multiple times a week) and spectroscopic (weekly) follow-up required to yield the greatest scientific return.

COMPUTATIONAL APPROACH

Data reduction, analysis, and storage are being performed using NERSC facilities. We are using a multiple instruction/multiple data (MIMD) approach utilizing Fortran 90, C, and MPI.

ACCOMPLISHMENTS

In total, the alliance discovered 35 supernovae during March 1999. Twenty Type Ia supernovae were caught before or at maximum light and were followed with UBVRI (ultraviolet, blue, visual, red, infrared) photometry and spectroscopy. These nearby supernovae will become the calibrators for high-redshift supernovae and will help us determine the fundamental cosmological parameters which describe our universe. This is the largest and most successful search for and follow-up of nearby supernovae in history.

SIGNIFICANCE

In order to draw any scientific conclusions from the high-redshift supernovae research, we need to be able to fully understand Type Ia supernovae. This is accomplished through careful analysis of several nearby supernovae in order to calibrate the high-redshift supernovae and ascertain possible systematic biases.

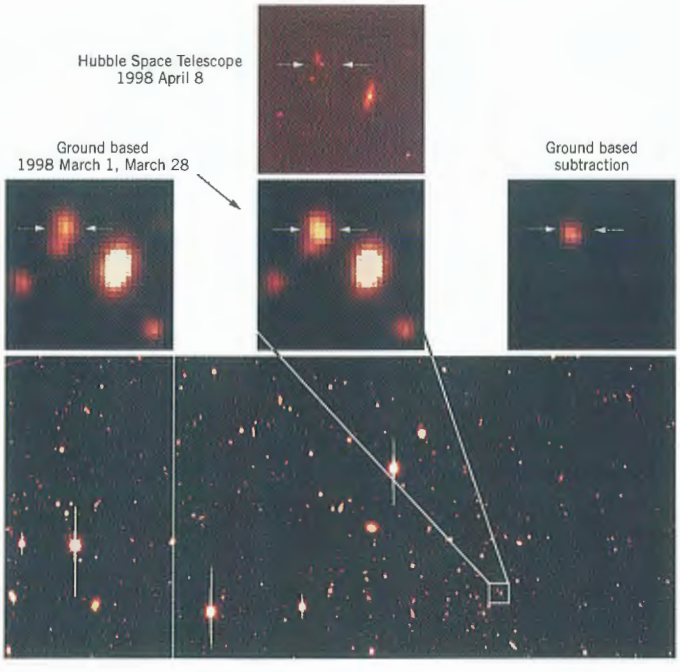
PUBLICATIONS

S. Perlmutter, G. Aldering, G. Goldhaber, R. A. Knop, P. Nugent, P. G. Castro, S. Deustua, S. Fabbro, A. Goobar, D. E. Groom, I. M. Hook, A. G. Kim, M. Y. Kim, J. C. Lee, N. J. Nunes, R. Pain, C. R. Pennypacker, R. Quimby, C. Lidman, R. S. Ellis, M. Irwin, R. G. McMahon, P. Ruiz-Lapuente, N. Walton, B. Schaefer, B. J. Boyle, A. V. Filippenko, T. Matheson, A. S. Fruchter, N. Panagia, H. J. M. Newberg, W. J. Couch, and the Supernova Cosmology Project, "Measurements of Ω and Λ from 42 high-redshift supernovae," Astophys. J. **517**, 565 (1999).

S. Perlmutter, G. Aldering, M. Della Valle, S. Deustua, R. S. Ellis, S. Fabbro, A. Fruchter, G. Goldhaber, D. E. Groom, I. M. Hook, A. G. Kim, M. Y. Kim, R. A. Knop, C. Lidman, R. G. McMahon, P. Nugent, R. Pain, N. Panagia, C. R. Pennypacker, P. Ruiz-Lapuente, B. Schaefer, and N. Walton, "Discovery of a supernova explosion at half the age of the Universe," Nature **391**, 51 (1998).

S. Perlmutter, B. Boyle, P. Bunclark, D. Carter, W. Couch, S. Deustua, M. Dopita, R. Ellis, A.V. Filippenko, S. Gabi, K. Glazebrook, G. Goldhaber, A. Goobar, D. Groom, I. Hook, M. Irwin, A. Kim, M. Kim, J. Lee, T. Matheson, R. McMahon, H. Newberg, R. Pain, C. Pennypacker, and I. Small, "High-redshift supernova discoveries on demand: First results from a new tool for cosmology and bounds on q0," Nucl. Phys. B Proc. Suppl. (in press).

http://panisse.lbl.gov:80/nearsearch/



By subtracting two charge-coupled device (CCD) images, obtained with the Cerro Tololo Inter-American Observatory's 4.0-meter telescope with a one month spacing, the Supernova Cosmology Project was able to detect SN 1998ba exploding in its host galaxy over 3 billion light-years away. One week after the discovery, SN 1998ba was observed by the Hubble Space Telescope. The dramatic improvement in resolution from the space-based image is readily apparent. The Supernova Cosmology Project has been using NERSC resources to determine the best way to reduce these types of images and improve upon our detection capabilities.

Domain-Wall Quarks at Finite Temperature

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RESEARCH OBJECTIVES

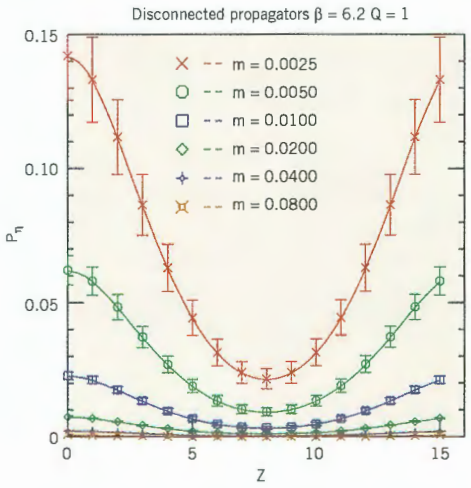
One problem which complicates lattice QCD simulations with the standard staggered or Wilson methods of putting quarks on the lattice is that chiral flavor symmetry is explicitly broken by these discretizations. Defining the quarks on a 5-dimensional lattice with open boundary conditions in the fifth dimension yields a lattice transcription whose 4-dimensional projection is explicitly chiral, but only when the lattice extent in the fifth dimension (N_5) becomes infinite. The question then is how well chiral symmetry is realized for a finite and manageable value of N_5. We are studying this question in the high temperature (plasma) phase on a set of $16^3 \times 8$ quenched configurations.

COMPUTATIONAL APPROACH

The calculation of the eigenmodes of the domain-wall Dirac operator and the inversion of this operator to calculate the required greens functions is performed using the conjugate gradient method. The code is vectorized for PVP execution over the sites of the 4-dimensional lattice. We use the red-black preconditioning developed for Wilson fermions.

ACCOMPLISHMENTS

We first determined the level crossings as a function of mass for Wilson fermions, which correspond to instantons in the gauge field configurations, for configurations with $\beta = 6/g^2 = 6.2$, $\beta = 6.1$ and $\beta = 6.0$. We then calculated lowest lying eigenmodes of the domain-wall Dirac operator on each configuration as a function of N_5. For $\beta = 6.2$, well above the transition, the eigenvalues separated into those which rapidly approached a non-zero limit as N_5 was increased, and those which appeared to be approaching zero exponentially with increasing N_5, and could be interpreted as the expected fermion zero modes corresponding to instantons. By $\beta = 6.0$, which is very near the finite temperature phase transition, there was no clear separation.



Configurations identified with topological charge one make large contributions to the disconnected propagators, contributions which increase with decreasing quark mass.

At our highest value of N_5 (10), we calculated the connected and disconnected contributions to the η/η' and σ/f_0 screening propagators at $\beta = 6.2$ and are repeating this analysis at $\beta = 6.0$. We are able to make an accurate calculation of the disconnected propagators by separating off the contribution of the lowest lying eigenmodes and using 20 noise vectors to get a stochastic estimator of the remainder. In the process of this calculation, we obtain estimates of the scalar and pseudoscalar chiral condensates for each configuration. The pseudoscalar condensate approximates the value predicted by the Atiyah-Singer theorem down to quark masses comparable with the value(s) of the would-be zero mode(s).

The screening propagators at $\beta = 6.2$ approximate the correct chiral behavior. Those configurations identified with having topological charge zero make contributions consistent with zero to the disconnected propagators, while those with topological charge one make large contributions to the disconnected propagators, contributions which increase with decreasing quark mass (see figure). In the topological charge one sector, the "zero" mode contributions extracted from the connected propagator are in good agreement with the disconnected propagator. Indications are that the situation at $\beta = 6.0$ is more complicated.

SIGNIFICANCE

When this analysis is repeated with two flavors of dynamical quarks, one should be able to demonstrate whether the $U(1)$ axial symmetry is restored at the chiral transition, revealing how chiral symmetry is realized in the excitations of the quark-gluon plasma. This information will be useful in interpreting data from experiments.

PUBLICATIONS

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J.-F. Lagaë and D. K. Sinclair, "Improved staggered quark actions with reduced flavour symmetry violations for lattice QCD," Phys. Rev. D **59**, 014511 (1999).

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.

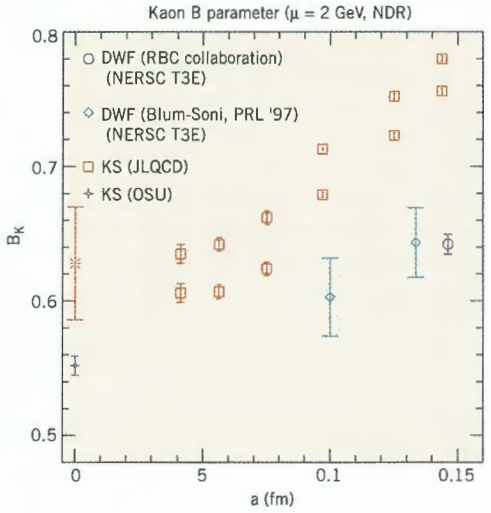

Figure 1: The kaon *B* parameter. The Kogut-Susskind result is from JLQCD and OSU. DWF indicate improved scaling in this case. The DWF values are not renormalized.

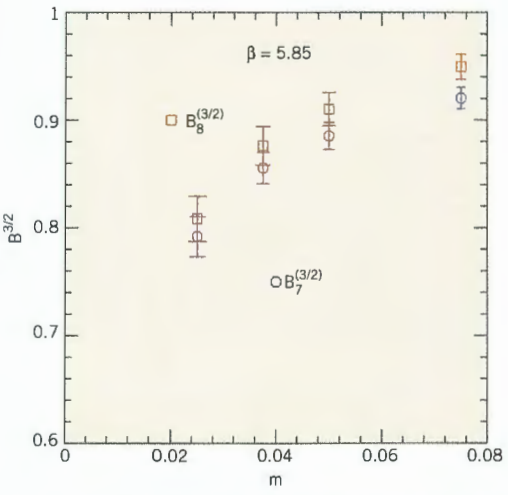

Figure 2: The $\Delta I = 3/2$ electroweak *B* parameters (not renormalized).

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-900 machine at NERSC is being 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 16 at $\beta \geq 6.0$. In the work finished so far, we have obtained a number of key results, including a calculation of the important matrix elements, B_K (see Fig. 1), $B_7^{3/2}$ and $B_8^{3/2}$ (Fig. 2), and the value of the strange quark mass. Furthermore, 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 compensate 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 the past 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 ϵ'/ϵ. Successful completion of this calculation should enable us to test for clues for the new physics that lies beyond the Standard Model.

PUBLICATIONS

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T. Blum and A. Soni, "QCD with domain wall quarks," Phys. Rev. D **56**, 174 (1997).

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QCD Simulations with Improved Staggered Quarks

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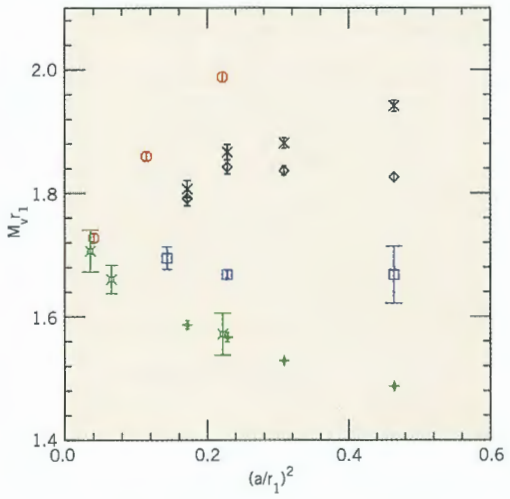
University of Arizona
Claude Bernard, Washington University
Tom DeGrand, University of Colorado
Carleton DeTar and Pierre Lacock, University of Utah
Steve Gottlieb, Indiana University
Jim Hetrick, University of the Pacific
Urs Heller, Supercomputer Computations Research Institute (SCRI),
Florida State University
Craig McNeile, Liverpool University
Kari Rummukainen, Nordic Institute for Theoretical Physics
(NORDITA)
Bob Sugar, University of California, Santa Barbara

RESEARCH OBJECTIVES

The MILC collaboration has developed and tested improved actions for Kogut-Susskind fermions in lattice QCD. These actions greatly reduce the effects of the nonzero lattice spacing on physical results. We are now ready to use these results, combined with a well-understood improved action for the gluon fields, in a large-scale simulation of QCD, including three flavors of dynamical quarks, as in the real world. Finer lattices will be used to study the hadron spectrum, form factors and decay constants of heavy-light mesons, and masses of hybrid mesons.

COMPUTATIONAL APPROACH

We use the standard "refreshed molecular dynamics" method to generate sample configurations, or lattices, with a probability proportional to their weight in the imaginary time quantum chromodynamics partition function. Expectation values of quantum mechanical operators can be estimated by averaging the operator over the set of configurations of the gluon fields. The computation of the force, or acceleration of the gluon fields, coming from the dynamical quarks requires the solution of a sparse matrix problem where the matrix is Hermitian and positive definite. We use the conjugate gradient algorithm to get an approximate solution to the sparse matrix problem. For each lattice link included in the quark action, the force on the corresponding gauge field is computed by parallel transporting the source and result of the sparse matrix computation from both ends of the path in the action to the lattice point where the force is being computed, and taking the outer product of these two vectors.



The vector meson mass in units of r_1 is plotted versus the squared lattice spacing for several combinations of gauge and quark actions. All of the points have been interpolated in quark mass to the point where the pion mass is 0.78 r_1.

ACCOMPLISHMENTS

We have developed code to simulate with fairly general fat gauge field link actions, and used this code to investigate flavor symmetry breaking in a number of different quark actions. We find that these fat link actions all reduce the flavor symmetry breaking, with the higher amounts of fattening giving greater reductions. These actions are now ready for use in full-scale simulations, generating lattices which can be used to study many aspects of QCD, including the effects of dynamical quarks on the hadron spectrum and on hadronic matrix elements.

SIGNIFICANCE

Our knowledge of the Standard Model is incomplete because it has been difficult to extract many of the most interesting predictions of QCD, those that require non-perturbative calculations. Due to steady improvements in algorithms and computational techniques, and rapid increases in the computing resources, these calculations are now having an important impact on high energy and nuclear physics.

PUBLICATIONS

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http://www.physics.arizona.edu/~doug/flavor_breaking

Numerical Simulation of Turbulent Reacting Flows

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RESEARCH OBJECTIVES

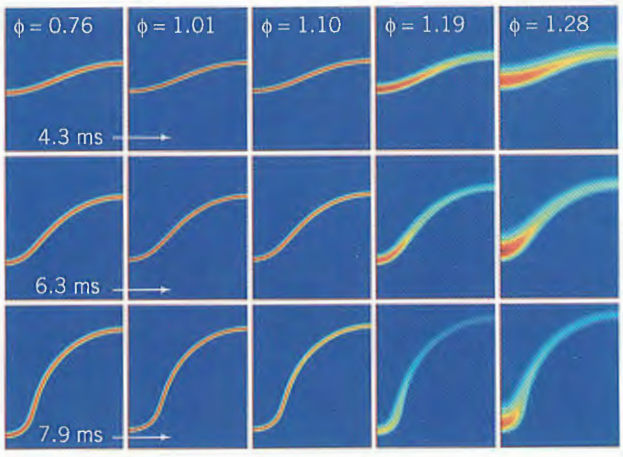
Our objective is to develop and validate high-fidelity numerical models that can accurately represent both the chemical and fluid-mechanical behavior of combusting hydrocarbons in a turbulent environment.

COMPUTATIONAL APPROACH

The principal computational tool for this project is the low Mach number adaptive mesh refinement algorithm developed by the CCSE at NERSC. This methodology provides an accurate and efficient approach for modeling reacting flows in the regime that is appropriate for engineering applications. The algorithm uses a fractional step discretization that easily facilitates the inclusion of complex kinetics mechanisms. The methodology uses a block-structured refinement approach that allows computational effort to be focused in regimes of the flow where it is required. The structured refinement approach provides a natural coarse-grained parallelism that has demonstrated excellent performance and scalability on distributed memory architectures.

ACCOMPLISHMENTS

During FY99, we have made substantial improvements to our methodology in two areas. In the algorithmic area, we have completed the parallelization of both the compressible and low Mach number versions of our adaptive methodology for distributed memory architectures. Computations using this methodology show that the data distribution and load balancing mechanisms we have developed provide an efficient scalable implementation of our adaptive algorithms in a framework that isolates the parallel implementation from the core physics modules for a particular application.



Mole fraction of CH in a premixed methane flame. The flame, initially flat, is perturbed by a counter-rotating vortex pair in the reactant stream. (The gas flows upward here, and only the left half of the symmetric vortex/flame interaction is shown.) The vortex pair modifies the gas composition ahead of the flame, and in fuel-rich cases, significantly alters the diffusion and chemical pathways that lead to CH formation. The computed results are in good agreement with experimental observation.

We have also generalized the low Mach number combustion methodology to allow for arbitrarily complex chemical kinetics and transport packages using an interface to CHEMKIN. The new methodology supports complex reaction mechanisms and differential diffusion in a low Mach number formulation that conserves both species and enthalpy while maintaining second-order accuracy of the overall discretization.

SIGNIFICANCE

The modeling of turbulent fluid flow in realistic engineering geometries, even in the non-reacting case, remains one of the great scientific challenges. For realistic combustion scenarios, the picture becomes more complex because small-scale turbulent fluctuations modify the physical processes such as kinetics and multiphase behavior. These processes, in turn, couple the small scales back to the larger fluid-dynamical scales as chemical constituents react. As a result of this coupling, we must capture the structure of the subgrid fluctuations to make predictions. The use of average quantities as inputs to physical processes will generate large errors through interaction of these models. Developing techniques that accurately reflect the role of small-scale fluctuations on the overall macroscopic dynamics would represent a major scientific breakthrough.

The range of length scales involved in practical engineering devices precludes the possibility of a direct numerical simulation in which all the relevant length scales are resolved. Consequently, any attempt to model realistic devices such as engines and furnaces requires some type of turbulent combustion model that represents the subgrid interplay between turbulence and kinetics. The goal of this project is to develop these types of models.

PUBLICATIONS

C. A. Rendleman, V. E. Beckner, M. Lijewski, W. Y. Crutchfield, and J. B. Bell, "Parallelization of structured, hierarchical adaptive mesh refinement algorithms," Computing and Visualization in Science (in press); LBNL-43154 (1999).

M. S. Day and J. B. Bell, "Numerical simulation of laminar reacting flows with complex chemistry," Combust. Theory Modelling (submitted); LBNL-44682 (1999).

J. B. Bell, N. J. Brown, M. S. Day, M. Frenklach, J. F. Grcar, and S. R. Tonse, "The effect of stoichiometry on vortex flame interactions," 28th Symp. (International) on Combustion (submitted); LBNL-44730 (1999).

http://www.seesar.lbl.gov/ccse/

Linear Algebra Algorithms on High Performance Computers

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Mark Adams, David Blackston, and Tzu-Yi Chen, University of California, Berkeley
Xiaoye Li and Osni Marques, NERSC, Lawrence Berkeley National Laboratory

RESEARCH OBJECTIVES

We have several goals:

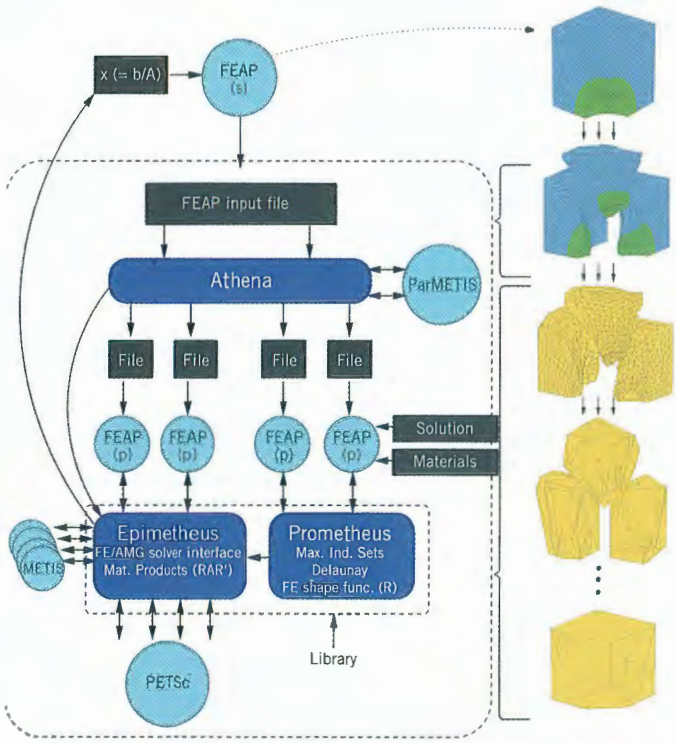
1. Produce a scalable sparse direct linear system solver.
2. Produce a scalable sparse incomplete factorization preconditioner.
3. Produce a scalable multigrid solver for partial differential equations (PDEs) on irregular meshes.
4. Produce a scalable symmetric eigensolver and singular value decomposition (SVD) for dense matrices.
5. Produce a scalable N-body code based on the fast multipole method (FMM) and the Barnes-Hut algorithm.

COMPUTATIONAL APPROACH

All codes are written with performance and portability across distributed memory architectures in mind. Some codes are also portable to shared memory systems and clusters of SMPs. MPI, C, C++ and occasionally some Fortran are the programming tools. The codes use state-of-the-art algorithms, many of which we designed.

ACCOMPLISHMENTS

1. The prototype sparse direct linear system solver is being used for computational chemistry research. An early version of the code is about to be released.
2. The sparse incomplete factorization preconditioner will be used as an iterative solver for linear systems too large for direct solvers.
3. The multigrid PDE code, which has been released in beta form, is designed for very large linear systems arising in finite element modeling in solid mechanics. Earlier versions of this system, developed by Mark Adams, have won two prizes for algorithms and scalability. The code will be integrated into a large earthquake modeling code.
4. An earlier version of the eigensolver/SVD code already in ScaLAPACK has been incorporated into a quantum chemistry code called MP-Quest at Sandia National Laboratories, and was runner-up for the Gordon Bell Prize at SC98. An early version of the code is about to be released.
5. The N-body code has been incorporated into a full-scale simulation of an electron-beam lithography device for semiconductor manufacturing and has been made available to an astrophysics data analysis project.



System architecture for Prometheus, a multigrid solver for finite element matrices on unstructured meshes in solid mechanics.

SIGNIFICANCE

All five projects will produce useful tools for high performance computing widely relevant to DOE research projects, with early versions already in use. In all cases, the code will be publicly available.

PUBLICATIONS

http://www.cs.berkeley.edu/~{demmel,xiaoye,madams,davidb}

Carbon-Climate Interactions

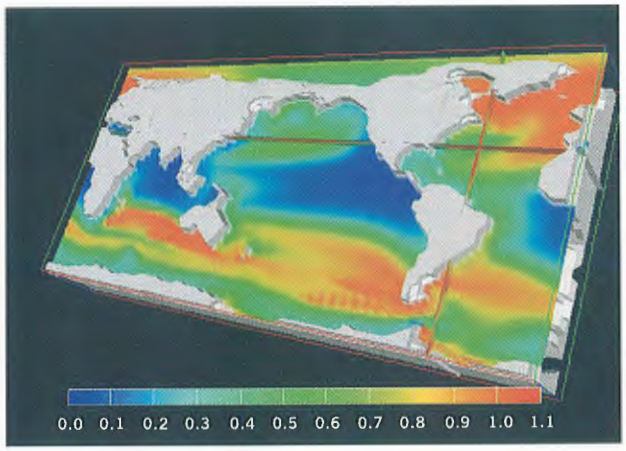
Inez Fung, University of California, Berkeley

RESEARCH OBJECTIVES

Paleo and historical records have shown that the concentrations of CO_2 and other trace species have co-varied with climate fluctuations on interannual to glacial-interglacial time scales. This research focuses on the mutual interaction between the carbon cycle and climate. It investigates how the terrestrial and oceanic carbon reservoirs may sequester or outgas CO_2 as climate changes, and hence determine the CO_2 abundance in the atmosphere. It explores how the rates of atmospheric CO_2 increase and climate change co-evolve and feed back on one another.

COMPUTATIONAL APPROACH

The global three-dimensional Climate System Model (CSM) of the National Center for Atmospheric Research (NCAR) is the principal tool. Fully interactive atmospheric, terrestrial, and oceanic carbon modules are implemented in the physical climate model. Three experimental themes are envisioned. The first focuses on the interannual variations of CO_2 since the 1980s, and attempts to simulate and explain the CO_2 growth rate variations observed. The second explores how climate change may alter terrestrial and oceanic carbon sinks, and the implications of these changes for achieving a target CO_2 level in 2050. The third prescribes a fossil fuel emission scenario, and lets the prognostic and fully interactive carbon and climate system co-evolve. Key to the analysis within each theme will be the sensitivity experiments that capture our confidence in and ignorance about carbon processing and how it may interact with climate.



The three-dimensional distribution of a hypothetical inert surface tracer through time demonstrates the pathways this tracer uses to go from the surface into the deeper ocean. The model was run for 50 years; this frame shows the values of the passive tracer at the 11th vertical level.

ACCOMPLISHMENTS

In the past year, we ran the atmospheric and oceanic modules of CSM, and because of our interest in the dispersal of CO_2 in the atmosphere and the ocean, we focused our analysis on the distribution of hypothetical inert surface tracers in the models. The three-dimensional distribution of the tracers through time clearly demonstrates the different circulation regimes between the Atlantic and Pacific oceans. The penetration of the tracer in the North Atlantic and the transport by the North Atlantic deep water is evident in the movie made with model output by the NERSC Visualization Group using AVS software. The results contribute to our understanding of how anthropogenic CO_2 may have penetrated the oceans, and to our evaluation of the ocean's capacity to store CO_2. We also used the NERSC Visualization facility to display the dispersal of anthropogenic CO_2 in the atmosphere. The results are crucial to the inversion calculations needed to infer the locations and magnitudes of the terrestrial and oceanic carbon sinks.

SIGNIFICANCE

This work will provide scientific input to national and international policy decisions about the feasibility of and strategy for managing the CO_2 level in the atmosphere. It complements the DOE's new focus on carbon sequestration.

PUBLICATIONS

J. T. Randerson, C. B. Field, I. Fung, and P. Tans, "Increases in early season ecosystem uptake explain changes in the seasonal cycle of atmospheric CO_2 at high northern latitudes," Geophys. Res. Lett. (in press).

J. T. Randerson, M. V. Thompson, T. J. Conway, I. Fung, and C. B. Field, "The contribution of terrestrial sources and sinks to trends in the seasonal cycle of atmospheric carbon dioxide," Global Biogeochemical Cycles **11**, 535 (1997).

I. Fung, C. B. Field, J. A. Berry, M. V. Thompson, J. T. Randerson, C. M. Malmstrom, P. M. Vitousek, G. J. Collatz, P. J. Sellers, D. A. Randall, A. S. Denning, F. Badeck, and J. John, "Carbon-13 exchanges between the atmosphere and biosphere," Global Biogeochemical Cycles **11**, 507 (1997).

http://www.atmos.berkeley.edu/ifgroup/

A Numerical Study of Acceleration-Driven Fluid Interface Instabilities

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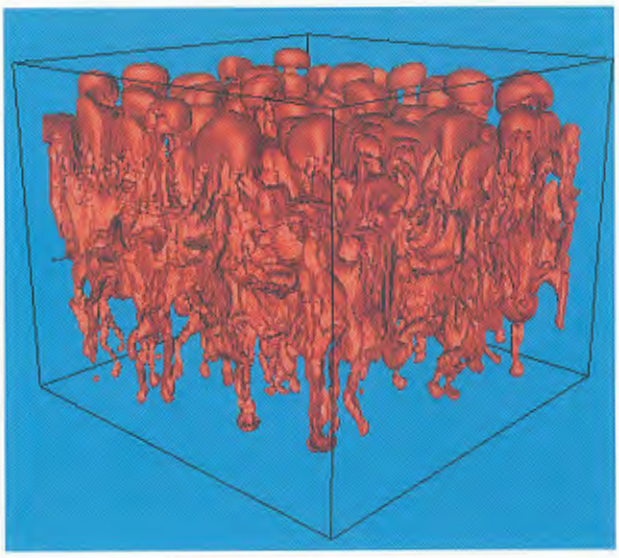
J. Grove and D. Sharp, Los Alamos National Laboratory

RESEARCH OBJECTIVES

We will conduct definitive simulations of acceleration-driven fluid mixing, including the steady acceleration driven Rayleigh-Taylor instability and the shock driven Richtmyer-Meshkov instability.

A Rayleigh-Taylor unstable mixing layer results from steady acceleration applied to a randomly perturbed initial interface separating fluids of distinct densities, with the light fluid pushing the heavy fluid. The reported experimental value for the effective acceleration rate, α, ranges from 0.04 to 0.077. Most simulation studies give lower values for α, ranging from 0.015 to 0.03. Our simulation of this problem has achieved an acceleration rate α between 0.075 and 0.08, which is probably somewhat high, but is consistent with reported experimental values. In view of this success, we propose to explore the dependence of α on numerical parameters such as mesh refinement, enlargement of the statistical ensemble, longer running time and compressibility, to obtain a definitive value of α. We also propose to determine the specific numerical issues responsible for the spread of the reported simulation values of α.

The shock-driven Richtmyer-Meshkov instability develops more slowly, and for this reason, the solution is more strongly dependent on initial parameters which are poorly understood. Our simulation study will explore these physical parameters.



The interface between heavy and light fluids is displayed in a late time simulation of the acceleration driven Rayleigh-Taylor instability. The simulation has undergone more than one generation of bubble merger.

COMPUTATIONAL APPROACH

We used the front tracking method to study RT and RM instabilities. Front tracking features high resolution of physical quantities at the material interface, thus giving a more accurate solution to the physical problem. Both grid-based and grid-free tracking methods are used at different stages of the simulation. We have implemented the front tracking method in a software package known as the FronTier. This code is written in C and is portable to various parallel computational platforms including the Cray T3E. FronTier has recently been extended to 3D and is ready for production usage.

ACCOMPLISHMENTS

A primary accomplishment was a simulation of the RT random surface instability in 3D which is consistent with experimental values for the growth rate of the bubble interface. We also extended FronTier to handle simulations in cylindrical (r, θ) geometry, which will enable 2D spherical simulations in the future. We are currently simulating a variety of random surface and single mode RM instability problems, to determine the dependence of the solution on the problem parameters. We are simulating the instability and breakup of a jet in 3D. Earlier studies showed control of mesh orientation for 2D implosion and agreement with Nova laser data for strong shock RM instability.

SIGNIFICANCE

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

PUBLICATIONS

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

Quantum Monte Carlo Simulations of Strongly Correlated Electron Systems in Reduced Dimensions

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Janez Bonca, Institut Jozef Stefan, Slovenia

RESEARCH OBJECTIVES

Our objective is to apply novel numerical methods to determine the properties of strongly interacting electron systems in reduced (mainly two) dimensions. A prototypical problem that we are considering is to identify a possible microscopic model for high temperature superconductivity.

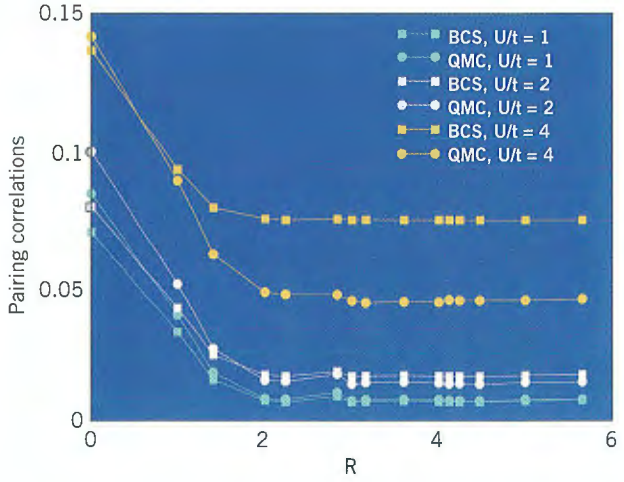
COMPUTATIONAL APPROACH

We developed the constrained path Monte Carlo (CPMC) method as a way to eliminate the "sign problem" that plagues many Monte Carlo simulations of fermion systems. In the CPMC method, the overlap of the wave function is constrained by a trial function, which prevents the probability associated with the Monte Carlo sampling from becoming negative. However, even with an approximate trial function, CPMC results for the two-dimensional Hubbard model compare quite well with exact diagonalization results, with much less computer time required than with other fermion quantum Monte Carlo (QMC) methods. Another advantage of CPMC over other methods is that it allows us to study larger system sizes, which is important for eliminating finite size effects that could bias the computed results.

ACCOMPLISHMENTS

We made several important improvements to our original version of CPMC. One was extending the method to use generalized Hartree-Fock wave functions as the initial, guiding, and constraining states. This allowed us to illustrate the remarkable lack of bias these states impose on the final solution. Another extension was to systems of electrons in strong magnetic fields. Here, instead of a sign problem, the simulations are faced with a phase problem, as Monte Carlo sampling from complex-valued distribution functions is required.

Our continued use of CPMC is focused on expanding the range of models and physical systems studied with it. We are in the midst of extensive simulations of the two-dimensional periodic Anderson Model, finding what we believe is an electron doping range where the ground state is one of partially saturated ferromagnetic. This range differs from that predicted by such commonly used approximators as dynamical mean field theory and the slave boson method. We just completed a series of simulations of the attractive Hubbard model, which is a system with no sign problem. Having now an exact method, we compared the results of the simulations with the predictions of the BCS approximation to determine empirically its range of fidelity. One result is illustrated in the accompanying figure.



The QMC and BCS on-site *s*-wave pairing correlation function as a function of the distance R between pairs for an 8 × 8, quarter-filled, attractive Hubbard model at U/t = 1, 2, and 4. U/t parameterizes the interaction strength.

SIGNIFICANCE

Reduced-dimensional systems typically exhibit a richness of novel phases which are accompanied by unusual magnetic and electrical properties. These phases and their properties present challenges to our understanding, but also present important opportunities for improving energy transmission and storage, optical switches and displays, computer memories and chips, etc. The identification of experimental probes that signal the appearance of such novel effects is an important goal of this project.

PUBLICATIONS

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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 **59**, 1706 (1999).

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bifrost.lanl.gov/~jeg/jeg.html

Global Optimization Approaches to Protein Fold Refinement and Tertiary Structure Prediction

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Betty Eskow, Richard Byrd, and Robert Schnabel,
University of Colorado, Boulder

RESEARCH OBJECTIVES

We have developed a joint global optimization approach to protein fold prediction based on sampling, perturbation, smoothing, and biasing, which has been successful working directly on the potential energy surfaces of small homopolymers, homopeptides, and α-helical proteins. We currently have DOE funding to extend the *ab initio* approach to β-sheet and mixed α/β proteins as well.

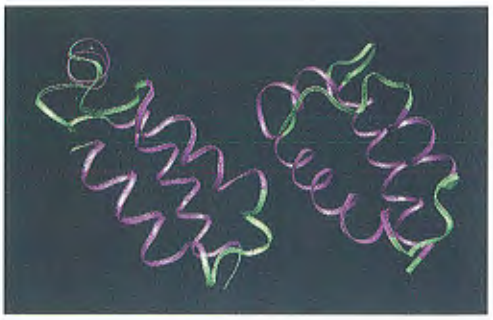
COMPUTATIONAL APPROACH

As the starting point, secondary structure is predicted by a neural network algorithm. Our approach then consists of two phases. The first phase starts with a completely extended conformer, with no secondary or tertiary structure, and performs local minimizations using the constrained energy function first and then the unconstrained potential energy function. The second phase starts with the outcome of the previous phase as the first member of a list of local minimizers. From the set of dihedral angles predicted to be coil, the algorithm randomly selects a subset, then performs a small-scale global optimization using the selected dihedral angles as variables while keeping the rest temporarily fixed at their current values. This optimization produces a number of local minimizers to the unbiased energy function on the subspace of dihedral angles chosen. A number of those conformations with low energy values are considered for further refinement, which is done by performing local minimizations (using the unconstrained energy function) on the full variable space. The new minimizers are merged into the current list, the lowest energy conformation is selected from this list, and the second phase repeats for a number of iterations.

ACCOMPLISHMENTS

We have included with the AMBER energy function a potential of mean force between hydrophobic carbons like that learned from our experimental and simulation studies of amino acid monomers in water. Using our global optimization approach with this new energy function, starting with the crystal structure of four α-helical proteins, we generated no new conformation that was lower in energy than the crystal/NMR structure.

We tested the stochastic/perturbation with soft constraints algorithm on the prediction of the α-chain of uteroglobin and a DNA binding protein (referred to as $2utg_{\alpha}$ and 1pou, respectively).



A comparison between the NMR structure of a four helix bundle DNA binding protein, 1pou (right), and the outcome from our global optimization algorithm (left). Purple indicates helical regions, while green indicates residues that are coil.

Both proteins were ~70 amino acids long and contained ~1200 atomic centers. We also have preliminary results on another 70-amino-acid protein, 3icb, and a 143-amino-acid protein, 3cln.

SIGNIFICANCE

During the next decade, the experimental acquisition of structural data for proteins will be driven by the need to define a "basis set" of fold topologies that will allow for generalization to the fold and function of all protein sequences from any genome. This experimental underpinning will allow the computational effort in structural genomics to establish a robust framework for reliably predicting the three dimensional architecture of proteins in order to gain insight into their function, and to integrate this functional annotation into systems level understanding.

PUBLICATIONS

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A. Azmi et al., "Predicting protein tertiary structure using a global optimization algorithm with smoothing," in *Proc. International Conference on Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches* (in press).

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http://polygon.lbl.gov/~thg
http://www.lbl.gov/~thg/ssi_cbi.html

Electron-Atom and Electron-Molecule Collision Processes

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Lawrence Berkeley National Laboratory
T. N. Rescigno, Lawrence Livermore National Laboratory
M. Baertschy and D. A. Byrum, University of California, Davis

RESEARCH OBJECTIVES

This project seeks to develop theoretical and computational methods for treating electron collision processes that are currently beyond the grasp of first-principles methods. We are developing methods for studying electron-atom and electron-molecule collisions at energies above that required to ionize the target, for calculating detailed electron-impact ionization probabilities for simple atoms and molecules, and for treating low-energy electron collisions with polyatomic molecules, complex molecular clusters, and molecules bound to surfaces and interfaces.

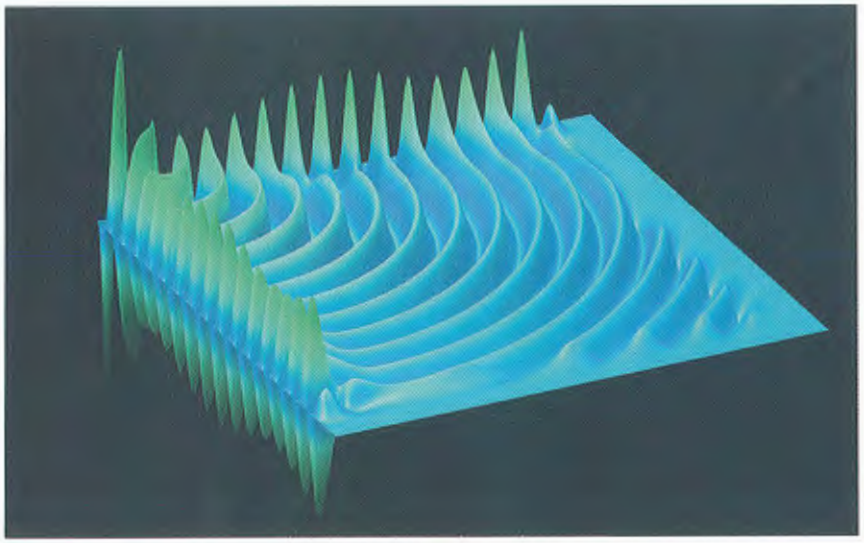
COMPUTATIONAL APPROACH

Our approach builds on the algebraic variational formalisms we have been developing to study electron-atom and electron-molecule scattering. These approaches have now been extended to include complex optical potential interactions, a scattered-wave/flux operator formalism, and a variety of techniques based on analyticity. These techniques allow us to treat a broad range of problems, from low-energy electron-molecule collisions using elaborate variational wave functions to direct solutions of the Schrödinger equation for simple atomic targets that provide detailed ionization cross sections. Our work uses the mathematics of complex analysis in numerical computations, and complex coordinates were the key to solving the electron-impact ionization problem completely for the first time.

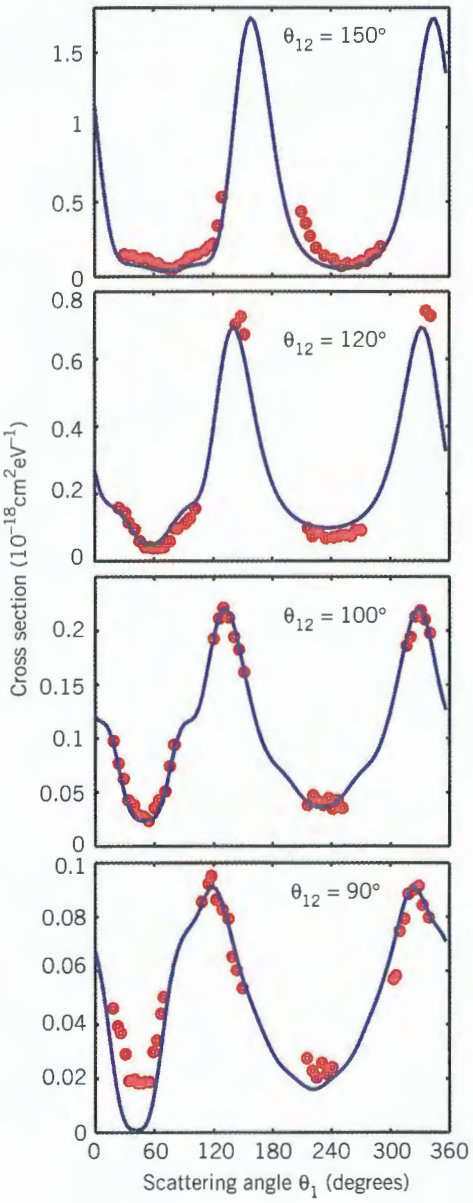
ACCOMPLISHMENTS

We have published major theoretical studies of low-energy electron scattering by CCl_4 and BCl_3—gases that are both used in the plasma etching of silicon and for which little experimental data exits. We have also completed the first *ab initio* study of low-energy electron scattering that has been able to produce results that are in quantitative agreement with measured cross sections. We successfully developed a code that allows for parallel computation of the most computationally intensive part of electron-molecule scattering calculations—the collision integrals needed to describe electron-exchange effects at low energies.

We demonstrated the first complete, first-principles numerical treatment of the electron-impact ionization problem. Our computational approach allows us to extract ionization cross sections (total and differential) directly from a scattering wave function that is constructed without explicit imposition of asymptotic ionization boundary conditions. We have obtained the first results of a complete treatment of the full three-body Coulomb problem with no approximations. Our approach requires the iterative solution of very large (several million by several million) systems of complex linear equations.



One component in an expansion of the wave function describing electron-hydrogen scattering plotted vs. the distances of the two electrons from the nucleus. The large-amplitude oscillations along the edges correspond to one outgoing electron, with the other remaining in a hydrogen bound state. The oscillations in the middle represent two outgoing electrons after ionization of the hydrogen atom.



Comparison between calculated (lines) and measured (dots) cross sections for electron-impact ionization of hydrogen. Each panel corresponds to a particular angular separation between the two outgoing electrons.

SIGNIFICANCE

Electron collision processes play a key role in such diverse areas as fusion plasmas, plasma etching and deposition, and waste remediation. Electron-molecule collisions play a central role in the plasma processing of silicon chips for the manufacture of very large-scale integrated circuits. All the interesting chemistry in these plasmas is electron initiated, and electron impact dissociation of etchant gases produces the reactive fragments that perform the relevant surface chemistry. The understanding and modeling of these low-temperature plasmas is severely hampered by the lack of a database of electron-molecule collision cross sections. This project will significantly add to that base of knowledge.

Our development of the first complete method for treating electron-impact ionization of atoms from first principles solved a fundamental problem in atomic physics that has resisted solution for more than 40 years. Electron impact dissociation, attachment, and ionization phenomena also occur in the condensed phase, notably in mixed radioactive waste. The primary radioactive decay events produce showers of secondary electrons which initiate the chemistry that produces a mixture very different from the one that was present originally. The tools we are developing will make it possible to understand and model this kind of electron-initiated chemistry.

PUBLICATIONS

T. N. Rescigno, M. Baertschy, W. A. Isaacs, and C. W. McCurdy, "Complete break-up of a colliding quantum system of three charged particles," Science 286, 2474 (1999).

T. N. Rescigno, D. A. Byrum, W. A. Isaacs, and C. W. McCurdy, "Theoretical studies of low-energy electron-CO2 scattering I: Total, elastic, and differential cross sections," Phys. Rev. A 60, 2186 (1999).

W. A. Isaacs, C. W. McCurdy, and T. N. Rescigno, "Low energy electron scattering from BCl3," Phys. Rev. A 58, 2881 (1998).

http://www.lbl.gov/Publications/LDRD/1998/CSD/index.html#McCurdy
http://www.nersc.gov/news/sciencecover12-24-99.html

Regional Scale Climate Variability and Impact Assessment for the Western United States

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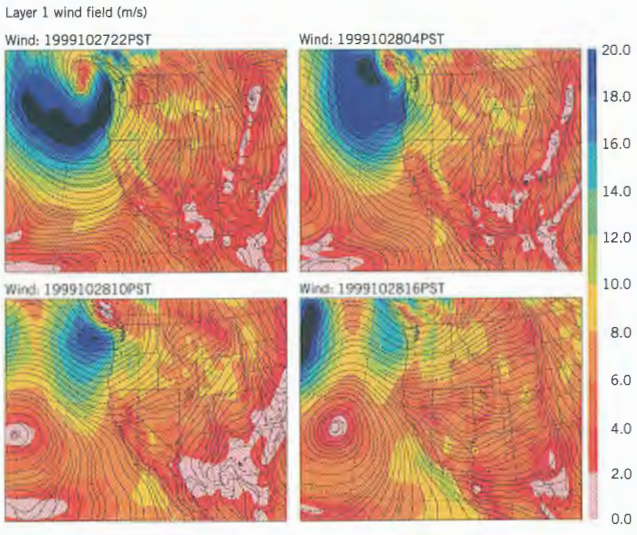
Lawrence Berkeley National Laboratory
Chris Ding and Andreas Mueller, NERSC,
Lawrence Berkeley National Laboratory

RESEARCH OBJECTIVES

The purpose of this project is to generate physically and dynamically consistent information on regional climate variability due to natural and anthropogenic factors and to assess its impacts on various sectors (e.g., water resources, agricultural production, ecosystems, etc.). An instrumental goal is to convert the present serial Regional Climate System Model (RCSM) to a high-performance parallel code.

COMPUTATIONAL APPROACH

The core of RCSM is a mesoscale atmospheric model that solves the stratified, quasi-2D flow equations for 3D advection and physical parameterizations with a third-order finite difference scheme. The parallel RCSM code uses a 2D domain decomposition with message passing for distributed memory architectures.



As part of a three-day weather forecast for the western U.S., RCSM produced this wind speed and direction forecast for six-hour intervals from 10 pm October 27 to 4 pm October 28, 1999.

It takes 15 minutes to simulate one model day on 14 nodes of the Cray T3E, with about the same performance on a Cray T90. Ongoing research includes improving scalability and load balancing as well as cross-platform portability and benchmarking.

ACCOMPLISHMENTS

We have produced a multi-year "hindcast" of the hydroclimate of the western U.S., which we are using to validate and improve our model and to analyze the observational data. The hindcast included a successful simulation of the streamflow in northern California's Russian River basin over a three-month period. The model has also been applied to eastern Asia. In addition, we completed a preliminary study of doubled CO_2 impacts on the western U.S. based on the HadCM2 ensemble projections.

SIGNIFICANCE

Generating information on regional-scale precipitation patterns and other aspects of climate variability requires high-resolution regional climate models. 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 regional climate research. The high performance RCSM will become a tool to generate science-based information to improve climate change impact assessments, as envisioned by the DOE Accelerated Climate Prediction Initiative (ACPI).

PUBLICATIONS

J. Kim, N. Miller, J. Farrara, D. Cayan, and K. Mo, "Winter-season hydroclimate study for the western US using the RCSM," in *Proc. 11th Conf. on Appl. Climatology* (Dallas, Texas, 1999), p. 350.

N. Miller, J. Kim, J. Farrara, K. Mo, and D. Cayan, "Short-term and seasonal streamflow predictions for a California coastal basin during the 97-98 winter," in *Proc. 14th Conf. on Hydrology* (Dallas, Texas, 1999), p. 255.

N. Miller, J. Kim, and R. Hartman, "Downscaled climate and streamflow study of the southwestern United States," J. Amer. Water Res. Assoc. (submitted).

http://ccs.lbl.gov/RCSM

Sparse Linear Algebra Algorithms and Applications for MPPs

Horst Simon, Chris Ding, Parry Husbands, Osni Marques, and Kesheng John Wu, NERSC, Lawrence Berkeley National Laboratory
Alan Edelman, Massachusetts Institute of Technology
Hongyuan Zha, Pennsylvania State University
Zhenyue Zhang, Zhejiang University, Hangzhou, China

RESEARCH OBJECTIVES

The goal of this research is to use high performance computing to help understand and improve subspace-based techniques for information retrieval, such as latent semantic indexing (LSI). In the past, LSI has been used only on very small data sets. We are developing an environment and scalable linear algebra algorithms with which LSI-based information retrieval can be applied to matrices representing millions of documents and hundreds of thousands of key words.

To improve the accuracy and efficiency of the retrieval algorithms, we hope to: (1) Further develop our subspace-based model and gain deeper understanding of the effectiveness of LSI. (2) Develop more robust and computationally efficient statistical tests for the determination of the optimal latent-concept subspace dimensions. (3) Further explore the low-rank-plus-shift structures of the term-document matrices and develop fast and memory-efficient numerical algorithms for the computation of low-rank matrix approximations. We will also investigate linear-time partial singular value decomposition (SVD) algorithms based on term and document sampling. (4) Investigate a variety of statistical methods such as canonical correlation analysis and a generalized linear model for translingual text retrieval.

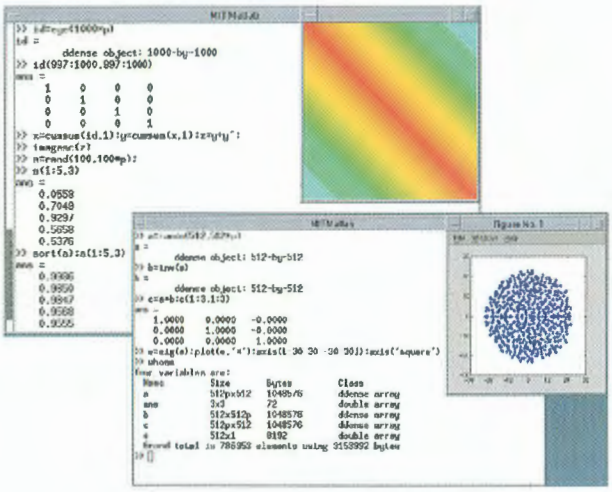
COMPUTATIONAL APPROACH

We currently plan to explore the use of SVD. In the future, other low-rank approximations to the document structure will be considered. For large-scale linear algebra operations we make extensive use of the ScaLAPACK, LAPACK, PARPACK, TRLAN, PETSc, and Aztec libraries.

ACCOMPLISHMENTS

We successfully ported the parallel computing extension MATLAB*P to NERSC's Cray T3E. This tool provides the ability to manipulate dense and sparse matrices stored on the T3E using the popular MATLAB environment. The goal is to reduce the programming overhead in setting up our numerical experiments.

Preliminary experiments on a large collection with over 500,000 documents have demonstrated the feasibility of our software. We have been able to perform LSI on the complete collection, whereas previous attempts have had to restrict their attention to a smaller subset of the data.



MATLAB*P provides a familiar, transparent interface for bridging the gap between workstations and supercomputers. It allows manipulation of dense and sparse matrices on MPP systems with little or no modification of scripts written for workstations.

SIGNIFICANCE

This project is one of the first to compute decompositions of complete, large, term-document matrices. The algorithms developed here will be useful not only in text retrieval, but also in more complicated settings such extraction of images with desired features from large collections. Combining effective search and classification algorithms for image problems with the computing and storage capabilities of future NERSC systems will position Berkeley Lab in a leadership position when it comes to the development of algorithmic techniques for the data and visualization corridors of the next decade.

PUBLICATIONS

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

Zhenyue Zhang, Hongyuan Zha, and Horst Simon, "Low-rank approximations with sparse factors I: Basic algorithms and error analysis; II: Penalized methods with discrete newton-like iterations," SIAM Journal of Matrix Analysis (submitted); LBNL-44003 and LBNL-44217 (1999).

Chris H. Q. Ding, "A similarity-based probability model for latent semantic indexing," presented at the 22nd International ACM SIGIR Conference on Research and Development in Information Retrieval, Berkeley, CA, December 1999; LBNL-43202 (1999).

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

APPENDIX A

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Mathematical, Information, and Computational Sciences Division

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As the flagship facility of the ASCR program, NERSC thanks the program managers with direct responsibility over the NERSC Division:

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Daniel Hitchcock
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Applied Mathematics

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Mary Anne Scott
Distributed Computing and Grid Technologies

Linda Twenty
OASCR Program Analyst

Projects in the NERSC Division also received support from the Office of Biological and Environmental Research. We acknowledge the support of David Bader, Climate Modeling, and Daniel Drell, Bioinformatics.

Index of Researchers

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

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in collaboration with NERSC researchers
and staff