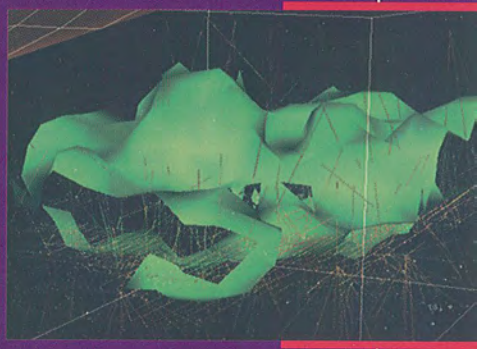
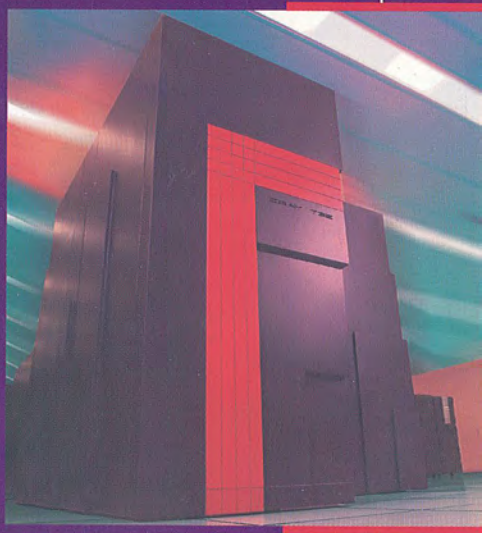
NERSC

NATIONAL ENERGY RESEARCH
SCIENTIFIC COMPUTING CENTER

1997 ANNUAL REPORT





BERKELEY LAB
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's Energy Research (ER) 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 ER 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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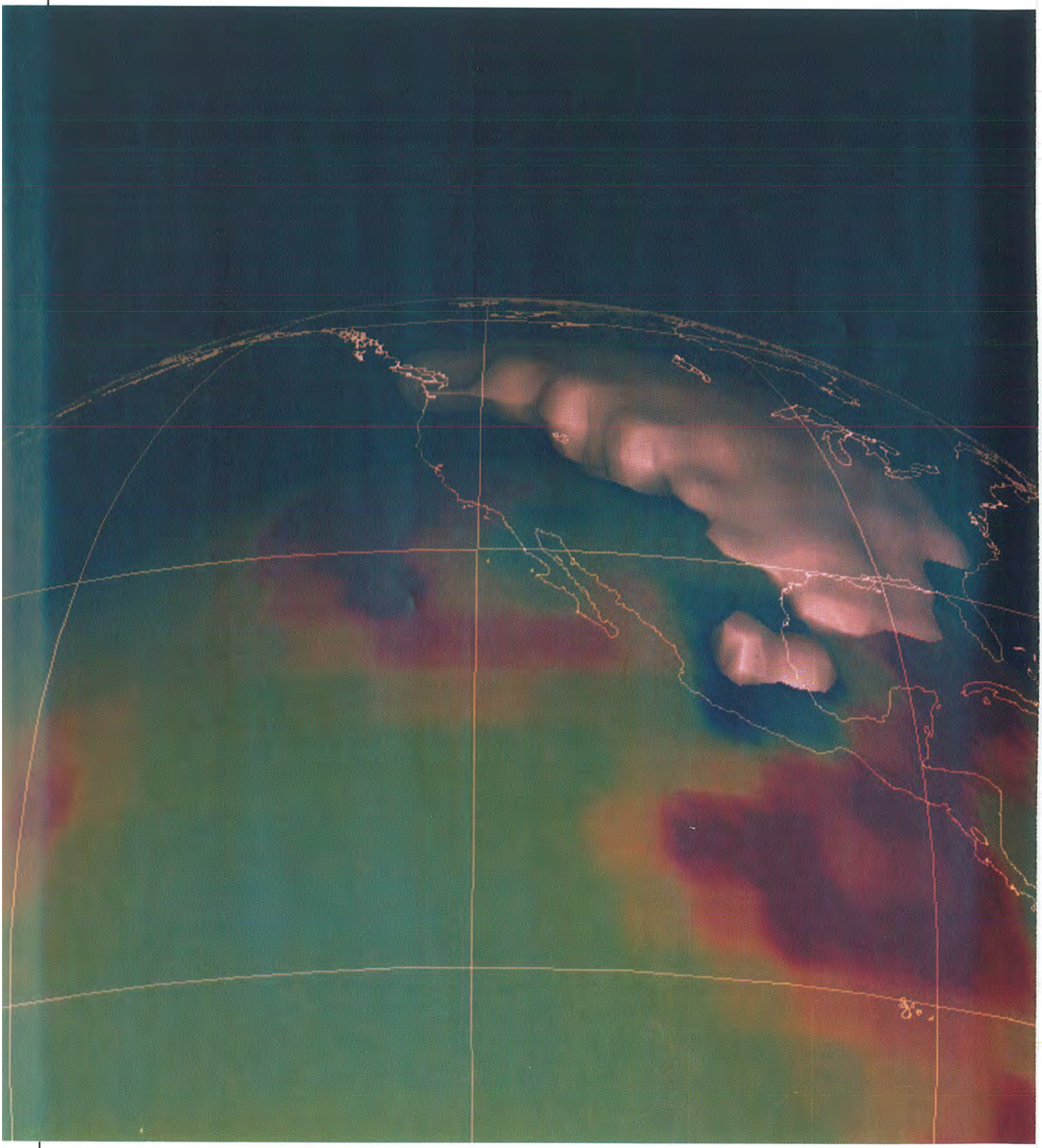
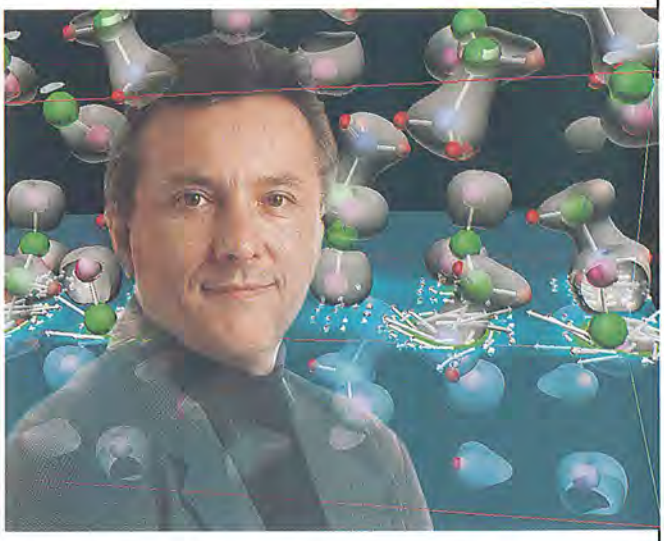
*DOE/ER Grand Challenge project



New images of deep geological structures were revealed when innovative algorithms and NERSC's Cray T3E were used to transform seismic data from around the world into models of the three-dimensional seismic structure of the earth's crust, mantle, and core. See pages 60 and 67 for further discussion. (Donald Vasco and Osni Marques, Lawrence Berkeley National Laboratory)

As we look back over the two years since NERSC relocated to Lawrence Berkeley National Laboratory, we feel a great sense of accomplishment. Some of the early successes are easily forgotten, so it is worthwhile to remind ourselves that together we achieved more than even the biggest supporters of the move envisioned. First, we accomplished the move with no disruption of service. I know of no precedent for a working supercomputer center the size of NERSC relocating, much less maintaining continuity. Second, while maintaining our parallel vector systems, we brought two new massively parallel processing systems into production, vastly increasing our computing capability. The evaluation and acceptance of the Cray T3E-900 was particularly difficult and time-consuming, straining our already stressed resources. These early difficulties were well worth the effort—today NERSC's T3E-900 is the largest unclassified computing resource in the U.S., and with innovations such as checkpoint restarting, we have demonstrated that a highly parallel machine can perform at high production standards. Third, we began implementing our new vision of what a high-performance computing center can be, providing computational science as well as computer science expertise to our clients, and conducting computational and computer science research to accelerate the pace of scientific discovery.

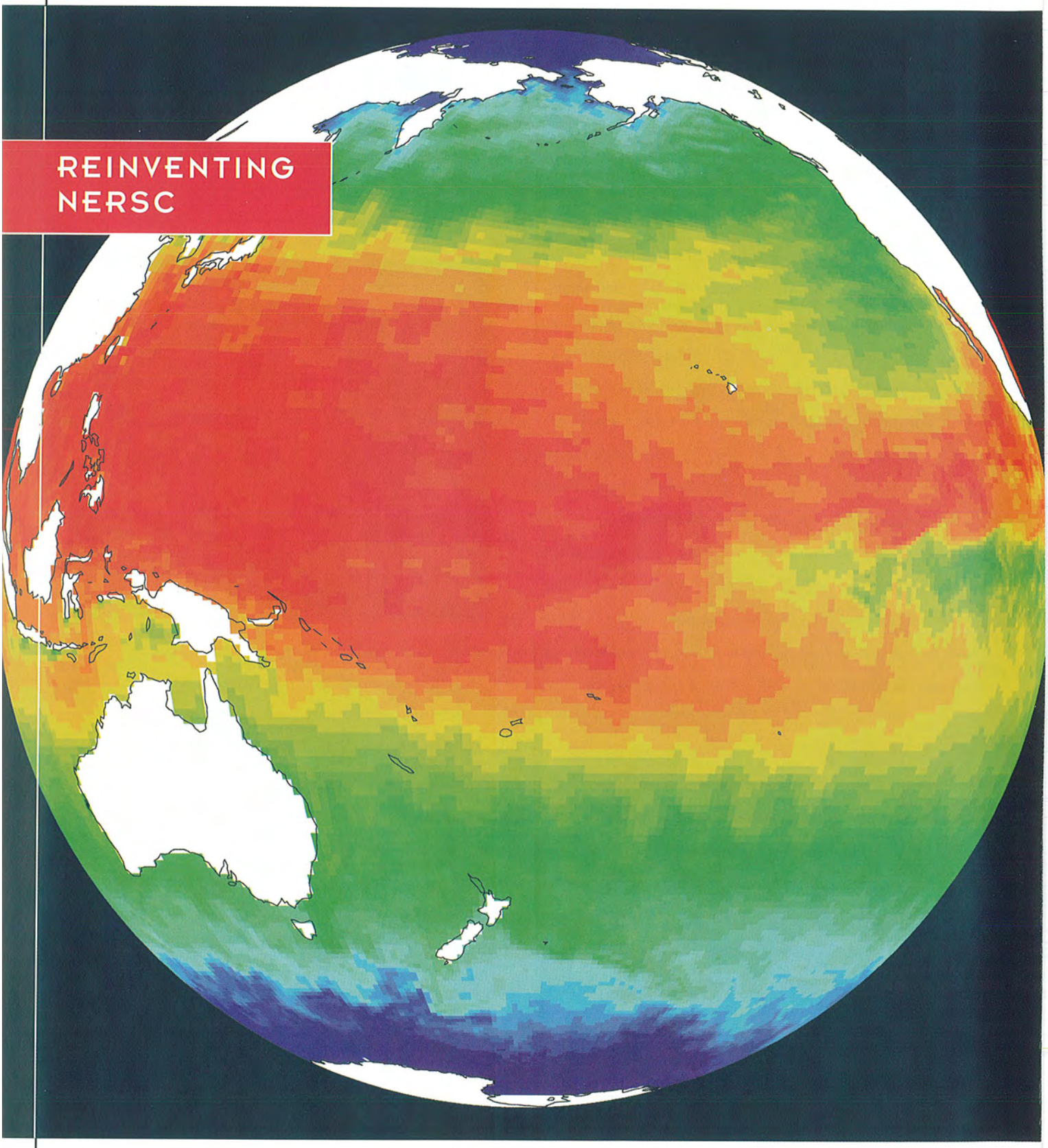


Many elements contributed to NERSC's early success, but it would not have been possible without the highly competent and dedicated effort of the NERSC staff. This transition has not been easy, but we have maintained our high level of client service and achieved significant scientific results, as summarized in this report. I am grateful to our DOE Office of Energy Research sponsors for their endorsement of our ambitious plans; to our clients, in particular ERSUG and EXERSUG, for their continued support in difficult times, for their willingness to embrace new technologies, and for their patience during occasional glitches; and to everyone at Berkeley Lab who worked hard to make NERSC welcome at its new home. My special thanks and congratulations, however, go to the NERSC staff for their skill, dedication, and tireless efforts to make NERSC the best scientific computing resource in the world.

But this is just the beginning. In an environment where technology changes every 18 months, NERSC cannot afford to stand still. We are beginning the crucial decision-making process for our next major system procurement, evaluating rapidly changing technologies and industry trends as well as architecture, hardware, and software issues. We are discussing new computational science initiatives that will enhance our contributions to the Energy Research scientific mission. We have ongoing efforts to strengthen our organization and to ensure the proper balance and integration of production and research. And we continue to build our computational and computer science expertise. These are more difficult tasks than we faced during the startup phase. Success will come more slowly and less visibly. We must continue working together in the spirit of our startup phase to assure NERSC's continuing success. I am counting on the continued support of our clients and stakeholders, as well as the dedication of the NERSC staff, to bring us closer to our vision of NERSC as a worldwide leader in high-performance computing.

Horst D. Simon

REINVENTING NERSC



The power of parallel computing is making it possible to begin combining high-resolution atmosphere, ocean, and sea ice models, with the goal of predicting the effect of greenhouse gases on the earth's climate. Representative climate research is described on pages 29, 32, 55, 59, and 68. (Robert M. Chervin, National Center for Atmospheric Research)

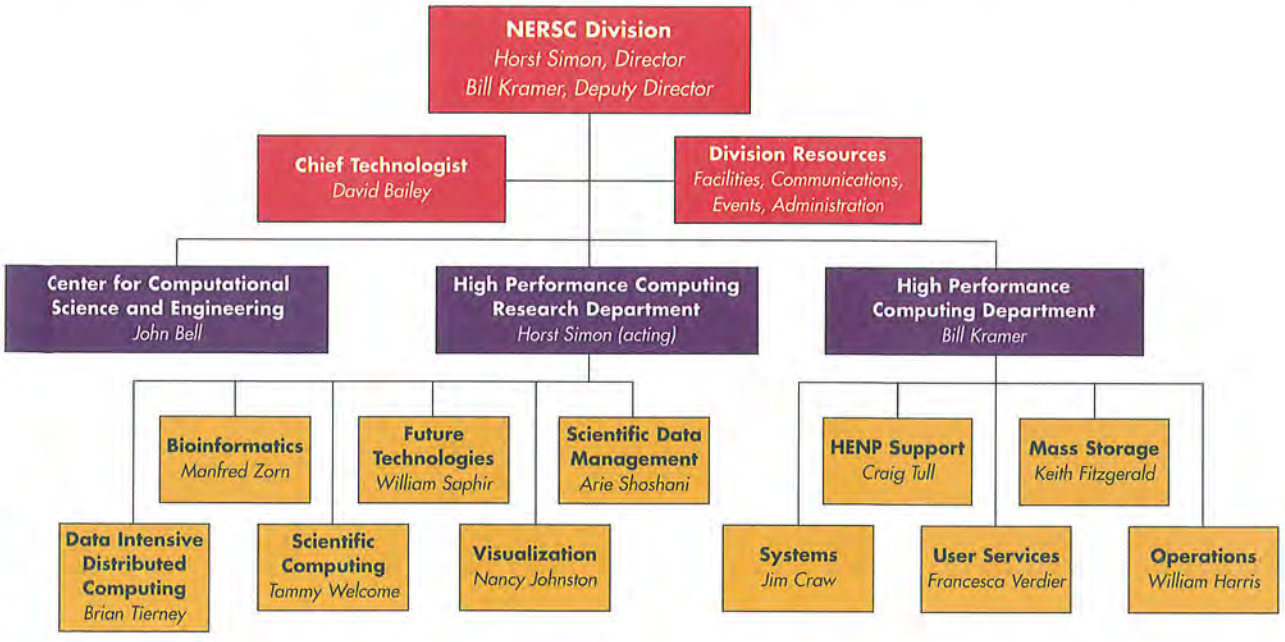
Founded nearly 25 years ago, the National Energy Research Scientific Computing Center was the first unclassified supercomputer center and was the model for those that followed. Our relocation from Livermore to Berkeley Lab in 1996 set the stage for reinventing NERSC to meet the computational science needs of the next century.

The new NERSC provides clients with not only state-of-the-art high-performance computers, but also an extensive range of services aimed at accelerating the pace of scientific discovery. The name change that accompanied the move—from "Supercomputer Center" to "Scientific Computing Center"—signaled a new philosophy, one of making scientific computing more productive, not just providing supercomputer cycles.

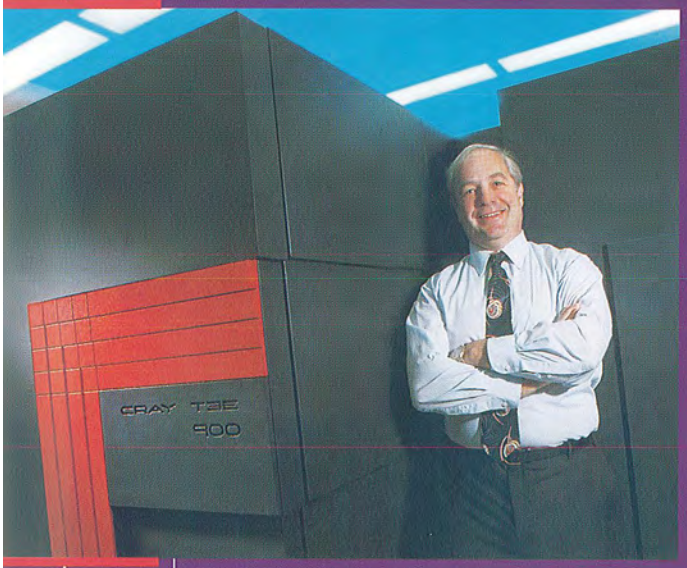
We have reinvented NERSC around that new philosophy. Our high-performance computing systems and excellent client services—the NERSC Program—are now complemented by expanded expertise in computational and computing science—the NERSC Division in Berkeley Lab's Computing Sciences organization. (This report describes both Program and Division activities.) Our goal is to give our clients both the computing and the intellectual resources necessary to conduct breakthrough computational research.

Our physical relocation set the tone for the changes to come. Through careful planning and extraordinarily hard work by the entire staff, the move was completed ahead of schedule and under budget—and with no interruption of services to our clients. During our first full year at Berkeley Lab, we welcomed more than 40 new employees from some of the top computing science organizations in the country to strengthen our scientific computing services. We further expanded our research capabilities by integrating several Berkeley Lab computational and computing science research groups into the NERSC Division. As a result, the Division has roughly the same number of staff engaged in research as we have providing day-to-day services, such as supporting our computing and storage systems.

By doing more with less, we have broadened our services without increasing our Program budget. For example, even though we are operating more machines than before,



CHECKPOINTING BRINGS RELIABILITY TO MASSIVELY PARALLEL PROCESSING



"As far as I know, no other MPP system is planning to do system-wide checkpoint/restart without having to reprogram applications," said Bill Kramer, Deputy Director of NERSC. "This is really a momentous step for those of us in the high-performance computing community."

In August 1997, NERSC achieved a milestone in high-performance computing: successfully stopping and restarting a number of scientific computing jobs on a Cray T3E supercomputer without any data processing loss or discontinuity. This accomplishment opened a new era of robust, reliable, production-mode MPP computing.

Called "checkpointing," the stop/restart procedure—achieved twice in one week—is believed to be the first time such a procedure has been accomplished on an MPP system. Checkpointing involves bringing all of the programs running on the computer to the same stage and stopping them, then recording all the information, transferring that information out of the machine, then, after the system is used for something else, putting the data back in and getting all the programs running again—on a machine capable of carrying out tens of billions of operations per second.

Successful checkpointing will allow the NERSC staff to use the T3E-900's 512 processors more efficiently by moving jobs between the processors and making larger pools of processors available quickly for bigger jobs. It will also allow NERSC to make the entire 512-processor computer available to tackle a single, complex problem when necessary, as well as carry out upgrades and maintenance without disrupting the work of researchers.

The checkpointing procedure was successfully demonstrated on both of NERSC's T3Es, the 512-processor T3E-900 and the 96-processor T3E-600. The restarted jobs were running on clusters ranging from 16 to 256 processors. After the machines were put back on line, James Craw, head of the NERSC Systems Group, commented, "It's kind of ironic that we achieved this major milestone and none of our users noticed—which was our objective."

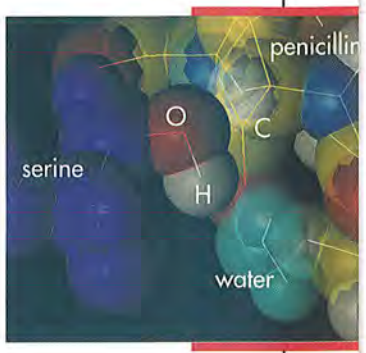
the technical staff dedicated to our core services is 20 percent smaller than it was three years ago.

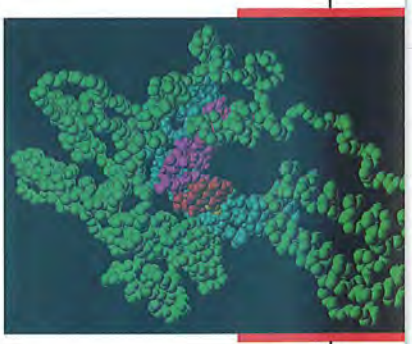
In the midst of all these changes, we reached a milestone that finally brought massively parallel processing (MPP) into full production mode—the checkpointing and restart of our Cray T3Es. Checkpointing has been a major goal in the MPP community for the 10 years since the first parallel machine was plugged in, and this is believed to be the first successful checkpointing of an MPP system (see opposite page).

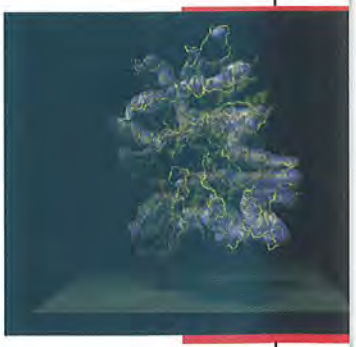
Our position as the nation's largest computing resource for unclassified research was confirmed by the November 1997 release of the TOP500 list of the world's most powerful computers (http://www.netlib.org/benchmark/top500.html). Our T3E-900 was listed as No. 5 in the world, and in this country is the No. 1 unclassified system.

We were also gratified to receive a favorable evaluation from an independent group of peers. The Lab Director's Review Committee, which met in May, assigned a rating of Outstanding/Excellent to Computing Sciences activities at Berkeley Lab. In their report, the committee wrote, "It is a remarkable achievement to continue to adhere to past high standards while integrating a major new activity and holding the new activity to the same high standards."

These achievements and many other highlights of the year are described in more detail in the following pages. Scientific accomplishments are presented in the "Science Highlights" section.







"Reinventing the Supercomputer Center at NERSC," an article by NERSC Director Horst Simon, was featured in the July-September 1997 issue of *IEEE Computational Science and Engineering*. You can find the article on the Web at http://www.nersc.gov/aboutnersc/reinventing.html. Another article by Horst, "The Recent Revolution in High Performance Computing," appeared in the Materials Research Society's *MRS Bulletin* in October. See http://www.nersc.gov/aboutnersc/revolution.html.

COMPUTING RESOURCES

The November 1997 TOP500 list of the most powerful computers ranked NERSC's Cray T3E-900 as No. 5 in the world, and in this country it is the No. 1 unclassified system.

Since NERSC moved to Berkeley, two Cray T3E supercomputers, a cluster of four Cray J90se computers, and a high-performance storage system have been added to NERSC's equipment roster, giving the center one of the most powerful lineups of computing resources in the country. As new machines are introduced to the center, systems experts carefully analyze performance and work with manufacturers to ensure that the equipment meets the high-performance needs of NERSC clients.

To provide state-of-the-art capabilities in scalable parallel computing, NERSC received delivery of the 512- processor Cray T3E-900 on July 14. The NERSC T3E-900 features the largest I/O system built to date and is a first-of-its-kind configuration. The fully configured machine offers 1.5 terabytes (TB) of disk storage, a read/write capability of 800 megabytes (MB) per second, and 128 gigabytes (GB) of memory. NERSC also has acquired a T3E-600 to provide a development platform for NERSC clients and to support Berkeley Lab's computing needs. The successful checkpointing/restart of the T3Es is described above.

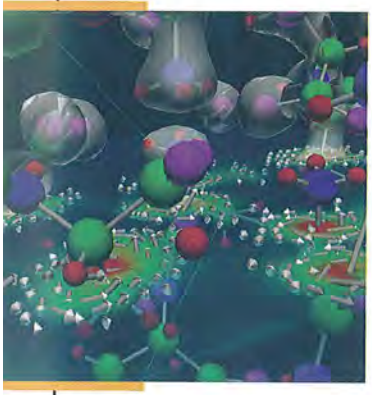
There are four systems in NERSC's Cray J90se cluster: Killeen is the interactive machine, while Franklin, Seymour, and Bhaskara perform batch processing. Franklin and Seymour now have queues that can accept jobs up to 1.6 GB, while Bhaskara has a queue limit of 4 GB, which represents half the physical memory on the machine. These expanded queues allow the J90 cluster to accept larger

In order to store and retrieve data gathered and used by researchers, NERSC operates two high-performance data storage systems. Together, these systems can hold 50,000 tapes, each storing from one to 20 gigabytes of compressed data. Not only have Wayne Hurlbert and Nancy Meyer helped keep NERSC's storage systems running at top efficiency, but they've also tracked down system design problems which could affect all users of such systems.

Members of NERSC's Operations and Systems groups ensure that the center's supercomputing facilities are up and running at optimum availability, reliability, and efficiency. Clayton Bagwell of the Operations Group and Jackie Scoggins of Systems are part of the team that has helped NERSC consistently provide clients with ever-improving service.

batch jobs. In a configuration that NERSC calls "SuperHome," the cluster machines mount Killeen's home directories via NFS so that user executables and files are available to each machine.

Requirements-based batch scheduling on the T3Es and J90s is managed by the Network Queuing Environment (NQE). With its intelligent scheduler, NQE automatically assigns the required processing resources to each computing task while balancing the workload among the processors. Clients specify their requirements (memory, number of processors, disk space, and processor time) for each batch job. The NQE scheduler examines each request and determines when and where the job is run, based on system load information from NQE execution servers.



To keep pace with improvements in processing capacity and capability, we also upgraded our storage systems and bandwidth. We installed uninterruptible power and increased the UniTree disk cache ninefold from 94 GB to 846 GB. We expanded the archival storage bandwidth from 27 MB/s to a potential 252 MB/s and expanded capacity from 33.6 TB to 106 TB (uncompressed). We added a second storage control processor and disks to store UniTree/HPSS databases. Finally, we acquired six IBM processors to use as mover machines for HPSS and to upgrade the local-area network within the machine room, increasing the bandwidth.

HPSS (High Performance Storage System) is the next-generation storage technology selected by NERSC after completing a market survey of storage systems and evaluating the options. The primary objective of HPSS is to move very large data objects between high performance computers, workstation clusters, and storage libraries at speeds many times faster than is possible with today's software systems. We set up an HPSS test environment in late 1997, and over the next year we will convert the UniTree and CFS environments to HPSS.

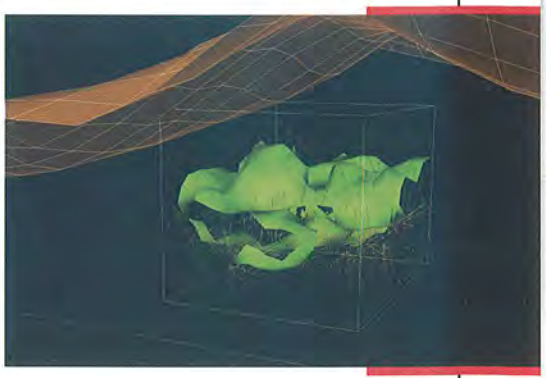
A new remote visualization server—an SGI Onyx 2—has also been installed to enable remote clients to create high-quality visualizations of data. The Onyx is integrated with the computing systems to provide a consistent environment for maintaining visualization software across NERSC systems.

Nationwide and international high-speed access to NERSC is provided by the Energy Sciences Network (ESnet), which is operated around the clock by the NERSC Operations staff.

The PDSF (Particle Detector Simulation Facility), a networked, distributed, production computing environment, supports the detector simulation, software development, and data analysis needs of large-scale high-energy physics and nuclear science investigations. The PDSF has brought a new client community to NERSC, with research teams from six experiments currently using the facility.

As part of NERSC's Advanced Systems Development program, we are collaborating with Sun Microsystems in the testing, evaluation, and development of a prototype single-system-image cluster of four symmetric multiprocessor systems. The cluster is designed to permit the systems, which have a total of 32 processors, to be deployed, managed, and viewed as a single operating system.

Implementing all of these new systems presented many challenges. For example, during the long and rigorous testing of the Cray T3E, NERSC and SGI/Cray representatives worked closely together to identify and resolve problems and make improvements. The end result was that NERSC clients had to wait a little longer, but were rewarded with a truly scalable production MPP machine. The solutions generated by the NERSC-Cray collaboration benefited other centers with T3Es as well.



COMPUTATIONAL AND COMPUTER SCIENCE RESEARCH

A shock wave exploding through the interface of two fluids provides a dramatic picture of the mathematical complexity of turbulence. (William Crutchfield and Jeffrey Greenough, Lawrence Berkeley National Laboratory)

The extent of NERSC's involvement in computer science research and the development of computational technologies sets us apart from most supercomputer centers. Our strategy for staying at the forefront of high-performance computing is to participate in the development of new technologies so that our clients will be among the first to reap the benefits.

This year we expanded our research groups and welcomed several groups from Berkeley Lab into the NERSC Division. The directions of their research are described below. Further information about staff research can be accessed from the NERSC "Research" Web page (http://www.nersc.gov/research).

CENTER FOR COMPUTATIONAL SCIENCES AND ENGINEERING

CCSE develops and applies advanced computational methodologies to solve large-scale scientific and engineering problems arising in the DOE mission areas involving energy, the environment, and industrial technology. CCSE's application-driven mathematical and numerical research enhances DOE scientists' ability to effectively use NERSC's computing resources as scientific and engineering tools.

CCSE's research is focused on high-resolution finite difference methods and adaptive mesh refinement. The primary areas of application are in fluid dynamics, such as turbulence and atmospheric models. Simulations of turbulence in combusting gases are a crucial part of current efforts to design more efficient and less polluting diesel and gasoline engines. CCSE is also investigating computational models for several types of atmospheric flow: stable boundary layers over land, mesoscale flows over complex terrain, and marine boundary layer clouds such as stratocumulus and trade cumulus.

CCSE's research involves significant software development, including BoxLib, a parallel library that will allow many higher-level codes to run efficiently in parallel without substantial code changes at the user interface level.

SCIENTIFIC COMPUTING GROUP

The Scientific Computing Group facilitates development of scientific applications that run on NERSC capability platforms, promotes optimal use of NERSC computing resources, and develops new computational approaches to scientific problems. The group's responsibilities include collaborating with strategic users to port and develop scientific applications, as well as evaluating, integrating, and creating new software tools and algorithms.

The group works on diverse scientific applications in the fields of computational fluid dynamics, computational

NERSC's Center for Computational Science and Engineering, headed by John Bell, develops algorithms and computational models aimed at gaining a better understanding of turbulence, one of the most common — yet least understood — problems occurring in such processes as combustion and fluid transport.

SCIENTIFIC COMPUTING GROUP WORKS TO BOOST RESEARCHERS' PRODUCTIVITY

Scientific Computing Group members (from left) Sherry Li, Andrew Canning, and Tammy Welcome work with NERSC users on scientific applications in such fields as physics, chemistry, fluid dynamics, earth sciences, materials science, and mathematics.

Scientific Computing Group staff members work with NERSC clients to make the scientist-supercomputer interface as productive as possible. They also help develop new tools for the benefit of the larger supercomputing community.

For example, group members Xiaoye "Sherry" Li and Osni Marques (not shown) played a key supporting role in the development of a new algorithm library for performing dense linear algebra calculations on distributed memory computers. Besides fine-tuning and testing various parts of the package, they also recorded the fastest performance for running the algorithms among the various supercomputers used. The library of algorithms, called ScaLAPACK for Scaled Linear Algebra Package, was placed in the public domain for researchers in such areas as physics, chemistry, engineering, and materials science.

As NERSC's 512-processor Cray T3E was being put through its specified acceptance tests, a small number of codes from NERSC clients were also being run to test the overall capabilities of the machine. Group member Andrew Canning, working with the Materials Science Grand Challenge team headed by Malcolm Stocks of Oak Ridge National Laboratory, helped produce some of the computer's first scientific results (see page 64)—even before it officially went on line. The code, which simulates 498 atoms and 996 electronic states, is a first-principles quantum calculation, "a state-of-the-art calculation that would push the memory and performance limits of any supercomputer," Canning said. "The T3E, with 512 processors, is one of the few machines capable of handling this type of calculation."

To work with the eight Grand Challenge teams using NERSC, the group rolled out a virtual red carpet to participating researchers around the country. "Our aim was to make NERSC an indispensable partner in solving these problems," said Scientific Computing Group Leader Tammy Welcome. "By assigning group members as points of contact and meeting with each team, we learned about their computational requirements and how they intend to use NERSC. At the same time, we let them know about our capabilities and the level of collaboration we can provide."

physics, computational chemistry, material sciences, structural biology, life sciences, data mining, and data-intensive computing, as well as fundamental problems in scientific computing such as numerical linear algebra (e.g., dense and sparse linear/eigen system solvers), mathematical libraries and templates, and parallel programming environments.

DATA INTENSIVE DISTRIBUTED COMPUTING RESEARCH GROUP

This group is working to push the state of the art in the storage and processing of huge data sets (greater than 1 terabyte). Their projects include:

- DPSS (Distributed Parallel Storage System)—A collection of wide-area distributed disk servers operating in parallel to provide logical block-level access to large data sets. Operated primarily as a network-based cache, the architecture supports cooperation among independently owned resources to provide fast, large-scale, on-demand storage to support data handling, simulation, and computation in a wide-area inter-networked environment.
- NetLogger Toolkit—A methodology and set of tools for network and distributed system performance analysis.
- WHERE agent/broker system (Wide-area Helpers Enabling Reliable Environments)—A heterogeneous system of brokers and agents that manage access to and information about a DPSS and its associated clients.

BIOINFORMATICS GROUP

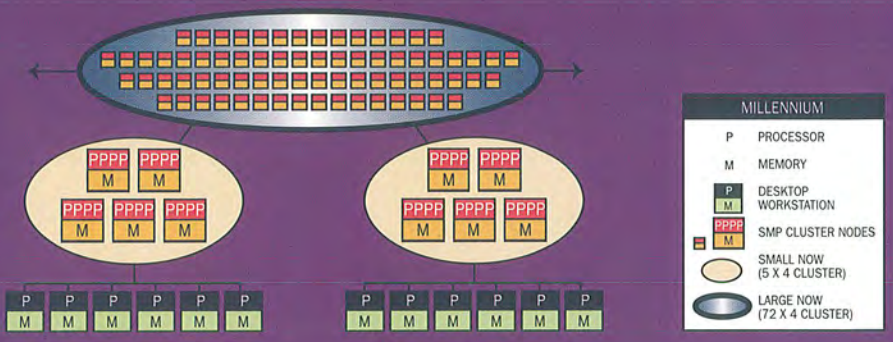
The Bioinformatics Group uses modern software engineering tools and methods for research and development efforts including:

- Supporting wet lab biology (laboratory information management systems, groupware).
- Analysis of biological sequences (sequence analysis, protein structure and function prediction, large-scale genome annotation).
- Access to biological information (database integration, data mining).
- Modeling of gene regulation.

The Bioinformatics Group, under the leadership of Manfred Zorn, carries out a wide range of R&D to further computational science in the field of biology. Their projects include laboratory information management systems, large-scale genome annotation, database integration and data mining, and modeling of gene regulation.

As researchers create ever-larger banks of shared data, enabling access to that information over computer networks becomes increasingly important. Brian Tierney's Data Intensive Distributed Computing Group is developing technologies that allow researchers to get there from here.

NERSC's key interest in the UC Berkeley/Intel Millennium architecture is in researching the high-performance potential of clusters based on SMP nodes rather than single-processor nodes.



FUTURE TECHNOLOGIES GROUP

The Future Technologies Group, which includes three faculty members from the UC Berkeley Computer Science Department, keeps NERSC on the technological leading edge by bringing research products into the NERSC production environment and shaping technology development. Two current research efforts involve shared-memory multiprocessor (SMP) clusters: the UC NOW (Network of Workstations) cluster and the UC/Intel Millennium project.

The Future Technologies Group strives to eliminate some of the guesswork about the immediate future of computing by researching, adapting, and experimenting with today's latest technologies to help develop tomorrow's standards. Bill Saphir leads this effort with help from Patrick Bozeman and Luigi Semenzato.

The group is also involved in developing software needed for scientific research, such as:

- MPI-2 (Message Passing Interface)—A library of routines for fast communication among processes in tightly coupled parallel applications.
- Globus project—A collaboration with Argonne National Laboratory, developing basic software infrastructure for computations that integrate geographically distributed computational and information resources.
- Titanium project—A collaboration with UC Berkeley, developing compiler and language support to optimize parallel programs on distributed memory multiprocessors.
- DOE2000 ACTS Toolkit—Improving the accessibility and usability of experimental parallel scientific software, enabling its introduction into the mainstream of parallel computing.

SCIENTIFIC DATA MANAGEMENT RESEARCH AND DEVELOPMENT GROUP

This group develops tools that enable scientists to manage and analyze massive amounts of data. Large-scale scientific simulations, experiments, and observational projects generate large multidimensional datasets. Typically, the time to access a subset from a large dataset stored on a mass storage system may take many minutes to hours. This slows down the effectiveness of data analysis to the point that much of the data may never be analyzed.

The Scientific Data Management Group is collaborating with Lawrence Livermore National Laboratory and the University of Maryland on the OPTIMASS project to enable rapid analysis of earth science and environmental data such as global warming and ozone layer depletion. By reorganizing the original datasets to match their intended usage and enhancing storage server protocols, the project has improved access time up to 100 fold.

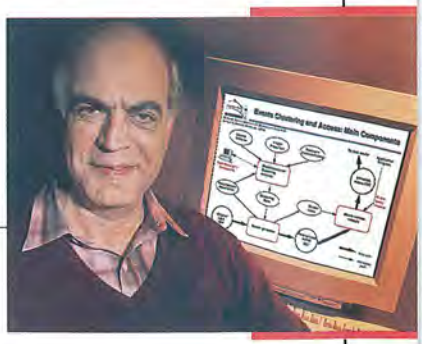
The group is also participating in the DOE Grand Challenge on High Energy and Nuclear Physics Data, which is developing techniques and tools that will enable efficient access to the massive datasets from the Relativistic Heavy Ion Collider (RHIC) STAR experiments (beginning in late 1999) in the search for the quark-gluon plasma. Simulated data generated at NERSC and the RHIC Computing Facility will be used in testing and developing these tools before experiment operations begin. (See page 54 for further discussion.)

VISUALIZATION GROUP

The Visualization Group supports NERSC clients by applying state-of-the-art practices in scientific visualization and computing, ranging from 3-D images and animated movies to virtual reality. They have developed virtual reality interfaces that allow interactive remote viewing and control of computer simulations, and are exploring new methods for visualizing extremely large data sets.

One recent example of their work involves nuclear magnetic resonance (NMR), which materials scientists use to determine chemical structure (see page 53). To better understand the results of NMR experiments, researchers are using NERSC's Cray T3E to simulate the response of crystalline structures to an applied magnetic field. The Visualization Group has developed stereoscopic displays of the results of computations on several different crystals, including two amino acids. The complex three-dimensional structure of the crystals can be very confusing when displayed on a 2-D monitor, but becomes quite obvious when viewed in stereo.

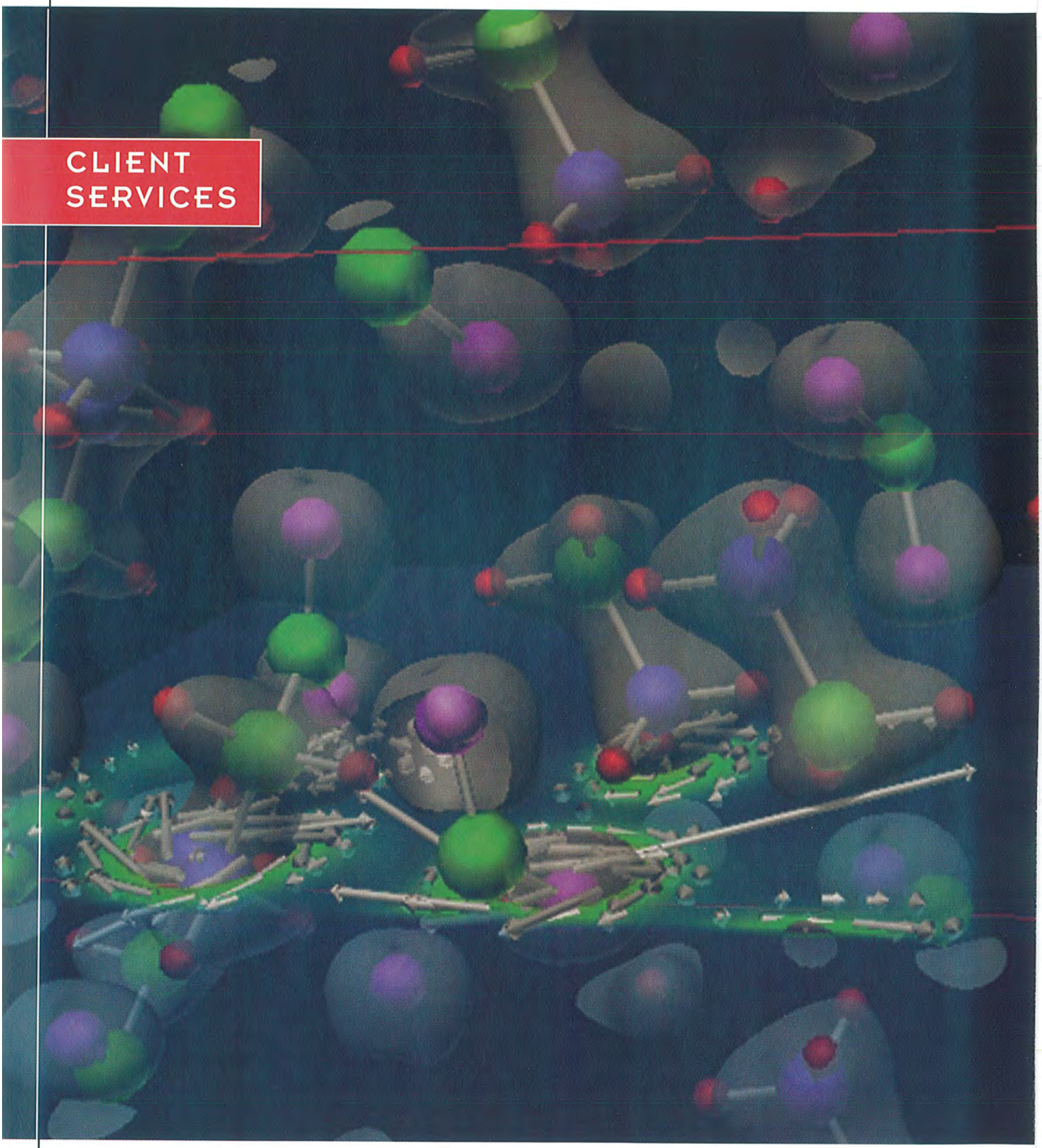
Other recent visualization projects have included DNA modeling, underground mineral and petroleum deposits, fluid dynamics turbulence studies, and quantum chromodynamics simulations.



Members of the Scientific Data Management Group, led by Arie Shoshani, help scientists avoid information overload by developing tools for managing scientific databases. The group addresses the specialized needs of scientific applications while taking advantage of commercially available software.

NERSC's Visualization Group helps scientists understand the results of their experiments and simulations by letting them see and manipulate the results in a three-dimensional virtual reality environment. From left: Kevin Campbell, Stephen Lau (kneeling), Terry Ligocki, Nancy Johnston, and Wes Bethel.

CLIENT SERVICES



To better understand the results of nuclear magnetic resonance (NMR) experiments, researchers are using the Cray T3E to simulate the response of crystalline structures to an applied magnetic field. For more information, see page 53. (Steven G. Louie, Marvin L. Cohen, and Bernd Pfrommer, University of California, Berkeley, and Lawrence Berkeley National Laboratory)

In FY 1997, DOE awarded parallel vector processing allocations on NERSC systems to 425 projects, and massively parallel processing allocations to 131 projects. A total of 1378 scientists (not including NERSC staff) made use of NERSC's computing resources. Our success is ultimately measured by the quality of science produced by these clients. Highlights of that science begin on page 22 of this report.

To help ensure that we are meeting our clients' needs, this year we established a set of ten performance goals pertaining to our systems and service. We developed these goals to set expectations for our own performance, then obtained our clients' endorsement of these goals as meaningful and useful.

We now proactively gauge just how well we are doing in meeting these common expectations. We have tried to ensure that they reflect our efforts from a client's perspective, as opposed to an internal one. For example, a measurement of system availability needs to reflect the number of hours a machine is available to our clients, not how long it takes to identify a problem and initiate corrective action on our end. Our performance goals cover the following areas:

- Reliable and Timely Service
- Innovative Assistance
- Timely and Accurate Information
- New Technologies
- Wise Technology Integration
- Progress Measurement
- High-Performance Computing Center Leadership
- Technology Transfer
- Staff Effectiveness
- Protected Infrastructure

Providing the necessary administrative support to keep NERSC functioning smoothly is a demanding job. Among those who have excelled in this arena are Eric Essman and Norma Early.

To give our clients, our sponsors, and our own staff a better idea of how we are performing, we produced a Client Services Report covering our work from October 1996 through September 1997. A few highlights of that report are summarized below along with other client service topics. We will share results of our self-evaluations with our client community on a regular basis.

RELIABLE AND TIMELY SERVICE

This performance goal addresses two general areas:

- How reliably our systems operate (i.e., availability to clients)
- How responsive we are to clients when they have a problem.

The table "System Availability Details" shows various aspects of our systems' reliability since NERSC moved from Livermore to Berkeley Lab. Figures in bold represent the

SYSTEM AVAILABILITY DETAILS

October 1996 Through September 1997
Measured (Goal)

Systems	Overall Availability	Scheduled Availability	MTBI* (Hours)	MTTR** (Hours)
Vector	**97.7%** (95%)	**99.3%** (96%)	**242** (96)	**5.3** (4.0)
Parallel	**95.2%** (85%)	**98.0%** (90%)	**43** (96)	**2.7** (4.0)
Storage	**98.9%** (95%)	**99.2%** (96%)	**85** (96)	**0.7** (4.0)
File Servers	**99.9%** (96%)	**99.9%** (96%)	**1460** (316)	**1.0** (8.0)
SAS	**99.9%** (97%)	**99.9%** (99%)	**973** (490)	**1.0** (4.0)

*Mean Time Between Interruptions **Mean Time to Restoral

measured time, while goals are shown in parentheses and red type. Scheduled availability refers to the amount of time the systems are expected to be available (accounting for scheduled maintenance and upgrades), while gross availability is based on 24 hours a day, seven days a week. MTTR (mean time to restoral) refers to the amount of time between a system failure and the point at which full service is restored to clients. Measured performance exceeded our aggressive goals in most cases, with the exception of time between interruptions for parallel and storage systems and time to restoral for vector systems. We are working to improve our performance in those areas.

NERSC's service goals are to respond to clients' problems within four working hours and to resolve at least 90 percent of those problems within two working days. Spot checks confirm that NERSC meets the goal of responding to problems within four hours. Between July 1, 1996, and May 15, 1997, 75.3 percent of all problems were resolved within two days. As the NERSC staff got up to speed, however, we made significant progress in meeting the 90 percent goal: between March 11 and May 15, 1997, 93.1 percent of all problems were resolved within two days.

Not all problems can be resolved within two days. Reasons for putting a problem on hold include software requests, ongoing coding projects, bugs waiting for a vendor-supplied fix, and a client not responding to a request for input within two days. Problems not resolved within 72 working hours are automatically escalated for more in-depth review to ensure that outstanding problems are addressed.

NERSC staff periodically review problems and client requests to ascertain areas needing attention with an eye toward fixing them to minimize disruptions in service.

INNOVATIVE ASSISTANCE

NERSC aims to provide its clients with new ideas, new techniques, and new solutions to their scientific computing issues.

For example, when DOE's Office of Energy Research announced that NERSC would be a partner in helping multidisciplinary teams from around the country solve eight of ER's twelve Grand Challenges, our computer scientists rolled out a virtual red carpet to participating researchers.

Through the Red Carpet Program, led by members of NERSC's Scientific Computing Group, NERSC staff are building individual working relationships with clients at other national labs and universities tackling such issues as cleaning up nuclear waste, supporting international research in magnetic fusion energy, designing particle accelerators, and understanding the structure of the smallest building blocks of matter.

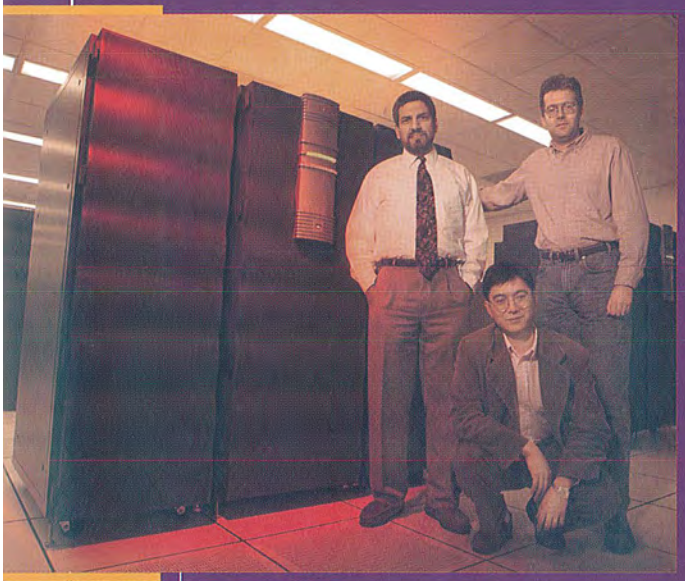
NERSC staff are holding site meetings with each Grand Challenge team to determine what services and support are needed. Services so far include providing training for new clients, integrating separate physics software packages into a cohesive program, developing new algorithms, and offering programming tips.

NERSC has also created a specialized group to support a particular field of science. The High Energy and Nuclear Physics (HENP) Support Group works with physicists around the globe to help develop solutions to the formidable computing challenges faced by the next generation of HENP experiments. The group provides access to and assistance with a combination of production systems such as the PDSF, advanced prototype storage systems such as HPSS and DPSS, and research and development projects such as contributing to the HENP Grand Challenge.

To address forefront scientific issues in high-energy and nuclear physics, complex experiments are being carried out by large collaborations to detect and analyze increasingly large numbers of final-state particles and/or events. The High-Energy and Nuclear Physics Support Group, led by Craig Tull, is helping scientists get the science out of massive amounts of data generated by experiments such as STAR (Solenoidal Tracker at RHIC). The challenge for the coming years is to provide cost-effective, high-performance computing capabilities and unprecedented data access which will allow widely distributed collaborations to process and analyze hundreds of terabytes of data per year.

Some of our client service experiments have worked well, while others sent us back to the drawing board. For example, to reduce travel time and costs, we tried using ISDN-based videoconferencing as a training tool. On our end, there were problems in learning how to present material via video, and clients had difficulty scheduling facilities, especially as we tried to scale up the sessions to reach more sites. As a result, we have decided to rely on Web-based technologies and are developing ways to provide reliable Web-based video. This will allow clients to tap our expertise at their desktop and on their own schedule.

CONSULTANTS SHOW INITIATIVE IN SOLVING PROBLEMS



Although User Services Group members Majdi Baddourah, Peter Tang, and Jonathan Carter spend some of their time answering queries from NERSC clients, they have also taken the initiative to identify and resolve applications issues before they turn into big problems.

As one of the NERSC consultants who routinely handles client inquiries, Majdi Baddourah provides timely help on difficult computing problems. But Majdi, a member of NERSC's User Services Group, decided to go a step further. He took the initiative and began monitoring jobs that were performing slowly on NERSC's C90 and J90 machines. He then called some of the clients and asked if they needed help in optimizing their source codes. Codes were optimized for both I/O and the processors, then returned to the clients for evaluation. This extra effort resulted in codes running up to 10 times faster, benefiting all users of the machines.

In another case, a Grand Challenge research group asked NERSC consultant Peter Tang for help in making a central piece of code run faster. Peter studied their code and went a step beyond optimization by suggesting use of a different algorithm. This algorithm accelerated processing time by a factor of four, and Peter is continuing to look at other algorithms to achieve even greater improvements.

Jonathan Carter of User Services has also developed innovative solutions to various problems. When one group of researchers was having trouble moving their Fortran 90 code to a new compiler, Jonathan went through 20,000 lines of code piece by piece and found bugs in the compiler. He then created a smaller test code, which helped debug the compiler. In another case, Jonathan worked with a researcher using a long-running code to create an automatic checkpoint/restart feature so that the data would be saved every 20 minutes, thereby saving hours or days of work in the event of a system shutdown. In a third case, Jonathan set up an autotasking feature for a fluid dynamics code that used 4 GB of memory, about half the capacity of a J90, but used only 20 percent of the processing power, leaving 80 percent of the processors idle. By distributing the work over more processors, autotasking allows the J90 to be fully utilized.

CLIENT TRAINING

NERSC has presented training sessions to proactively help clients adapt to using the newest computing technologies. Here are some examples:

- While NERSC's new Cray T3E was being installed and put through its acceptance testing, we held a series of six classes to help prepare clients for using this new machine.
- In conjunction with the semi-annual Energy Research Scientific Computing Users Group (ERSUG) meeting at Princeton Plasma Physics Laboratory in January 1997, NERSC provided an overview of parallel computing and four sessions on optimizing code for the T3E.
- The NERSC staff also gave a presentation for researchers using the Cray C90 who began using the J90 cluster. The presentation highlighted the differences between the two machines and helped prepare clients for the transition.

TECHNOLOGY TRANSFER

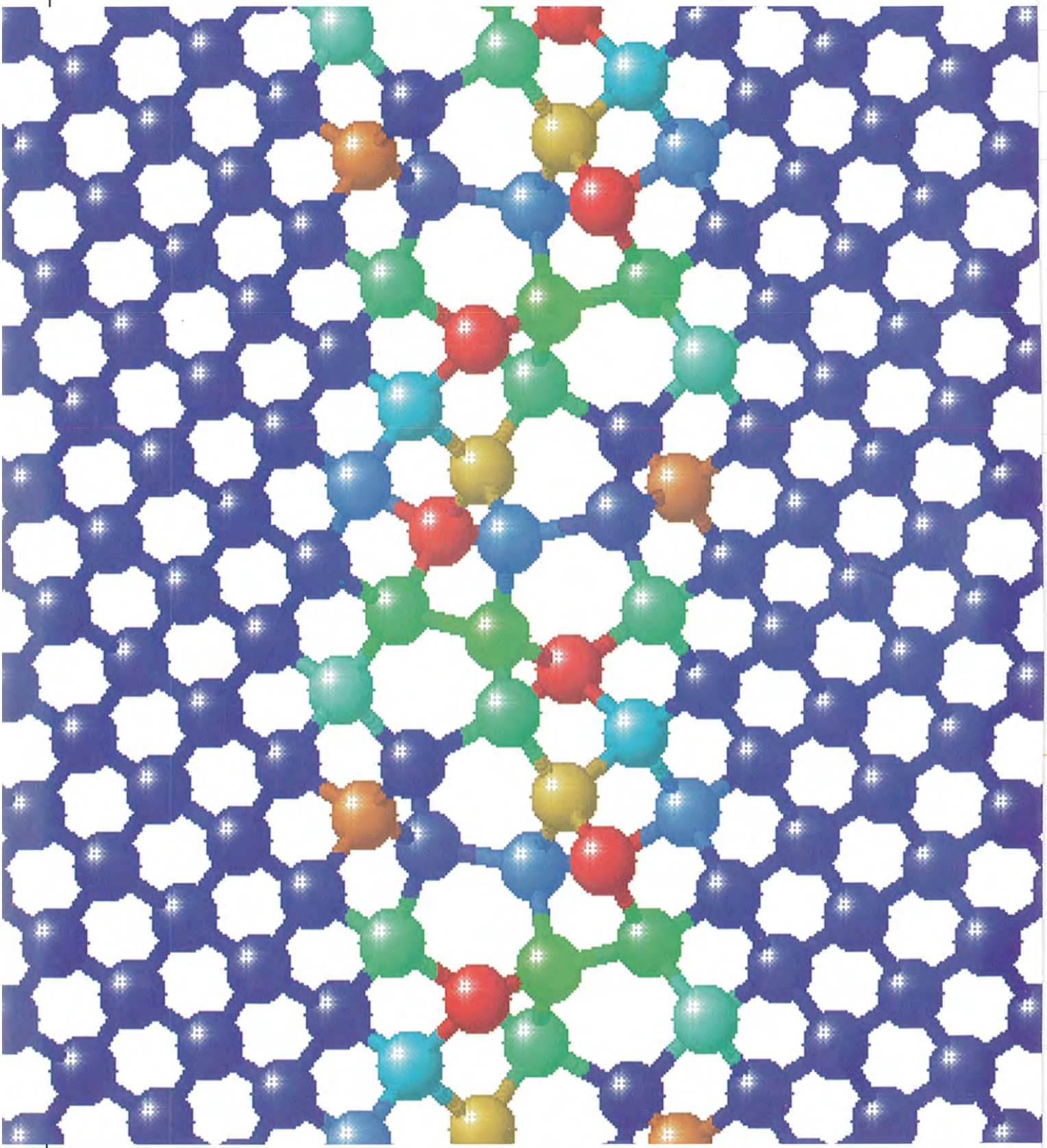
Many organizations look to NERSC to provide expertise in high-performance computing. As one of the world's first computing centers to put a Cray T3E into a demanding production environment, we are regularly contacted by others considering such a move. The U.S. Army Corps of Engineers, the National Computational Science Alliance, Georgia Tech, and computing centers in France and Korea have all tapped our experience as part of their planning process. NERSC routinely hosts visitors from educational and research institutions around the world.

NERSC staff members participate in various organizations that set the pace for new technology development. For example, the head of our Systems Group is a member of Silicon Graphics' customer advisory board; members of our Mass Storage Group serve on the HPSS executive and technical committees; and our Future Technologies Group leader serves on the MPI standards committee.

NERSC staff also share their expertise through software releases, articles in technical journals, tutorials and presentations at professional conferences and workshops, and invited talks at universities, laboratories, and high-tech industries.

ERSUG

The Energy Research Scientific Computing Users Group is composed of user representatives from the NERSC customer laboratories and university sites. This group provides guidance to both NERSC and the Office of Energy Research about current services offered by NERSC and the direction of future development. When appropriate, ERSUG appoints task forces and working groups to address specific issues related to NERSC services. ERSUG meetings for 1997 were held on January 28-29 at NERSC and June 5-6 at Princeton Plasma Physics Laboratory. Recent ERSUG activities include development of a guidance document for NERSC's next major system procurement.



The mechanical and electrical properties of silicon grain boundaries can adversely affect the performance of semiconductors. Simulation of the atomic structures of these extended defects can reduce the need for difficult and costly high-resolution experimental studies. See page 42 for further discussion of interface modeling.
(J. R. Morris, K.-M. Ho, D. M. Ring, Z.-Y. Lu, and B. Harmon, Ames Laboratory; C.-L. Fu, Oak Ridge National Laboratory)

NERSC AND THE FATE OF THE UNIVERSE

If you're trying to determine whether the universe will collapse or continue expanding—and you plan on announcing your findings to the world—it's a good idea to cross-check your work. That's what the Supernova Cosmology Team has done. To analyze their data from 40 supernovae for errors or biases, and to simulate 10,000 exploding supernovae, they used the Cray T3E supercomputer at NERSC.

Their conclusion?

Our universe, which began with the Big Bang, will never come to a standstill or collapse in a Big Crunch, but will expand forever, according to findings announced in January 1998 by Saul Perlmutter, leader of the international Supernova Cosmology Project and a member of the Center for Particle Astrophysics, based at Berkeley Lab.

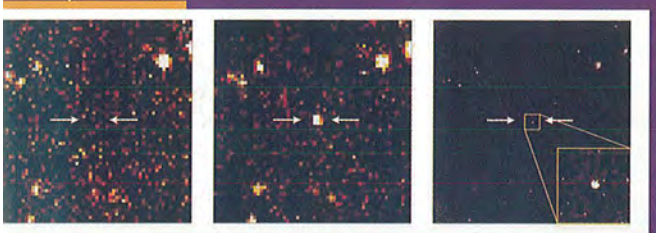
Using several ground-based telescopes, the Hubble Space Telescope, and the NERSC T3E, the Supernova Cosmology Project has determined that the universe was expanding faster seven billion years ago (roughly half the time since the Big Bang) than it is today. Although expansion has slowed, the deceleration is not enough to suggest that gravity can bring outwardly rushing galaxies and other celestial matter to a halt.

"On the basis of both the ground-based data and the new Hubble data, we find evidence for a universe which may ultimately expand indefinitely," Perlmutter said.

Berkeley Lab astrophysicist Saul Perlmutter, with supernova 1987a in the background. (Supernova image: ©Anglo-Australian Observatory, David Malin, photographer)

The evidence comes from observing Type Ia supernovae in very distant galaxies. To look at a distant object in space is to look into the distant past. To measure that distance, astronomers use "standard candles," objects whose intrinsic brightness is the same wherever they are found. Type Ia supernovae at their maximum brightness can be brighter than entire galaxies, bright enough for their light to have traveled billions of light-years and still be visible.

To double-check their work, the supernova team had to compare the light from nearby supernovae with that of the distant ones. The light measurements from the more distant supernovae (which have been shifted to the red part of the spectrum due to the expansion of the universe) and the closer ones (which are in the blue) were altered slightly to



The first two images, from an Earth-based telescope, show a small region of sky just before and just after the appearance of a Type Ia supernova that exploded when the universe was about half its present age. The third image shows the same supernova as observed by the Hubble Space Telescope. Because their intrinsic brightness is predictable, such supernovae help to determine the deceleration, and so the eventual fate, of the universe. (Perlmutter et al., The Supernova Cosmology Project)

examine the effects of dust along the line of sight to the supernovae as well as slightly different explosion scenarios. The measurements were then compared to make sure the team's observations matched their theoretical calculations. Because the measurements involved readings from 40 supernovae taken many times over a 60-day period, making the comparisons "is a task you only want to send to a supercomputer," said Lab postdoctoral fellow Peter Nugent.

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

"This work takes about an hour using 128 processors on the T3E," Nugent said. "It's wonderful to be able to run six or seven of these in just one day and then compare the results."

The group also used the T3E to simulate the explosions of 10,000 supernovae at varying distances, given a universe with a particular cosmology, in an effort to study their observation techniques. The cosmological values from the fits to the simulations were then plotted and compared with their known input to determine any biases which could have influenced the interpretation of the original data.

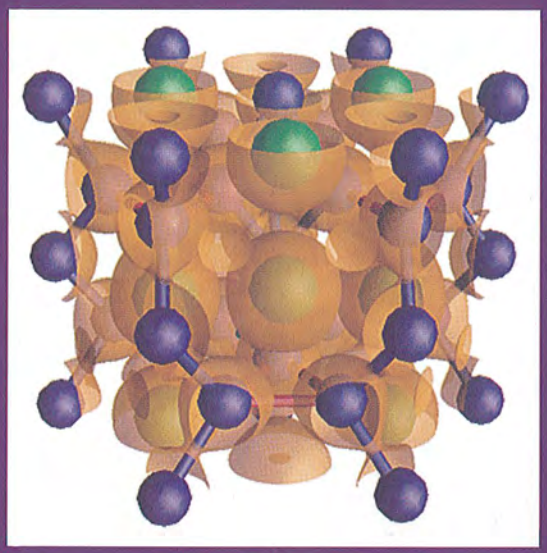
Finally, Nugent is tapping NERSC for help in preparing a paper in which he and researchers from the University of Oklahoma compare spectra from nearby and distant supernovae. They are studying whether or not the environments in which the supernovae occur influence how they explode. One theory holds that supernovae which exploded several billion years ago in metal-poor environments may look quite different from those which are used as calibrators, which occur relatively nearby in more metal-rich environments.

So far, the results show not much difference between earlier and more recent events, Nugent said. The conclusion is that these supernovae are good standard candles for comparative measurements. See http://panisse.lbl.gov/public/ for more information.

RESEARCHERS ELIMINATE ONE THEORY IN THE MYSTERY OF THE MISSING XENON

Scientists looking into the "mystery of the missing xenon" have found strong evidence against one leading theory and, along the way, discovered new information about the behavior of the element. The findings were published in the August 15, 1997 issue of Science magazine.

A team of investigators headed by professors Steven Louie of the University of California, Berkeley, and Lawrence Berkeley National Laboratory and Raymond Jeanloz, also from UC Berkeley, used both experimental and computational science to try to determine if xenon, which makes up only 0.000009 percent of Earth's atmosphere, could also be found elsewhere on Earth, such as inside the planet's core.



Within the Earth's core, can pressure cause xenon to react with iron? This simulation shows that even under extreme pressure, iron (blue) does not bond with xenon (green).

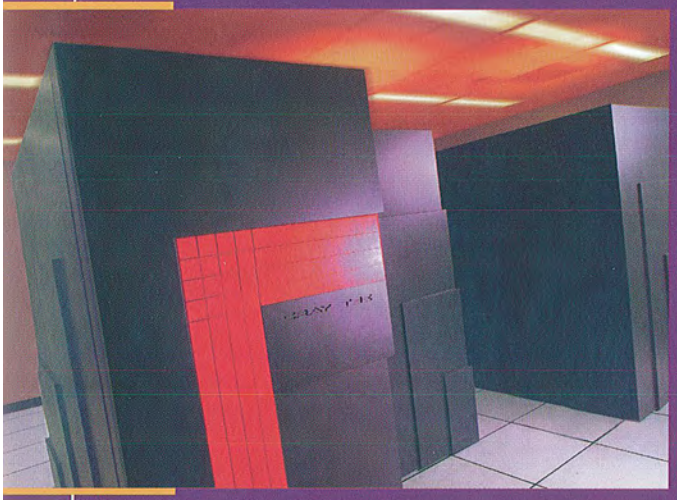
Two Berkeley graduate students, Sander Caldwell and Bernd Pfrommer (who is also associated with the Berkeley Lab Materials Sciences Division and NERSC), were key contributors to the project.

According to Caldwell, xenon is more abundant on the other rocky planets (Mars, Venus, and Mercury), and scientists have long thought more of the noble gas should be present on Earth. One theory is that xenon, usually found as a gas, could have bonded with iron in the Earth's core, and it was this theory that Caldwell tested in his lab. Despite subjecting a sample of xenon and iron to pressures up to 70 gigapascals (or 700,000 times atmospheric pressure at sea level), the two elements did not form a compound.

Using the computational capabilities of the Cray T3E at NERSC and other parallel computer platforms, Pfrommer performed quantum mechanical calculations and reached similar conclusions. "With our calculations, it is much easier to simulate high pressures than in an experiment," Pfrommer said. Even at pressures as high as 500 gigapascals, the calculations showed no sign of a chemical bond between xenon and iron.

Caldwell also aimed an industrial heating laser at his sample of xenon and iron, trying to cause the two elements to bond. While bonding did not occur, comparisons of the samples at different pressures and temperatures did clear up one mystery—xenon's phase changes.

At low pressure, xenon's structure is face-centered cubic. At higher pressures, above 75 gigapascals, the structure



changes to a hexagonal close-packed structure. In between, the thinking went, was a third structural form that was not entirely understood.

However, by using calculations from NERSC and observing samples, Caldwell and his colleagues determined that there is no third structural form. Rather, at those pressures, xenon "can't decide which phase it should be in."

Calculations showed that there was a very small energy difference between the two phases. "In fact, we had to keep crunching the numbers because the difference is so small, it was hard to calculate," Caldwell said.

By heating the sample, Caldwell provided energy for the sample xenon to change from one phase to the next without going through the predicted middle phase. "We cleaned up the area in the middle," said Caldwell. "There is no xenon II phase—it is actually part of the two known phases."

Ironically, it was the iron in the sample that absorbed enough energy from the laser to help solve the mystery of the missing phase.

"Although the question of xenon's presence is still up in the air, so to speak," Caldwell said, "we've probably ruled out that it's sequestered in the core of the Earth. Now we need to seek another explanation."

VERTICAL DISPLACEMENT EVENTS IN SHAPED TOKAMAKS

Ahmet Y. Aydemir,
Institute for Fusion Studies, University of Texas at Austin

Research Objectives

The goal of this research is to investigate the currents generated on plasma-facing components during large scale, macroscopic displacements of the plasma column in elongated tokamaks, caused by disruptions or loss of positional control.

Computational Approach

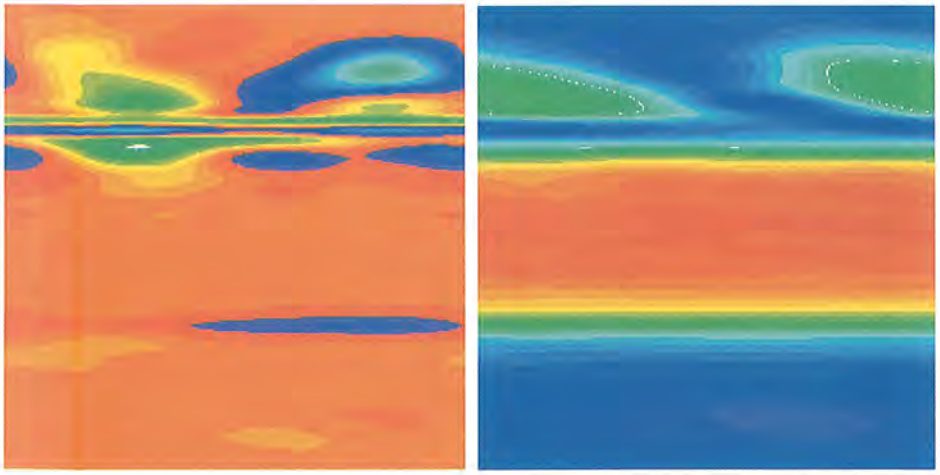
Vertical stability of tokamaks has been studied extensively in the past, using sophisticated, but one- or two-dimensional, computational models. Our approach here is a self-consistent and three-dimensional reexamination of the problem, using our nonlinear magnetohydrodynamic code CTD that has been appropriately modified to handle nonlinear free-boundary problems without any built-in symmetry assumptions. The plasma region, described by the MHD equations, is surrounded by a wall of finite thickness and resistivity. Toroidal equilibrium and plasma shaping are provided by external currents assumed to be flowing in circuits of large inductance, so that the currents can be taken to be constant in time. To date, production runs have been done on the vector machines (C90), but CTD is gradually being rewritten in C++ and ported over to the T3E at NERSC.

Accomplishments

In double-null equilibria self-consistently generated with CTD, we are examining the nonlinear evolution of vertical displacement events (VDEs). We have qualitative observations of large poloidal and toroidal nonuniformities in the currents generated in the resistive wall. The electric field set up by the decaying plasma current, in conjunction with the eddy currents generated by the motion of the plasma column, leads to a very large poloidal nonuniformity in the toroidal component of the wall current, with a possible reversal of the current near the strike point. The poloidal halo currents in the wall, mainly due to coupling of the diamagnetic plasma currents to the conducting wall after the column comes in contact with it, are by their very nature poloidally localized; but they also exhibit toroidal nonuniformities when the VDE is coupled with an n=1 MHD mode. A more quantitative characterization of these processes and an extension of the work to single-null geometry are under way.

Significance

Loss of vertical stability, due to a disruption or a failure in the feedback system, is an event that probably cannot be completely avoided in the operation of a tokamak. Thus, a quantitative understanding of the currents generated by a VDE and the electromagnetic forces generated by them on the conducting structures around the plasma column is essential for the design and operation of the next generation of tokamaks.



Distribution of poloidal (left) and toroidal (right) currents on the resistive wall during a downward moving VDE. Horizontal axis is the toroidal angle. Poloidal angle, measured from the outboard midplane, is on the vertical axis.

PATTERN FORMATION IN POLYMER FILMS

Anna C. Balazs, University of Pittsburgh

Research Objectives

The aim of our research is to isolate conditions for creating patterned polymer films. Tethering polymers onto a substrate and immersing the system into a poor solvent provides a unique opportunity for creating such patterned layers. For example, tethered homopolymers form arrays of "pinned micelles" on the surface. We extended this concept by investigating the behavior of tethered copolymers in poor solvents. By introducing greater chemical complexity within the chains, we could drive the system to form more complicated surface patterns.

Computational Approach

In carrying out this research, we used numerical self-consistent field calculations, Monte Carlo simulations, and scaling theory.

Accomplishments

We determined the behavior of tethered polyelectrolytes confined between two walls and the properties of thin films of ABC triblocks confined between smooth plates. In the case of polyelectrolytes, we demonstrated that surfaces covered with like-charged polymers and immersed in a poor solvent show an attraction as the layers are compressed. Furthermore, at high degrees of ionization, compressing the layers results in a novel first-order phase transition: the stretched, charged chains spontaneously associate into aggregates on the surfaces. At both low and high degrees of ionization, the free energy versus distance profiles reveal distinct minima, which indicate an optimal separation between the surfaces. The results provide guidelines for driving highly concentrated solutions of mesoscopic particles to self-assemble into ordered arrays, or colloidal crystals. Such colloidal crystals can be used as Bragg defraction devices or optical switches.

In the case of confined ABC triblocks, the B segment is chosen to be the central block, and all the blocks are incompatible. The chains microphase segregate into a lamellar phase, with the stripes either perpendicular or parallel to the walls. When all the monomer-surface interactions are identical, the perpendicular orientation has the lowest free energy. When a repulsion is introduced between the surface and the A and C monomers, the surface interactions further stabilize the perpendicular orientation. At strong surface interactions, the morphology of the perpendicular structure is controlled by the overall thickness of the molten layer.

Significance

In comparing diblocks to triblocks as candidates for forming laterally patterned films, our work indicates that triblocks possess distinct advantages over diblocks. Therefore, triblocks can be used to fabricate patterned polymer surfaces whose features are in the tens of nanometers scale and, thus, an order of magnitude smaller than typically achieved through photolithography. These surfaces can be used for novel optical or electronic applications. Both of the above studies illustrate the dramatic effect that confinement has on the phase behavior of polymeric systems.

Publications

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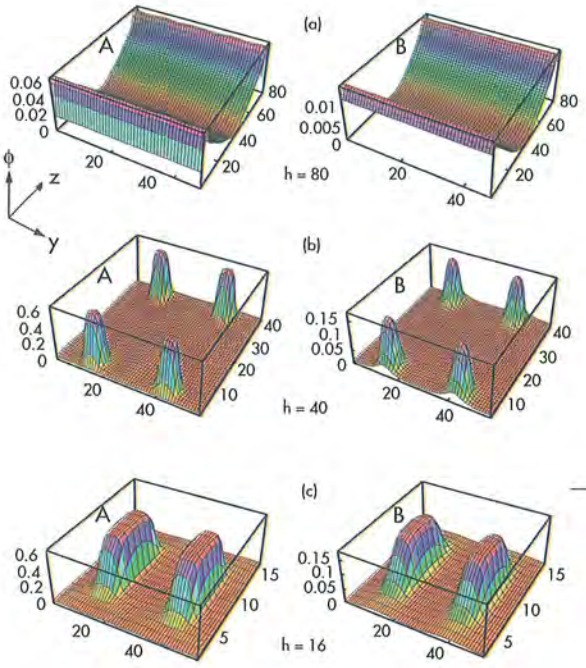

Density profiles for two surfaces coated with end-grafted polyelectrolyte chains. The plots show the effect of decreasing the separation between the surfaces and reveal that the stretched, charged chains spontaneously associate into aggregates as the surfaces are brought closer together. The parameter f denotes the polymer density. Here the shape of the profiles for the counterions are qualitatively the same as those for the polymers. (a) At surface separation h = 80, the grafted chains form homogeneous layers. (b) At h = 40, micelles form on each of the surfaces. (c) At h = 16, compression causes the micelles from the surfaces to merge.

THE INDONESIAN THROUGHFLOW AND THE GLOBAL CLIMATE SYSTEM

Tim Barnett and Niklas Schneider,
Scripps Institution of Oceanography

Research Objectives

To determine the role in the coupled ocean-atmosphere system of oceanic transport from the Pacific to the Indian Ocean through the Indonesian Seas.

Computational Approach

A sophisticated climate model that couples general circulation models of the ocean and atmosphere was integrated with both open and closed Indonesian passages. Climate and Indonesian throughflow simulated by the first integrations compare favorably with observations. Effects of the Indonesian throughflow on the earth's climate are determined by contrasting this climate state with the simulation obtained after closure of the oceanic passages between Australia and Asia.

Accomplishments

The Indonesian throughflow affects the circulation and thermocline depth around Australia and in the Indian Ocean. It shifts the western Pacific/eastern Indian Ocean warm pool and centers of deep atmospheric convection to the west by increasing surface temperatures in the eastern Indian Ocean and reducing temperatures in the equatorial Pacific. This control on sea surface temperature and deep convection affects atmospheric pressure in the entire tropics and, via atmospheric teleconnections, in the mid-latitudes. As a result, surface wind stresses in the entire tropics change, and meridional and zonal gradients of the tropical thermocline and associated currents increase in the Pacific and decrease in the Indian Ocean. The response includes an acceleration of the equatorial undercurrent in the Pacific, and a deceleration in the Indian Ocean. Thus, the Indonesian throughflow exerts significant control over the global climate in general, and the tropical climate in particular. Results also indicate that feedbacks of the throughflow transport and its wind forcing are negative, and suggest that this interplay can not excite growing solution or lead to self-sustained oscillations of the ocean-atmosphere system.

Significance

In addition to increasing understanding of the oceanic transport through the only low latitude connection of the world's oceans, this research serves the continuing effort of evaluating and improving climate models that play a pivotal role in the prediction of natural climate variability and of anthropogenic climate changes.

Publications

Schneider, N. 1997. The Indonesian throughflow and the global climate system. *J. Climate*, in press.

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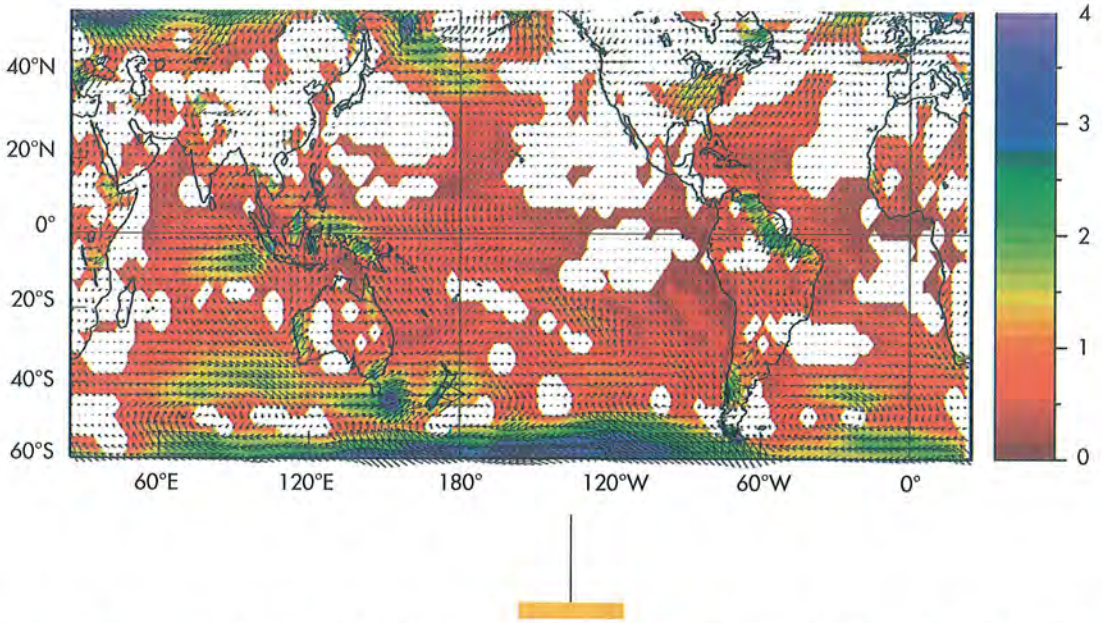

Changes of the surface wind stress (arrows) due to closure of the Indonesian throughflow. Changes of the stress that are significantly beyond the natural climate variability are color coded, where the color corresponds to changes of the wind stress magnitude in N/m*m.

COMPUTATIONAL ENZYMOLOGY

Paul A. Bash, Argonne National Laboratory

Research Objectives

Advances in protein crystallography have enabled scientists to determine the three-dimensional structures of enzymes and explore the mechanisms by which enzymes achieve both strict specificity in recognizing their substrates and extraordinary efficiency in catalyzing chemical transformations. Some aspects of the reaction mechanism, however, lie outside the reach of experimental methods, due in large part to the short-lived nature of the key steps along the reaction pathway.

In our program, we are attempting to develop numerical tools, based on first-principles physical and chemical models, that can provide information complementary to that obtained from experiment. Our goal is a basic understanding of the reaction mechanism in enzyme systems. Our methods are designed to fill in some of the details missing from present experimental studies of enzyme systems and complete the picture of how enzymes achieve such remarkable catalytic efficiencies and substrate specificities.

Computational Approach

Our principal computational tool is a hybrid, quantum mechanical/molecular mechanical (QM/MM) method developed to simulate the behavior of biological molecules in the condensed phase. Relatively few atoms in the active site of the enzyme are treated quantum mechanically; the bulk of the atoms are represented by a molecular mechanics hamiltonian. The method enables us to investigate the critical events of bond formation and cleavage catalyzed by the enzyme and yet retain the principal effects of the protein environment. To calibrate the quantum hamiltonian parameters, we rely on large quantum chemistry calculations conducted on the J90 cluster using the code GAUSSIAN-94. Our molecular dynamics simulations are performed with the code CHARMM on the T3E, using the parallel architecture to routinely simulate systems involving twenty thousand atoms.

Accomplishments

We have investigated the reaction mechanism in the class of enzymes known as beta-lactamases, the primary source of antibiotic resistance in bacteria. These enzymes hydrolyze antibiotic agents such as penicillin with great alacrity. We have performed a number of molecular dynamics simulations aimed at defining the so-called Michaelis complex: the state in which the enzyme has captured the substrate but prior to any bond reorganization. We have found two possible mechanisms for the initial attack of the enzyme on its penicillin substrate to be consistent with the results of our simulations. Our next efforts will be directed to understanding the relative energetics of these two possible pathways.

Significance

Recent experiments have indicated that once bacteria develop a resistance to antibiotics, that resistance is not lost even after many thousands of generations of bacteria cultured in the absence of antibiotics. Additionally, bacteria seem able to find mechanisms to develop resistance to new antibiotics. An understanding of how the beta-lactamase enzymes function at an atomic level may provide new insights into the development of new antibiotics or enzyme inhibitors.

Publications

Bash, P. A., L. L. Ho, A. D. MacKerell, Jr., D. Levine, and P. Hallstrom.1996. Progress toward chemical accuracy in the computer simulation of condensed phase reactions. *Proc. Natl. Acad. Sci.* USA 93:3698-3703.

Cunningham, M A., L. L. Ho, D. T. Nguyen, R. E. Gillilan and P. A. Bash. Simulation of the enzyme reaction mechanism of malate dehydrogenase. 1997. *Biochemistry* 36:4800-4816.

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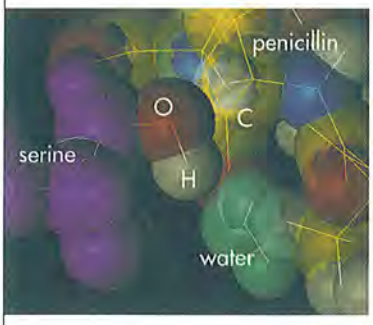

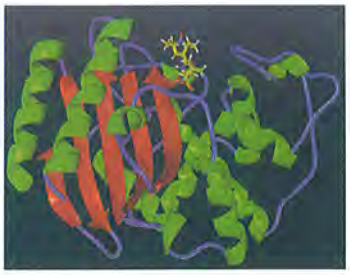

CPK rendering of the active site of beta-lactamase. The catalytic serine residue (in blue) is positioned to transfer a proton (H) to the water molecule (in cyan). This transfer will activate the serine in preparation for its oxygen atom (O) to attack the carbon atom (C) of penicillin substrate (in yellow).

Ribbon diagram of the enzyme beta-lactamase from TEM-1. Helices are rendered in green and beta sheets in red. Connecting loops are indicated in blue. The penicillin substrate is drawn as a stick figure with carbon atoms in yellow, nitrogen in blue, oxygen in red, hydrogen in white, and sulfur in orange. The penicillin molecule is located in the active site of the enzyme.

ADAPTIVE ALGORITHMS FOR MODELING LOW MACH NUMBER FLOWS

John Bell, Ann Almgren, Vincent Beckner, Phillip Colella, William Crutchfield, Marcus Day, Louis Howell, Michael Lijewski, Richard Pember, Charles Rendleman, and David Stevens, Lawrence Berkeley National Laboratory

Research Objectives

Many phenomena in fluid dynamics are described by low Mach number models. Examples of low Mach number flows range from propagation of flames and the breakup of sprays to the dynamics of the atmosphere and the oceans. The goal of this project is to develop new computational tools for modeling these types of flows.

Computational Approach

Our approach for modeling low Mach number flows is based on a projection formulation that incorporates modern high-resolution upwind difference methodology for discretizing advective transport. This formulation forms the basis for a hierarchical adaptive-mesh refinement algorithm that localizes computational effort where it is required to preserve accuracy.

Accomplishments

We completed a serial version of the adaptive-mesh refinement algorithm for the incompressible Navier-Stokes equations, which is a prototype for more general low Mach number flows in both two and three dimensions. This basic framework has also been extended to model laminar flame propagation. We are currently developing a parallel version of the algorithm for the T3E, based on a coarse-grained parallelization strategy.

Significance

Successful completion of this work will provide us with a dramatic improvement in our ability to model low Mach number flows. This improvement in modeling capability will enable us to gain new insights into fundamental scientific questions about turbulent flows and combustion and will form the basis of a new generation of modeling tools that can be used for designing combustion systems such as engines and industrial furnaces.

Publications

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Pember, R. B., P. Colella, L.H. Howell, A. S. Almgren, J. B. Bell, W. Y. Crutchfield, V. E. Beckner, K. C. Kaufman, W. A. Fiveland, J. P. Jessee. 1997. An adaptive projection method for the modeling of unsteady, low Mach number combustion. Fall Meeting of the Western States Section of the Combustion Institute. WSS/CI 97F-125. LBL-38551.

Howell, L. H., R. B. Pember, P. Colella, J. P. Jessee, and W. A. Fiveland. N.d. A conservative adaptive-mesh algorithm for unsteady, combined-mode heat transfer using the discrete ordinates method. *Numerical Heat Transfer, Part B: Fundamentals*, submitted.

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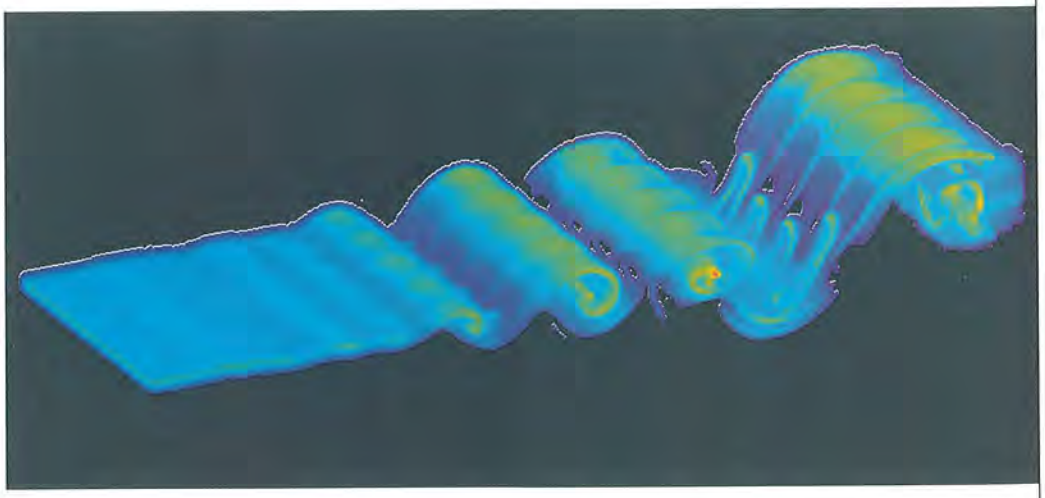

Vorticity magnitude from the 3D simulation of a variable density shear layer using adaptive mesh refinement.

CHAMMP COUPLED CLIMATE MODEL DEVELOPMENT AND APPLICATION

Robert M. Chervin, National Center for Atmospheric Research

Research Objectives

The coupled atmosphere, ocean, and sea ice model being developed (now designated the Parallel Climate Model, or PCM) is a multi-institutional effort involving NCAR, the Naval Postgraduate School (NPS), and the Los Alamos National Laboratory (LANL), under the sponsorship of the Department of Energy's Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP) Program on Climate Research. This coupled model will be used for sensitivity studies on century-long time scales to address questions related to the climatic impacts of greenhouse gas and other radiative forcings.

Computational Approach

The ocean component is the Parallel Ocean Program (POP) developed by Smith, Malone and Dukowicz (LANL). The model uses second-order finite differencing in space and leapfrog finite differencing in time. An implicit technique is used for the free-surface calculation. The model uses a generalized curvilinear coordinate system which permits displacing the North Pole to a location such that the convergence of meridians does not place an excessive restriction on the allowable time step. POP has recently been reformulated in terms of data structures and the use of memory and cache and completely rewritten for enhanced performance in a message-passing environment.

The sea ice component was derived from an eddy-resolving Arctic Ocean model by Zhang (NPS) and optimized for MPP architecture by Craig (NCAR). It uses the Zhang and Hibler ice dynamics with line relaxation for solving the viscous-plastic ice rheology. The thermodynamics are from the Semtner and Parkinson-Washington models. The grid is transformed such that the resolution is constant, thus avoiding the problem of convergence near the pole as on a latitude-longitude grid. For the coupled model, an ice model grid with 27 km resolution has been designed that includes all of the present day ice-coveraged areas in both hemispheres, minimizing the grid space required.

The atmospheric component for the coupled model is the massively parallel version of the NCAR Community Climate Model version 3 (CCM3), which is based on the spectral transform technique to use spherical harmonics as basis functions for the spatial discretization. Leapfrog finite differencing is used in time, and semi-Lagrangian transport is used for advection. This model includes the latest versions of radiation, boundary physics, and precipitation physics.

The method of tying the components together and allowing the exchange of fluxes and state variables is the flux coupler concept developed at NCAR for the Climate System Model. Since the grids of the various components are quite different, a conservative interpolation scheme developed by Jones (LANL) is being used for passing information between components.

Accomplishments

Four codes (CCM3, old POP, the prototype PCM, and new POP) were made operational on the T3E at NERSC. Several performance bottlenecks were identified and corrected. The PCM version of new POP was optimized by Wayland (NCAR) for the NERSC Cray T3E and demonstrated excellent scalability using 4, 8, 16, 32, 64, 128, and 256 PEs.

Significance

The scientific purpose of the production runs will be to assess the impact of greenhouse and other radiative forcings on decade to century time scales.

Publications

Washington, W. M., J. W. Weatherly, and R. M. Chervin. 1998. A new DOE coupled parallel climate model with high resolution ocean and sea ice. *Proc. Ninth Symposium on Global Change Studies*. Boston: American Meteorological Society, in press.

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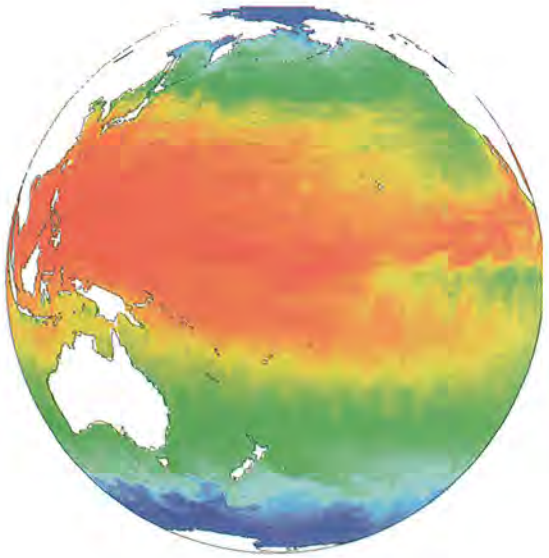


Snapshot of ocean temperature.

ELECTRONIC STRUCTURE CALCULATIONS ON LITHIUM POLYMER ELECTROLYTES

Larry A. Curtiss, Argonne National Laboratory

Research Objectives

This project involves a fundamental study of lithium polymer electrolytes used in lithium battery systems. We are investigating the effects of the polymer host on ion solvation and the attendant effects of ion pairing, which strongly affect the ionic transport in these systems.

Computational Approach

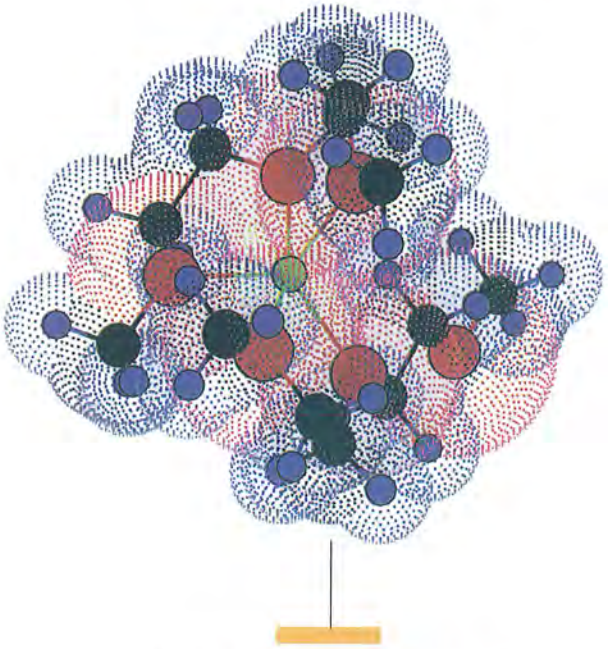
Ab initio molecular orbital theory is being used to investigate energetic, structural, and dynamical properties of ion-ion and ion-polymer interactions at a molecular level in combination with molecular dynamics simulations being carried out at the University of Minnesota. The polymer is being modeled using alkyl oxides chains. The interaction of a lithium cation with the oxygens from one and two chains is being investigated to examine the stability of different coordinations of lithium with the polymer model and barriers to migration of the lithium cation from one coordination site to another coordination site. The calculations are being done on both the Cray C90 and J90 computers.

Accomplishments

Structures were located corresponding to coordination of a lithium cation with one to six oxygens of either one or two alkoxide chains. The binding energies of the complexes were found to increase with coordination of the cation by oxygen, although the binding per Li-O bond decreases. The barriers for lithium cation migration between coordination sites and transition states were located. While the barriers were found to be small for lithium cation migration from lower to higher coordination of lithium with oxygen, the barriers were large for higher to lower coordination.

Significance

Much is unknown about the nature of the ion association processes, the ion-polymer interactions, and the role that they play in ionic conductivity of lithium polymer electrolytes used in batteries. These electron structure computations in combination with molecular dynamics simulations at the University of Minnesota and neutron scattering measurements at Argonne National Laboratory will provide fundamental insight into the ionic conductivity mechanism in these materials.



Coordination of lithium cation (green) with six oxygens (red) from two ethylene oxide chains.

Publications

Boinske, P. T., L. A. Curtiss, J. W. Halley, B. Lin, and A. Sutjianto. 1996. Lithium ion transport in a model of amorphous polyethylene oxide. *Journal of Computer-Aided Materials Design* 3:385-402.

Sujianto, A., and L. A. Curtiss. 1997. Theoretical study of the potential energy surface of diglyme. *Chemical Physics Letters* 264:127-133.

http://www.cmt.anl.gov/mcp/lipeo.htm

NUMERICAL TOKAMAK TURBULENCE PROJECT

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J. M. Dawson, University of California, Los Angeles
V. K. Decyk, University of California, Los Angeles
W. D. Dorland, University of Texas at Austin
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
J. V. W. Reynders, Los Alamos National Laboratory
R. E. Waltz, General Atomics

Research Objectives

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

Computational Approach

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

Accomplishments

Detailed parameter studies have been conducted with our GK and GLF simulations, addressing discharge #81499 in the General Atomics DIII-D tokamak as a base case because of its relevance to the International Thermonuclear Experimental Reactor (ITER). Careful comparisons have been made between the results of the GLF and GK simulations of shot 81499 and variants to determine parametric dependences and points of agreement and disagreement between the simulation algorithms (the Cyclone study). Elsewhere, GLF and GK simulation results have been compared to experimental findings with good agreement in some cases. As part of the Cyclone study, a GK flux-tube PIC simulation has been the object of a vigorous study of its convergence properties, with results so far suggesting that statistical convergence is being obtained. Although the differences between the results for the turbulent ion thermal diffusivity in GK and GLF simulations are not large (GK results are often a factor of 2 to 3 lower than GLF results), the implications of these differences for the projected fusion performance of ITER can be significant.

The NTTP simulations have also demonstrated the importance of flow shear and negative central magnetic shear in reducing drift-wave turbulence in tokamaks as observed in experiments. GK simulations have verified the improved confinement in the TEXTOR tokamak due to a small percentage of Ne impurity which has a stabilizing effect on ion-temperature-gradient turbulence. Many NTTP codes have been successfully ported to the T3E in the last year, and a new global GLF code is yielding physics results (see graphic). Progress has been made in including realistic geometrical effects (for example, shaped cross sections and magnetic X-points needed to model plasmas with divertors) and realistic equilibrium plasma profiles in the simulations.

Significance

The NTTP simulations are 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 improved performance. This simulation work builds a bridge between theory and experiment, and provides a basis for reduced transport models intended to fit current experimental databases, 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 like ITER, reliable NTTP simulations can lead to significant cost savings and improved performance in future experiments.

Publications

Fivas, M., T. Tran, K. Appert, J. Vaclavik, and S. Parker. 1997. Stabilization of ion-temperature-gradient-driven tokamak modes by magnetic-field gradient reversal. *Phys. Rev. Lett.* 78:3471.

Cohen, B. I., and A. M. Dimits. 1997. Implicit, partially linearized, electromagnetic particle simulation of plasma drift-wave turbulence. *Phys. Rev. E* 56:2151.

Waltz, R. E., R. L. Dewar, and X. Garbet. N.d. Theory and simulation of rotational shear stabilization of turbulence. *Phys. of Plasmas*, in press.

http://www.acl.lanl.gov/GrandChal/Tok/tokamak.html
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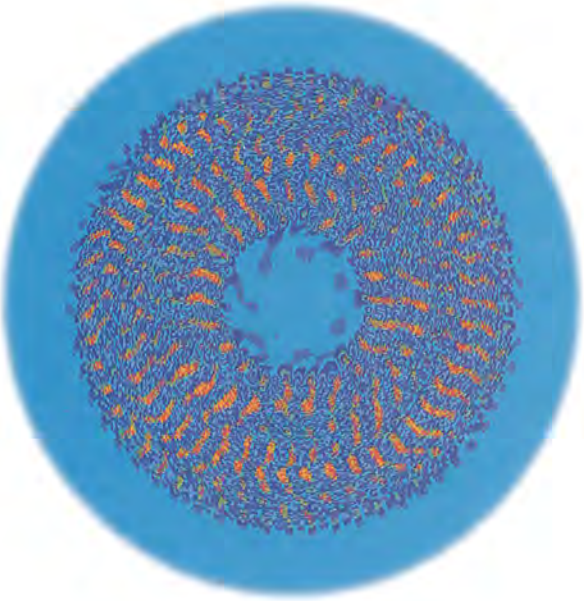


Researchers completed cross-section calculations of cylindrical multi-helicity ion-temperature-gradient-driven turbulence with previously unattainable resolution on NERSC's Cray T3E-600. Work is in progress to increase the resolution, improve the performance of the parallel code, and include toroidal geometry in calculations on the T3E-900. (V. E. Lynch, J-N. Leboeuf, B. A. Carreras, Oak Ridge National Laboratory; J. D. Alvarez, L. Garcia, Universidad Carlos III de Madrid)

GLOBAL TURBULENT TRANSPORT MODELING IN TOROIDAL PLASMAS USING GYROKINETIC PARTICLE SIMULATION

John Dawson, Richard Sydora, and Viktor Decyk,
University of California, Los Angeles

Research Objectives

This project focuses on the development and application of low frequency particle-in-cell simulation models for the study of fluctuation-driven heat and particle transport in magnetically confined fusion plasmas, such as the tokamak, and addresses a problem recognized as a grand challenge in plasma physics.

Computational Approach

Our simulation approach is based on the particle-in-cell method applied to the gyro-drift dynamical equations of motion for charged particles in external electric and magnetic fields, along with the self-consistent fields created by the particles. Collisional interactions between like and unlike species of particles were analyzed by Monte Carlo methods. The model has been implemented on a number of shared and distributed memory computing platforms such as the Cray C-90 and the T3E at NERSC. The distributed memory version of the model uses a domain decomposition method for the particles and fields along with message passing, and this allows us to take advantage of the enormous amount of memory, as well as speed, on these machines. It is a computationally intensive model and exploits all 512 processors on the T3E.

Accomplishments

We have recently demonstrated that full-scale, global simulations of tokamak transport with parameters typical of current high temperature experiments such as DIII-D at General Atomics, San Diego, are possible on massively parallel distributed computing architectures such as the Cray-T3E at NERSC. As we are now in the production mode, we are investigating the complex interplay between short and long wavelength fluctuations. We have found a considerable amount of radial structure and propagation effects in the turbulence which has not been included in local simulations. We have also explored the possibility of suppressing turbulent fluctuations by locally reversing the radial variation of the magnetic field line pitch (or magnetic shear) as well as adding small amounts of impurity ion species such as neon or argon.

Both of these effects are shown to suppress the turbulent fluctuations to a certain degree and are similar to the experimental observations. Finally, we have been contributing to the validation and benchmarking of fluid-based codes with kinetic closure schemes, such as the gyro-Landau fluid model which has been applied to local turbulent transport simulations and is currently being developed into a global model.

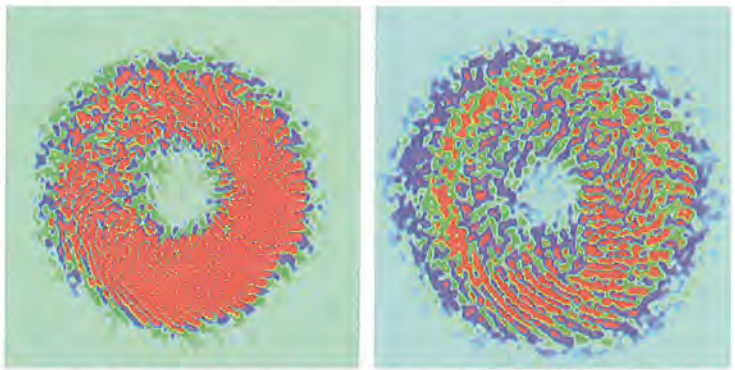
Significance

One of the primary scientific goals for fusion is to obtain a predictive capability of turbulent transport in different magnetic configurations so that effects from turbulence can be minimized and a cost-effective design for the next generation fusion devices can be achieved. With full-scale simulations of anomalous transport now possible, we are beginning to approach this goal.

Publications

Sydora, R. D., V. K. Decyk, and J. M. Dawson. 1996. *Plasma Phys. Control. Fusion* 38:A281.

Electrostatic Potential Fluctuations (Poloidal Cross-Section)



Pre-Saturation Phase **Post-Saturation Phase**

Amplitude of electrostatic potential fluctuations taken at two different time slices during the evolution of the turbulence. The turbulent eddies cause transport of heat and particles. These simulations were performed on the T3E and had a reverse magnetic shear equilibrium.

SIMULATION OF MICROSTRUCTURAL CHANGES

Tomas Diaz de la Rubia and Maria J. Caturla,
Lawrence Livermore National Laboratory

Research Objectives

We are studying, at a microscopic level, the damage produced in metal irradiated by an energetic atom, and how this damage is distributed into vacancies and interstitials. In particular we are interested in the clustering of the different defects after the irradiation and their effects in the later evolution of these defects under annealing of the material. Our final goal is to understand how microstructural changes occur under irradiation conditions.

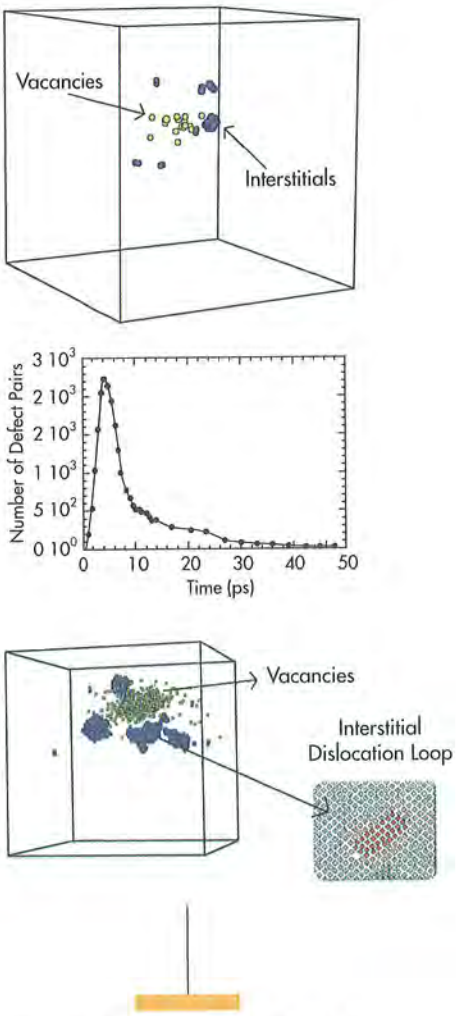
Computational Approach

We use a classical molecular dynamics code to study radiation damage in metals. Our molecular dynamics code has been implemented to be used on the Cray T3E. It uses standard PVM for message passing, and the programming language is Fortran 90. This code was previously running on a Cray T3D and was easily implemented to run on the T3E.

Accomplishments

From the simulations performed on the T3E we are extracting a data base of the number and distribution of the vacancies and interstitials produced by different energetic ions. This data base will be used as the input for a later Monte Carlo simulation of defect diffusion at elevated temperatures, facilitating the study of defect clustering and, therefore, microstructure evolution and mechanical property changes. Other parameters needed for this Monte Carlo simulation have been extracted using the parallel molecular dynamics code, such as vacancy and interstitial diffusivities and binding energies of vacancies and interstitial clusters.

In particular, we have studied the damage produced by self-irradiation of lead with energies between 10 keV and 30 keV, both in the bulk of the material and at the surface. The low melting point of this metal, together with its low thermal conductivity and softness, results in very large cascades produced by the energetic atoms. In order to model this damage in a realistic manner with molecular dynamics, it is necessary to use simulation boxes that include between 250,000 and 106 atoms. A typical simulation of 30 keV Pb irradiation on Pb requires a simulation box with 60 lattice units in each direction (864,000 atoms). The forces on each of these atoms are calculated at every time step and the location of the atoms updated according to those forces. Each time step is on the order of fentoseconds, and the total simulation time is typically of 50 picoseconds, due to the large relaxation times for this material. The CPU time for a time step using 64 processors and 864,000 atoms is approximately 3.5 seconds. Therefore, a total of 48 CPU hours are needed to complete each one of these large cascades.



Vacancies (light color) and interstitials (dark color) produced by a 30 keV Pb in Pb. Observe the large interstitial clusters produced. The interstitial clusters are forming dislocation loops as can be observed by looking at a single plane on the lattice.

Significance

We are now performing Monte Carlo simulations of defect diffusion using the results from the parallel molecular dynamic code. These results provide a physically based model for defect production and migration. These simulations will increase understanding of the controversial problem of void swelling in metals.

MICROSCOPIC CALCULATIONS OF NUCLEAR SCATTERING: FULL-FOLDING OPTICAL POTENTIALS FOR ELASTIC NUCLEON-NUCLEUS SCATTERING

Charlotte Elster and S. P. Weppner,
Ohio University

Research Objectives

An important goal in the application of multiple scattering theory to nuclear systems is to determine the nonrelativistic optical potential for elastic nucleon-nucleus scattering within the framework of the Spectator Expansion of multiple scattering theory. A consistent *ab initio* calculation of the first order term of this expansion implies the construction of full-folding optical potentials from realistic single particle wave functions (describing the ground state of the target nucleus) convoluted with nucleon-nucleon (NN) t-matrices (derived from nuclear forces based on meson exchange) as well as the modification of the optical potential through the nuclear medium.

Computational Approach

The exact calculation of the optical potential requires a three-dimensional integration in which the integration variable is coupled to the energy of propagation of the projectile and target nucleon. This very fact leads to a full-folding optical potential which treats the off-shell behavior and the energy dependence of the NN t-matrix when carrying out the integration. When integrating to negative energies, the pole structure of the NN t-matrix has to be taken carefully into account. This pole structure—a true bound state in the $3S_1$-$3D_1$ channel, the deuteron, and a virtual state in the $1S_0$ channel, the di-proton—gives rise to an additional channel in the optical potential, the deuteron pickup channel.

Accomplishments

We calculated elastic scattering observables for 16O, 40Ca, and 208Pb at projectile energies ranging from 65 to 200 MeV projectile energy and compared the full calculation to calculations in which the energy of the NN t-matrix is fixed at half the projectile energy. We found that this fixed-energy prescription describes the full calculation remarkably well for proton scattering at 200 MeV projectile energy. For energies below 200 MeV, we found that the influence of the deuteron and di-proton state slowly gains importance as lower energies are approached.

We also tested the validity of the factorized off-shell tp approximation in the energy regime between 65 and 400 MeV and found that this approximation, which only retains the non-locality given through the NN t-matrix, is, even at lower energies, a very good representation of the full-folding calculation based on a fixed energy in the NN t-matrix as far as the elastic nucleon-nucleus observables are concerned.

Significance

A long-standing aim of classical nuclear physics has been to apply the nuclear force as obtained from two nucleon data and to predict many body phenomena from it. In recent years the PI and collaborators have made considerable progress towards this goal in the area of proton and neutron scattering from nuclei at intermediate energies. This progress has partially been due to the rapid developments in high-performing computing technologies.

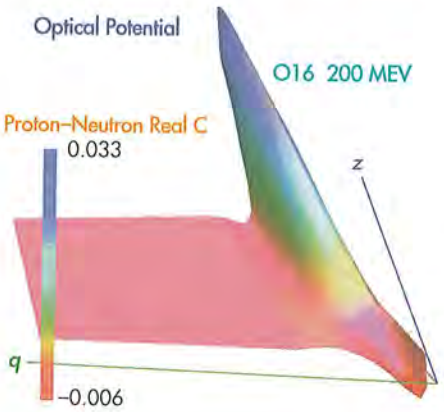
Publications

Elster, C., S. P. Weppner, and C. R. Chinn. 1996. Microscopic optical potentials for elastic nucleon-nucleus scattering. In *Proceedings of the Specialists' Meeting on the Nucleon-Nucleus Optical Model up to 200 MeV*, Bruyeres-le-Chatel, France, November 13-15. http://db.nea.fr/html/science/om200

——. 1997. Full-folding optical potentials for elastic nucleon-nucleus scattering based on realistic densities. *Phys. Rev. C* 56:2080. http://xxx.lanl.gov/ps/nucl-th/9611045

Elster, C., and S. P. Weppner. 1997. Energy dependence of the NN t-matrix in the optical potential for elastic nucleon-nucleus scattering. *Phys. Rev. C.*, in press. http://xxx.lanl.gov/ps/nucl-th/9708010

http://plato.phy.ohiou.edu/~elster/nersc97/nersc97.html



The full-folding optical potential for 16O at 200 MeV projectile energy as function of the momentum transfer q and the nonlocal, orthogonal variable K. The proton-neutron part corresponding to the Wolfenstein amplitude C is shown, which corresponds to the imaginary part of the spin-orbit potential.

ENERGETICS, BONDING MECHANISM AND ELECTRONIC STRUCTURE OF CERAMIC/CERAMIC AND METAL/CERAMIC INTERFACES

Arthur J. Freeman, Northwestern University

Research Objectives

To determine the structural, electronic, and magnetic properties of metal/ceramic interfaces (notably transition metals/BST interfaces); and to understand the effects of lattice distortions and magnetic canting in the colossal magneto-resistance (CMR) materials, using highly precise all-electron local-density total-energy methods.

Computational Approach

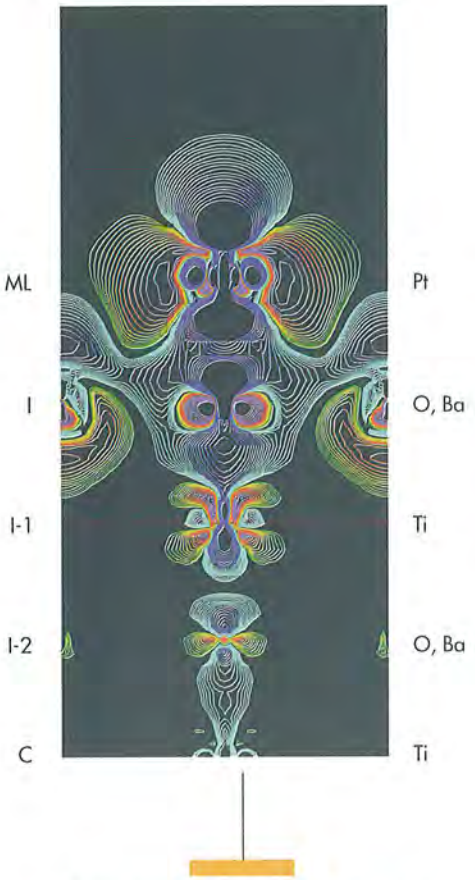
For several of our projects, we used the full-potential, linearized, augmented plane wave (FLAPW) method. The underlying concept is the partitioning of real space into spherical regions around atoms, and into interstitial and vacuum regions. This expands the charge, potential, and wave functions without any shape approximation, which makes it the most suitable and highly precise method for solids. One of the most important capabilities of FLAPW is the ability to calculate atomic forces and predict the total energy as a function of nuclear positions, which allows the determination of structural properties.

To further increase our capability of handling large complex systems to a new level and to exploit the computational power of massively parallel machines, we have parallelized our FLAPW code. The generalized eigenvalue equation has been solved by the newly developed parallelized QR (PQR) pack age, which is a portable eigen-solver written for distributed memory computers for solving the eigenvalues and vectors. We achieved good acceleration and reasonable scalability.

Accomplishments

We performed first-principles modeling of the leakage behavior of metal/BST (barium strontium titanate) thin film devices and found significant hybridization between metal d states and the O 2p-Ti 3d states. The Fermi levels of the metals lie in the gap of BST, and metal-induced gap states were observed. The issues of how to achieve low leakage current (through calculation of the Schottky barrier height), the bonding mechanism and structure of the interface have been addressed.

We determined from first-principles the magnetism in CMR materials and investigated the effects of lattice distortions on the competition between double exchange (DEX) and superexchange. We found that both global and internal lattice distortions dramatically influence the character of the exchange interactions. Distortions associated with typical Mn-O bond variations promote the DEX contribution; the bending of the Mn-O bonds in the (a-b) plane suppresses the DEX; and the tilting of the octahedra promotes non-Heisenberg contributions to the exchange interaction energy.



Charge density difference upon Pt adsorption on a slab of $BaTiO_3$.

Significance

Our simulations on metal/BST systems provide information that helps direct the search and expedites the corresponding experimental work by steering the selection of materials for new metal electrode materials that lead to low leakage current for metal/BST/metal capacitors. The investigation on the CMR material helps us to understand its exchange coupling, which goes beyond the Heisenberg model.

Publications

Rao, F., M. Kim, A. J. Freeman, S. Tang, and M. Anthony. 1997. Structural and electronic properties of transition-metal/$BaTiO_3$(001) interface. *Phys. Rev. B* 55:13953.

Mryasov, O. N., R. F. Sabiryanov, A. J. Freeman, S. S. Jaswal. 1997. Effect of lattice distortions on the competition between the double and superexchange mechanisms in $LaMnO_3$. *Phys. Rev. B* 56:7255.

QUANTUM MONTE CARLO SIMULATIONS OF EXTENDED AND THREE-BAND HUBBARD MODELS IN ONE AND TWO DIMENSIONS

James E. Gubernatis, Los Alamos National Laboratory

Research Objectives

To study strongly correlated electron effects in various Hubbard models using the constrained-path Monte Carlo method.

Computational Approach

We are using a parallelized version of the constrained-path Monte Carlo method recently proposed by Zhang, Carlson, and Gubernatis. This method projects the ground-state wavefunction from a trial wavefunction by a branched random walk, and eliminates the infamous fermion sign problem by eliminating any random walker that develops a negative overlap with a constraining wavefunction. If this constraining wavefunction were the exact ground-state wavefunction, the procedure would be exact. Because only an approximate ground state can be used, a variational upper bound to the exact ground-state energy is produced. Benchmarking has demonstrated that this bound is tight and that the Monte Carlo representation of the wavefunction produces good approximations to other physical quantities like pairing correlation functions.

Accomplishments

We focused on simulations of the two-dimensional, three-band Hubbard model, one of the three most studied possible models of high temperature superconducting materials. We completed a series of computations of the hole-binding energy and the superconducting pairing correlations functions. We found that over a wide range of physically relevant parameters two doped holes bind, but the pairing correlation functions decay rapidly with distance. In particular, these correlations decay much more rapidly for extended s-wave correlations than they do for d-wave correlations. Furthermore, increasing the strength of the copper-site Coulomb repulsion suppressed the longer-ranged pairing correlations. These longer-ranged correlations are also suppressed with increasing system size.

Presently we are developing extensions of the constrained-path Monte Carlo method that will permit the use of a greater variety of constraining wavefunctions, such as the fixed-particle number BCS and the spin-density-wave wavefunctions. We are also considering a study of the effects of a dimerized lattice on hole binding.

Significance

We do not find evidence of off-diagonal long-range superconducting order. Because of the variational nature of our computational method, our results do not necessarily prove that the three-band Hubbard model, the most studied model of high temperature superconductivity, does not superconduct. However, our results, plus previous similar null results on the one-band Hubbard model, darken hopes that these models will serve as useful paradigms for the superconducting phase of high temperature superconducting materials.

The reported activity is a sub-project of a broader project applying a variety of computational methods to various models of strongly interacting electrons in novel materials in reduced dimensions.

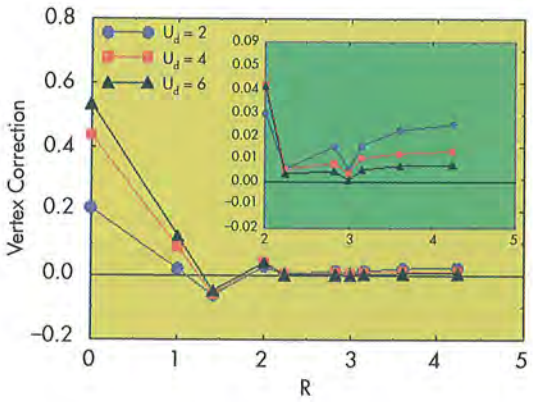
Publications

1. Shiwei Zhang, J. Carlson, and J. E. Gubernatis. 1997. Constrained path Monte Carlo method for fermion ground states. *Phys. Rev. B* 55:7464.

2. Shiwei Zhang, J. Carlson, and J. E. Gubernatis. 1997. Pairing correlations in the two-dimensional Hubbard model. *Phys. Rev. Lett.* 78:4486.

3. M. Guerrero, J. E. Gubernatis, and Shiwei Zhang. N. d. Quantum Monte Carlo study of pairing correlations in the three-band Hubbard model. *Phys. Rev. B*, submitted.

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



Distance dependence of the vertex contribution to the d-wave pairing correlation function for different values of the copper-site Coulomb repulsion.

ELECTROMAGNETIC TURBULENCE AND TRANSPORT BARRIER FORMATION IN THE TOKAMAK EDGE REGION

P. Guzdar, B. N. Rogers, and J. F. Drake,
University of Maryland

Research Objectives

A predictive model of turbulence and transport barrier formation in the tokamak edge.

Computational Approach

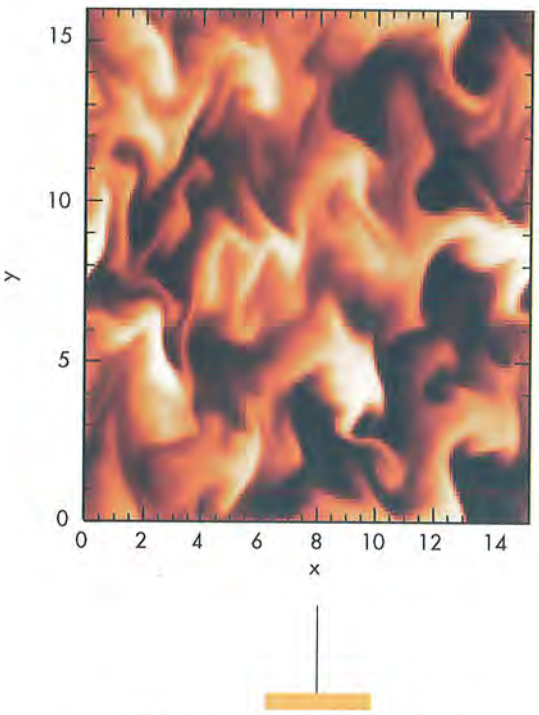
We model anomalous transport in the edge region of tokamaks with three-dimensional, electromagnetic simulations of plasma turbulence in a torus. The simulations are based on the Braginskii equations in a shifted-circle toroidal geometry, and are carried out in a poloidally and radially localized, flux-tube-like domain. Typical simulations are computationally intensive, requiring a grid resolution of roughly 128 x 128 x 128 and exceeding 10^5 time steps. We therefore rely heavily on the multiprocessing capabilities of J90s.

Accomplishments

In contrast to earlier electrostatic turbulence studies, we observe two distinct, new regimes in the electromagnetic system: an L-mode-like regime at low temperature (weak diamagnetic regime), in which the transport increases sharply as the plasma pressure approaches a small fraction of the ideal ballooning instability limit (see figure), and an H-mode-like regime at high temperature (high diamagnetic regime), in which complete suppression of the turbulence occurs as the ideal limit is approached. This suppression is due to local, sheared, self-generated ExB and diamagnetic flows. In the early stages of the formation of the barrier, strong ExB flows develop. The ion pressure then rapidly evolves so that the local ion pressure gradient balances the radial electric field, the total ion poloidal rotation being small. The magnetic perturbations and finite ion temperature are essential for the development of the barrier. These results suggest that a transport barrier in the edge region can form spontaneously when local diamagnetic effects are strong and the pressure gradient exceeds a threshold.

Significance

The study of tokamak edge transport and related phenomena, such as the L-H transition, the structure of the pedestal profiles, the density limit, and edge-localized modes, is among the most critical efforts in the controlled fusion community, and is vital to the accurate assessment of future tokamak designs.



Turbulent density perturbations caused by the nonlinear development of drift-resistive ballooning modes.

Publications

Drake, J., Y. Lau, P. Guzdar, A. Hassam, S. Novakovski, B. Rogers, A. Zeiler. 1996. Local negative shear and the formation of transport barriers. *Phys. Rev. Lett.* 3:494.

Rogers, B. and J. Drake. 1997. Enhancement of turbulence in tokamaks by magnetic fluctuations. *Phys. Rev. Lett.* 79:229.

FIRST-PRINCIPLES AND TIGHT-BINDING CALCULATIONS OF INTERFACES IN MATERIALS

Bruce Harmon, J. R. Morris, K.-M. Ho, D. E. Turner, Z.-Y. Lu, C. Z. Wang and G. D. Lee, Ames Laboratory
C.-L. Fu and M. H. Yoo, Oak Ridge National Laboratory

Research Objectives

Interfaces in materials, such as surfaces, grain boundaries, stacking faults and twin boundaries, control many properties. These include strength, growth dynamics, ductility, and electronic states. We are currently addressing the accurate quantum mechanical modeling of these features on the scale of thousands of atoms. Only with the advent of massively parallel computers and order-N electronic structure methods have such first-principles and tight-binding calculations become feasible.

Computational Approach

Our recent advances in algorithms, combined with the power of the new Cray T3E computers at NERSC, allow us to perform first-principles plane wave pseudopotential calculations using up to 1000 Si atoms. We are currently implementing our density-matrix, order-N tight-binding molecular dynamics code on the T3E, and are also examining parallel matrix diagonalization techniques for practical, direct solutions for the tight-binding electronic structure problem.

Accomplishments

The first-principles code is now in production mode on the T3E. We have completed the first-principles calculation of the structure and energy of eight different {510} grain boundary structures, for both Si and Ge. Each of these calculations involves approximately 400 atoms. A new tight-binding potential is being tested against these calculations, and reproduces the energetics quite well. We have begun calculating the electronic structure of the Si 7x7 reconstructed (111) surface, using a system of approximately 500 atoms, to understand surface electronic states. We are doing finite temperature simulations on this system to understand the phase transitions taking place on Si(111).

Significance

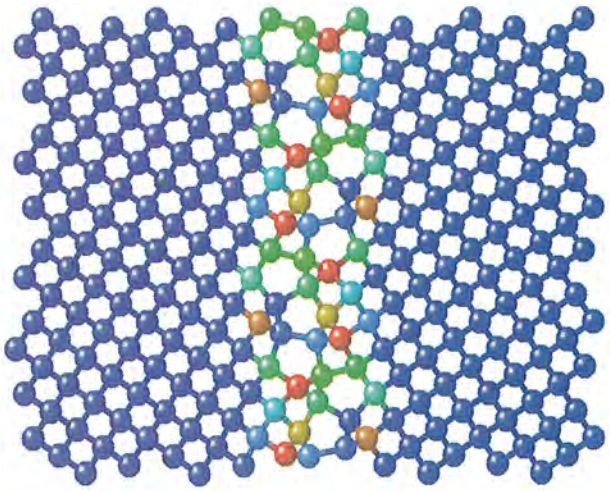
The ability to evaluate the consequences of extended material defects, requiring large numbers of atoms to simulate, is an important challenge for materials science. We are currently using the tools and techniques applied here to such problems, using fundamental science to solve key technical issues involving mechanical and electronic properties.

Publications

Morris, J. R., K. M. Ho, and C. L. Fu. 1996. Tight-binding study of tilt grain boundaries in diamond. *Phys. Rev. B* 54:132.
http://cmp.ameslab.gov/~jrmorris/highlights/grainHL.html

Morris, J. R., J. Scharff, K. M. Ho, D. E. Turner, Y. Y. Ye, and M. H. Yoo. 1997. Prediction of a {11-22} hcp stacking fault using a modified generalized stacking-fault calculation. *Phil. Mag. A* 76:1065.
http://cmp.ameslab.gov/~jrmorris/papers/gamma.html

Morris, J. R., Z.-Y. Lu, D. M. Ring, J.-B. Xiang, K.-M. Ho. C.-Z. Wang, and C.-L. Fu. N.d. First-principles determination of the {510} symmetric tilt boundary structure in Si and Ge. In preparation.
http://cmp.ameslab.gov/~jrmorris/highlights/sigrain.html



Atomic structure of the lowest energy (510) symmetric tilt boundary in Si.

COMPUTATIONAL CHEMISTRY FOR NUCLEAR WASTE CHARACTERIZATION AND PROCESSING: RELATIVISTIC QUANTUM CHEMISTRY OF ACTINIDES

Robert J. Harrison, Pacific Northwest National Laboratory

Research Objectives

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

Computational Approach

The work involves determination of the electronic structure of molecules, including relativistic effects necessary for heavy elements. Most calculations are very challenging and well suited to the Cray-T3E. There are five 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 fewer still for systems containing actinides.

Application work: We are studying the speciation of aqueous uranium (VI) carbonates. A detailed understanding of the actinide-carbonate-water system is essential to modeling the fate and transport of actinides in the environment.

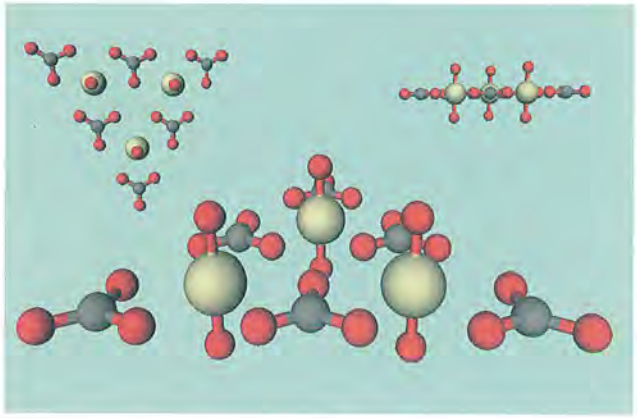
Method and computer program development: Existing programs are being parallelized and extended to enable calculations on larger molecules at higher levels of accuracy.

Computer Science: Extensions of Global Arrays, parallel I/O, new linear algebra, metacomputing, and prototyping of new parallel programming tools.

Collaboration tools: We use Internet video conferencing to augment weekly telephone voice conferences and are evaluating CORE-2000 and other collaboration tools.

Accomplishments

All components of the project are well underway. For benchmark purposes, we have parallelized existing all-electron Dirac-Hartree-Fock and four-component second-order perturbation theory which treat relativistic effects very rigorously. Calculations at these levels of theory can take several hours on 64 nodes of the T3E. These results are being used to validate calculations using relativistic effective core potentials on larger molecules. Determination of the vibrational frequencies of the molecule in the figure took about 30 hours on 256 nodes of the T3E using the NWChem DFT module. The data from calculations on a sequence of related molecules is being correlated with experiment data. A spin-orbit configuration interaction code has also been parallelized and has just commenced production use on the T3E.



DFT/RECP calculations have been performed on this polymeric uranium carbonate, and results agree well with experimental observations.

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 massively parallel computers will provide capabilities for modeling heavy-element compounds similar to those currently available for light-element compounds. The theoretical and computational methodology so developed will supplement current, very expensive experimental studies of the actinides and lanthanides. This will allow limited experimental data to be extrapolated to many other regimes of interest.

The program objectives will be attained through a multi-laboratory, multi-university and multi-disciplinary collaboration. These techniques will be applied to important molecular systems and processes, including the interaction of actinides with: (1) organic complexing agents present in tank wastes; (2) natural aqueous systems (carbonates), in order to better understand fate and transport in the environment; and (3) new materials, such as phosphates and amides, for the design of *in situ* remediation technologies and separation systems.

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

EXTENDING THE SCALE OF MOLECULAR SIMULATIONS

Martin Head-Gordon, David Chandler, and William H. Miller,
Lawrence Berkeley National Laboratory

Research Objectives

Our research focuses on the development of methods to attack the three principal bottlenecks to extending molecular simulations: (1) the timescale bottleneck in molecular simulations, (2) the particle number bottleneck in electronic structure calculations, and (3) the dimensionality bottleneck in quantum reactive scattering.

Computational Approach and Accomplishments

We have developed action functionals for directed paths that connect reactants and products via rare crossings of transition states. With the algorithms for sampling these functionals we have developed over the past year, this is now a practical computational method for obtaining meaningful simulations of reactive processes which occur on timescales far too long for conventional simulations. A range of problems of increasing realism and complexity have been studied, facilitated by use of the NERSC T3E. These include hydrogen bond breaking in liquid water, and the dissociation of NaCl in water.

We have developed improved methods for constructing the effective Hamiltonian in electronic structure theory with effort scaling only linearly with molecule size. This includes exchange interactions, and Coulomb interactions for periodic systems. We have also addressed the related problem of converting an effective Hamiltonian into a density matrix in linear scaling effort, via a novel Chebyshev analysis, which is of both formal and practical value.

Simulation methods based on the direct and correct evaluation of rate constants for chemical reactions have been generalized to approximately include the effect of pressure on a primary chemical reaction of interest. This has been applied to the $O + OH \rightarrow HO_2 \rightarrow O_2 + H$ reaction, which is of central importance in modeling hydrocarbon combustion.

Additionally we have made progress of semiclassical initial value representations as a general way of including quantum effects in molecular simulations without the prohibitive cost of a formally exact treatment. Particularly interesting is the generalization we have made that provides a description also of electronically non-adiabatic processes.

Significance

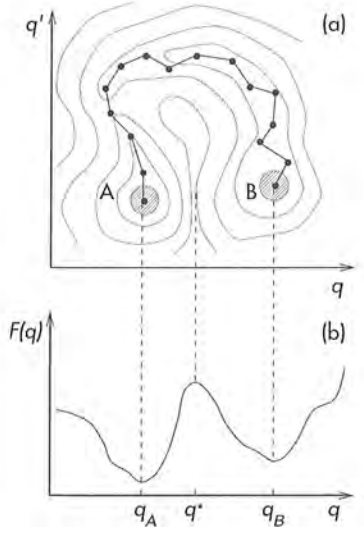
Progress in these areas leads to better possibilities for leveraging new supercomputing capabilities into changes in the scale of simulations that are feasible. For example, consider the particle number bottleneck. A method whose complexity rises as the cube of molecular size means that the availability of a computer eight times faster translates into the ability to study a molecule that is only two times larger. By contrast, a linear scaling method would permit a system eight times larger to be modeled. Similar considerations apply in our other two areas of focus, and illustrate the need for improvements in the algorithms of molecular simulations to go hand in hand with improvements in supercomputing resources.

Publications

Schwegler, E., M. Challacombe, and M. Head-Gordon. 1997. Linear scaling computation of the Fock matrix. II. Rigorous bounds on exchange integrals and incremental Fock build. *Journal of Chemical Physics* 106:9708-9717.

Baer, R., and M. Head-Gordon. 1997. Sparsity of the density matrix in Kohn-Sham density functional theory and an assessment of linear system-size scaling methods. *Phys. Rev. Lett.* 79:3962-3965.

German, T. C., and W. H. Miller. 1997. Quantum mechanical pressure-dependent reaction and recombination rates for O+OH → H+O-2, HO2. *Journal of Physical Chemistry* 101:6358-6367.



(a) Schematic energy landscape with reactant region A and product region B. The chain of beads is a discretized path as used in our path simulation. It reproduces the correct reaction coordinate which depends both on q and on q'.

(b) Schematic free energy along coordinate q. The coordinate q adequately characterizes the stable states near $q=q_A$ and $q=q_B$. The free energy F(q) has a maximum at $q=q^*$. This value of q is far from that associated with the dynamical bottleneck separating the two stable states.

PREDICTION OF PROTEIN TERTIARY STRUCTURE: MODELING ENERGY SURFACES, GLOBAL OPTIMIZATION, AND HIGH PERFORMANCE COMPUTING

Teresa Head-Gordon, Lawrence Berkeley National Laboratory

Research Objectives

To predict protein structure in the size range of 1000-2500 atoms, for which no *ab initio* prediction method can reliably solve. To characterize the energy surface by determining the global minimum and all relevant low-lying minima using sophisticated mathematical optimization techniques.

Computational Approach

For a-helical proteins, we designed an algorithm to (1) predict protein class; (2) make a neural network prediction of 2° structure helix, sheet, and coil for each amino acid; (3) optimize the energy surface; and (4) use stochastic perturbation to find the global optimum in sub-space, where the sub-space is defined as the coil regions predicted by the neural network. We have ported our algorithm to the Cray T3E.

Accomplishments

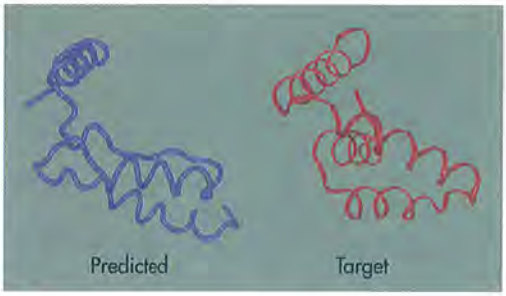
In collaboration with University of Colorado researchers, we are developing a global optimization approach based on sampling, perturbation, smoothing, and biasing that has worked successfully on potential energy surfaces of small homopolymers and peptides. We have developed new techniques that incorporate secondary predictions in order to focus more effectively on tertiary structure by determining the global minimum in a succession of small configuration subspaces.

An equally important consideration is the adequacy of the model energy surface. It is thought that existing gas-phase protein force fields do not discriminate between correct folds and misfolds, since such potentials consider both structures to be energetically comparable. However, correct folds can be distinguished from misfolds by incorporating an additional energy term which describes the stabilizing influence of aqueous solvation.

From simulation and neutron and x-ray scattering, we are extracting simple mean force potentials for the interaction of amino acid sidechains in the presence of water. The enormous reduction in complexity means that we can evaluate the energy of polypeptide chain conformations with the water environment implicitly present, a calculation totally intractable using explicit water models and more accurate than empirical solvent surface area terms. On the J90s and the C90, we are using molecular dynamics to simulate neutron scattering data of single leucine and glutamine dipeptides in solution and are backing out the potential of mean force profiles by combining the simulation and experimental data.

Significance

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



A comparison of the crystal structure of the A-chain of uteroglobin progesterone binding protein and that predicted by a global optimization strategy developed by our group. The current predicted structure was found at the end of three 4-hour runs with 64 processors on the T3E-900, but is not yet converged.

Publications

Pertsemlidis, A., A. M. Saxena, A. K. Soper, T. Head-Gordon, and R. M. Glaeser. 1996. Direct, structural evidence for modified solvent structure within the hydration shell of a hydrophobic amino acid. *Proc. Natl. Acad. Sci.* 93:10769-10774.

Pertsemlidis, A., R. M. Glaeser, and T. Head-Gordon. 1997. Differences in hydration structure near hydrophobic and hydrophilic amino acid side chains. *Biophysical Journal* 73:2106-2115.

Yu, R. C., and T. Head-Gordon. N.d. Improved neural networks for protein secondary structure prediction without use of sequence or structural homologies. *J. Comp. Biol.*, in preparation.

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

MOLECULAR UNDERSTANDING OF MUTAGENICITY

Brian E. Hingerty, Oak Ridge National Laboratory
Suse Broyde, New York University
Dinshaw J. Patel, Memorial Sloan Kettering Cancer Center

Research Objectives

To elucidate why certain DNA base sequences are mutational hotspots when damaged by carcinogenic environmental chemicals.

Computational Approach

Molecular mechanics calculations in combination with data from NMR experiments in the form of distances between hydrogens on the carcinogen-damaged DNA molecule are employed to produce molecular views of the damaged DNA that are in agreement with the data. The computations are carried out with the molecular mechanics program DUPLEX on the Cray C90.

Accomplishments

The aromatic amines are a category of environmental carcinogens present in tobacco smoke, automobile exhaust, dyes and other industrial products, and broiled meats and fish. These substances, when activated biochemically, can bind to DNA and subsequently cause a mutation when the DNA replicates. Such mutations are widely believed to be the initiating event in carcinogenesis by these substances. Often, the target base in the DNA to which the carcinogen binds is guanine (G). Interestingly, it has been found that a carcinogen-bound guanine may be highly mutagenic (a hotspot) or weakly or non-mutagenic, depending on what the neighbor bases are. One example of such a sequence that has been of considerable interest comes from the E. coli bacterium. It is known as the NarI sequence and contains the bases G1-G2-C-G3, where C is the base cytosine. Surprisingly, G3 is a mutational hotspot when bound by certain aromatic amine carcinogens while G1 and G2 are not. The underlying reason for this difference has been a mystery and is of great importance because it is a paradigm for mutational hotspots, such as in the p53 gene, which are found mutated in many human tumors.

We have elucidated the structure of a DNA duplex containing the NarI sequence linked at G1, G2, or G3 with a model aromatic amine carcinogen known as 2-aminofluorene (AF), using a combination of high-resolution NMR solution studies and molecular mechanics computations. These studies have revealed a striking difference in structure when the carcinogen damage is at G3, compared to G1 or G2. When the AF is at G1 or G2, it resides preponderantly in the major groove of an unperturbed B-DNA double helix. However, when the AF is at G3, it resides half the time in a position where it is inserted into the helix, causing the damaged guanine to be displaced from its normal helix-inserted position. It is plausible that this structural distortion, if also present during DNA replication in the cell, could be responsible for the failure of the DNA to replicate normally when the hotspot is damaged, leading to the mutatagenic consequence.

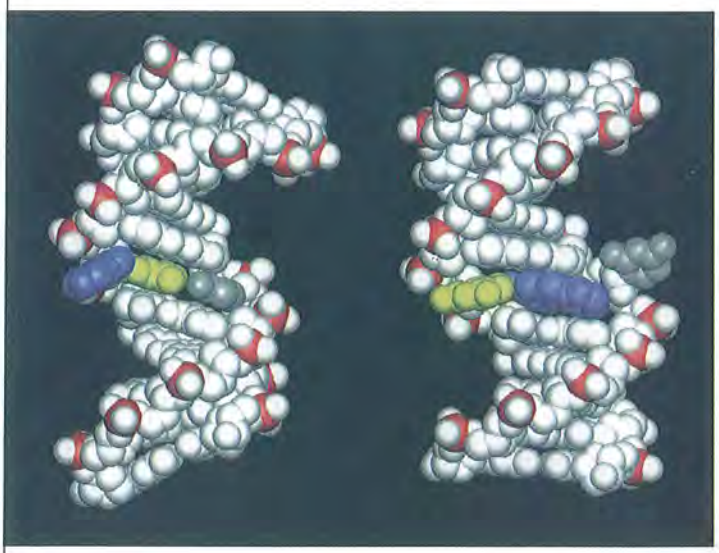
Significance

This work is the first delineation of structural distinctions between mutagenic hotspots and coldspots, revealing how subtle differences in base sequence can produce remarkable differences in structure that can explain the hotspot phenomenon.

Publications

Mao, B., Z. Gu, B. E. Hingerty, S. Broyde, and D. J. Patel. N. d. Solution structure of the aminofluorene [AF]-intercalated conformer of the syn [AF]-C8-dG adduct opposite dC in a DNA duplex. *Biochemistry*, in press.

Mao, B., Z. Gu, B. E. Hingerty, S. Broyde, and D. J. Patel. N. d. Solution structure of the aminofluorene [AF]-external conformer of the anti [AF]-C8-dG adduct opposite dC in a DNA duplex. *Biochemistry*, in press.



Structures of DNA damaged by the carcinogenic aromatic amine 2-aminofluorene (AF). Left: AF in the B-DNA major groove, the predominant structure at a mutational coldspot. Right: AF inserted into the helix with displacement of the damaged guanine, the predominant structure at a mutational hotspot. Color code: AF: blue; AF-damaged guanine: yellow; cytosine partner to damaged guanine: gray.

AB INITIO RELATIVISTIC DIRAC-FOCK SELF-CONSISTENT FIELD CALCULATIONS FOR COMPOUNDS OF THE TRANSLAWRENCIUM ELEMENTS

Darleane Hoffman, Lawrence Berkeley National Laboratory
G. L. Malli, Simon Fraser University

Research Objectives

Our goal is to investigate the effects of relativity in atomic and molecular structure, physical and chemical properties, bonding, volatility dissociation energy, and covalency for the superheavy translawrencium elements and their lighter homologs.

Computational Approach

We used our relativistic self-consistent field (SCF) formalism for molecules, with our universal Gaussian basis sets, using the MOLFDIR code assuming a finite Gaussian nuclear model to perform *ab initio* all-electron fully relativistic Dirac-Fock (DF) and nonrelativistic Hartree-Fock (NR HF) SCF calculations for a large number of molecules of the translawrencium elements. We used the Cray C-90 at NERSC for the evaluation of billions of matrix elements. We performed matrix diagonalization for the SCF part of our DF calculations.

Accomplishments

1. We optimized the bond distance for tetrachlorides of rutherfordium and its lighter homologs, assuming tetrahedral geometry, by performing calculations at four bond distances and by fitting the results to a polynomial.

2. We optimized the bond distances in hexachlorides of seaborgium, tungsten, and molybdenum, assuming octahedral geometry, and we predict that $SgCl_6$ is the most stable of the hexachlorides of the group 6 elements.

3. We performed the first all-electron fully relativistic DF as well as NR HF SCF calculations on seaborgium hexabromide $SgBr_6$, which has 316 electrons, assuming octahedral geometry. We optimized the bond distance by performing NR HF SCF calculations at four internuclear Sg-Br separations and fitting the results to a polynomial.

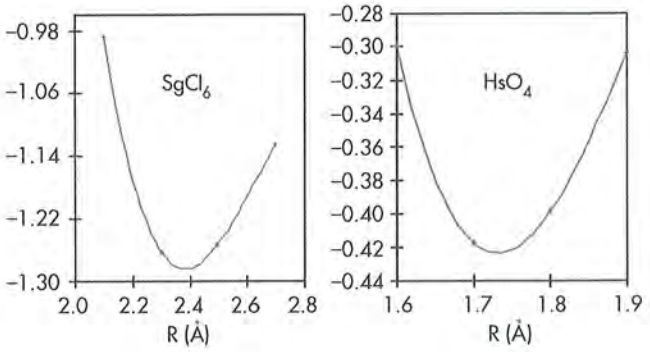
4. We performed calculations for pentachlorides of hahnium, tantium, and niobium, assuming a trigonal bipyramidal geometry.

5. We performed *ab initio* DF SCF calculations on hassium tetroxide HsO_4.

6. We performed the first *ab initio* all-electron DF and HF SCF calculations for a number of molecular systems of E112.

Significance

We have investigated the relativistic effects for systems involving superheavy elements and developed a groundwork for inclusion of the next most significant effects due to electron correlation, starting from our DF SCF calculations. Electron correlation effects are very significant for such systems with hundreds of electrons, and cannot be neglected in any accurate prediction of the physical and chemical properties of these systems.



Left: Dirac-Fock total energies for octahedral $SgCl_6$ at various Sg-Cl bond distances.

Right: Total Dirac-Fock energy of Hassium tetroxide (Td) at various Hs-O distances.

Publications

Malli, G. L. 1997. *Ab initio* relativistic quantum chemistry of superheavy transactinide elements: rutherfordium through eka-astatine. *Proceedings of the Welch Foundation Conference on Chemical Research XXXXI: The Transactinide Elements*, Houston, Texas, October 27-28.

Malli, G. L. 1997. *Ab initio* all-electron fully relativistic Dirac-Fock-Breit calculations for the compounds of the heaviest elements: the transactinides rutherfordium through eka-astatine (Z=117). Invited talk, Fourth Workshop on the Physics and Chemistry of the Heaviest Elements, Stenungsund, Goteborg, Sweden, June 5-9.

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http://www.sfu.ca/chemistry/faculty/malli.htm
http://csa5.lbl.gov/~gamma/

ITER DESIGN BASIS PLASMA DISRUPTION SIMULATIONS

S. C. Jardin, Princeton Plasma Physics Laboratory
R. O. Sayer, Oak Ridge National Laboratory

Research Objectives

The International Thermonuclear Experimental Reactor (ITER) is to be a multi-billion-dollar tokamak that will produce on the order of 1 billion watts of fusion power in a quasi-continuous mode of operation. The U.S. is one of four partners in the design of this experiment (together with Japan, Europe, and Russia). This tokamak is being designed to operate with over 20 million amperes of electrical current in the plasma ring. In the unlikely event that ITER suffers a disruptive instability, most of this current will be transferred to the steel vacuum vessel that surrounds the plasma. We are attempting to calculate how that current will be distributed in the structure so that the electromagnetic forces can be calculated and the vessel can be designed with the appropriate safety margin. During the disruption, current will be transferred by both inductive and conductive processes.

Computational Approach

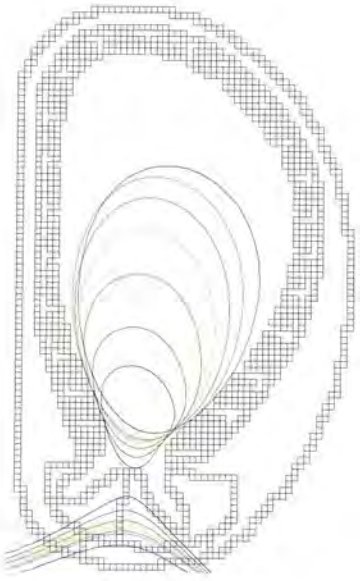
The Tokamak Simulation Code (TSC) solves the appropriate axisymmetric resistive magnetohydrodynamic (MHD) equations in a domain that includes a plasma region, a surrounding plasma halo region, a vacuum region, and solid conductors. We used many techniques to overcome the severe time scale disparity in MHD, particularly between wave phenomena and diffusion time scales, and between diffusion parallel and perpendicular to the magnetic field. The potential functions describing the electromagnetic field that are advanced in time are those that are continuous across regions, allowing accurate computation of current transfer from plasma to solid conductor. To develop and calibrate the TSC disruption model, we used many comparisons with TSC results of simulations of existing experiments. The TSC code is well suited to vector computers such as the NERSC C90 and J90.

Accomplishments

A detailed TSC filamentary structural model was built, and seven TSC worst-case disruption scenarios were developed for the present ITER design. TSC time history files have been made available to the project engineers for stress analyses. These files contain details of the toroidal plasma current distribution, toroidal and poloidal structure currents, and plasma-wall poloidal currents at different points in time during the disruption. Each calculation has slightly different initial conditions, and each leads to different stress patterns for the forces and pressures on the ITER structural components. In each of these seven cases, for example, the net vertical force evolution differs significantly for the different structural components.

Significance

Plasma-disruption-induced electromagnetic effects drive the design of ITER structures. Poloidal halo currents flowing between the first wall and plasma, observed on several operating tokamaks, can prove very destructive. The TSC numerical model provides the most realistic method of scaling existing experimental observations to a machine which is an order of magnitude larger in most parameters.



Outlines of the plasma-vacuum interface (last closed flux surface) during a plasma disruption. Several million amperes of current are transferred to the structure, producing forces that must be designed for.

PARTICLE PHYSICS PHENOMENOLOGY FROM LATTICE QCD

Gregory Kilcup, Ohio State University
Rajan Gupta, Los Alamos National Laboratory
Stephen Sharpe, University of Washington

Research Objectives

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

Computational Approach

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

Accomplishments

Using several ensembles of lattices with varying lattice spacing, we were able to do a definitive continuum extrapolation for one weak interaction quantity, B_K, which gives the rate at which kaons turns themselves into anti-kaons. In a similar vein, we began the calculation of several quantities (prosaically known as B_1 through B_8), which enter into the decay rate of kaons into pions. Further calculations are required to determine their final values. Along the way we found the first evidence from a lattice calculation for the famous "delta I= 1/2" rule in kaon decays, a longstanding and puzzling phenomenon in weak interactions.

Significance

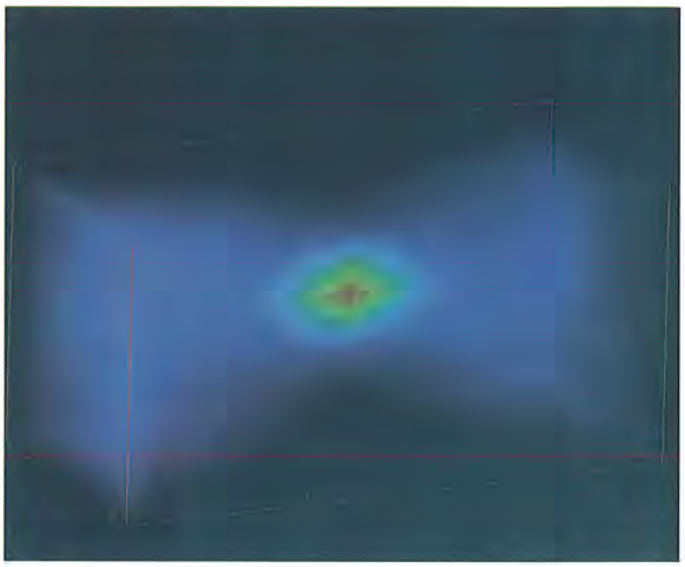
Together with results from particle physics experiments currently under way at labs in the U.S. and Europe, these calculations allow direct and detailed tests of the so-called Standard Model of particle physics. At a minimum they will help determine some of the fundamental constants of nature. Eventually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

Publications

Kilcup, G., R. Gupta, and S. Sharpe. 1997. Staggered fermion matrix elements using smeared operators. E-print hep-lat/ 9707006. *Physical Review D*, in press.

Pekurovsky, D. and G. Kilcup. Weak Matrix Elements: On the way to the delta I=1/2 rule and epsilon-prime/epsilon with staggered fermions. 1997. E-print hep-lat/9709146. *Nuclear Physics B (Proc Supp)*, in press.

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



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

QUANTUM AND CLASSICAL SIMULATIONS OF CLUSTERS, NANOSTRUCTURAL MANIPULATIONS, AND NANOTRIBOLOGY

Uzi Landman, Georgia Institute of Technology

Research Objectives

To investigate, through the development of large-scale classical and quantum simulation methodologies, the size-dependent evolution of materials properties; atomic-scale formation mechanisms of interfacial nanojunctions and wires and their structural, mechanical, dynamic, electronic, and transport characteristics; nanocrystalline assemblies; and the atomistic origins of nanotribological and thin-film lubrication phenomena.

Computational Approach

Large-scale classical and quantum molecular dynamics (MD) simulations (where the phase-space trajectories of a large number of interacting particles are generated via solution of the appropriate equations of motion) are used to explore materials physical and chemical processes on refined spatial and temporal scales. These simulations include: (1) first-principles quantum MD simulations involving concurrent calculations of many-particle potential energy surfaces using density functional theory in conjunction with nonlocal pseudopotentials and plane-wave basis sets, used in studies of size-evolutionary physical and chemical patterns in clusters, nanocrystals and their assemblies, and atomic, electronic, mechanical, and transport properties of metal and semiconductor nanowires; and (2) grand-canonical ensemble classical MD simulations of confined molecular liquid systems, with up to a million atoms interacting through tested many-atom potentials, used in investigations of nanotribology and thin-film rheology and lubrication.

A selected atomic configuration of a sodium nanowire obtained via first-principles molecular dynamics. Atoms are shown as spheres. Superimposed are two isosurfaces depicting a wavefunction near the Fermi level which contributes to the electronic conductance of the nanowire.

Accomplishments

(1) First-principles quantum MD simulations of finite temperature dynamics, atomic and electronic structures, and transport in simple metal nanowires, predicting formation of "magic wire configurations" of enhanced stability and dynamical conductance fluctuations. (2) Elucidation of the energetic and entropic origins of solvation forces, rheological transitions, and structural and phase transformations in equilibrium and sheared interfacial films, and their dependencies on molecular shape, size, and structural complexity, as well as on interfacial morphology.

Significance

The development of large-scale atomistic simulation methodologies, coupled with high-performance computational platforms, allows explorations, with predictive capabilities, of the origins of physical and chemical processes in complex materials and under extreme conditions. Investigations of size-dependent evolution of material properties in clusters, atomic and electronic structures and dynamics in nanowires and nanocrystalline assemblies, and energetics, structure, rheology, and dynamics of highly confined complex fluids yield deep insights into the nature of these systems. These investigations allow interpretation of experiments, predict novel phenomena, guide laboratory synthesis and probing of novel materials systems, and address issues pertaining to future technologies, particularly in the areas of atomic-scale materials manipulations for device, sensor, and machine miniaturization, and tribology in ultra-high-density information storage systems.

Publications

Barnett, R. N., and U. Landman. 1997. Cluster-derived structures and conductance fluctuations in nanowires. *Nature* 387:788.

Gao, J., W. D. Luedtke, U. Landman. 1997. Layering transitions and dynamics of confined liquid films. *Phys. Rev. Lett.* 79:705. *J.Phys.Chem. B* 101:4013.

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ION TEMPERATURE GRADIENT-DRIVEN TURBULENCE CALCULATIONS

Jean-Noel G. Leboeuf, Vickie E. Lynch, and Ben Carreras,
Oak Ridge National Laboratory
J. Diego Alvarez and Luis Garcia,
Universidad Carlos III, Madrid, Spain

Research Objectives

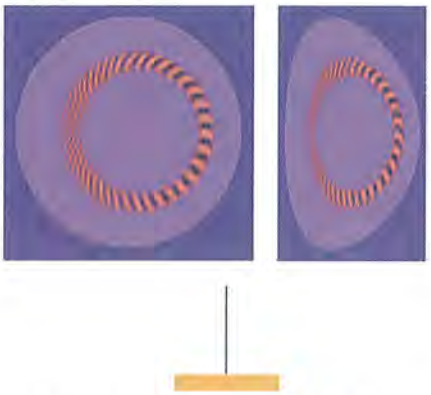
Modeling of ion temperature gradient-driven turbulence as a cause of anomalous plasma transport in magnetic fusion devices is at the core of the Numerical Tokamak Turbulence Project (NTTP), one of the Department of Energy's Phase II Grand Challenges. The model developed at Oak Ridge National Laboratory is a full-torus gyrofluid model for this type of tokamak turbulence, covering the entire plasma cross section. This model is complementary to global gyrokinetic models and local flux tube gyrofluid and gyrokinetic models currently in use within the NTTP to understand and control plasma turbulence and transport in tokamak fusion devices.

Computational Approach

The three-dimensional toroidal gyrofluid model under development solves a set of fluid equations, augmented by a closure describing linear wave-particle resonances leading to Landau damping over the whole plasma cross section. The linear terms are treated implicitly in time, while the nonlinear terms give rise to convolutions which are treated explicitly in time. Finite differences are used in the radial direction, while Fourier mode expansion is used in the angles covering the long way around the torus (toroidal direction) and the short way around the torus (poloidal direction). This model has been implemented in parallel on the vector parallel machines at NERSC and on the massively parallel Cray T3E. Message passing for the T3E version was implemented using PVM (Parallel Virtual Machine). Both linear and nonlinear calculations have been performed on these machines.

Accomplishments

Appropriate gyrofluid equations for describing ion temperature gradient turbulence over the full plasma cross section have been derived and implemented in both cylindrical and toroidal geometry. This model of core plasma transport in tokamak fusion devices has been parallelized for the Cray T3E using message passing and PVM. Large-scale nonlinear calculations performed on the T3E show that the turbulence in steady-state is dominated by short-scale structures on the order of a few plasma Larmor radii, much smaller than the full plasma cross section. Extensive linear tests have been performed in toroidal geometry in anticipation of large-scale nonlinear calculations. These studies are part of the fusion community-wide Cyclone Team's effort at benchmarking the various approaches to modeling ion temperature gradient-driven turbulence pursued to date.



A typical linear toroidal eigenmode for circular and D-shaped tokamak plasmas.

Significance

This work contributes to the fundamental understanding of anomalous transport in magnetic plasma fusion devices. Control of anomalous transport is one of the key issues for present and future fusion reactors to become efficient energy-producing devices.

Publications

Lynch, V. E., J.-N. Leboeuf, B. A. Carreras, J. D. Alvarez, and L. Garcia. 1997. Plasma turbulence calculations on the Cray T3E. SC '97, San Jose, California, November 15-21. http://www.supercomp.org/sc97/proceedings/TECH/LYNCH/INDEX.HTM

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

NUCLEON STRUCTURE FROM LATTICE QUANTUM CHROMODYNAMICS CALCULATIONS

Keh-Fei Liu, Shao-Jing Dong, and Terrence Draper,
University of Kentucky

Research Objectives

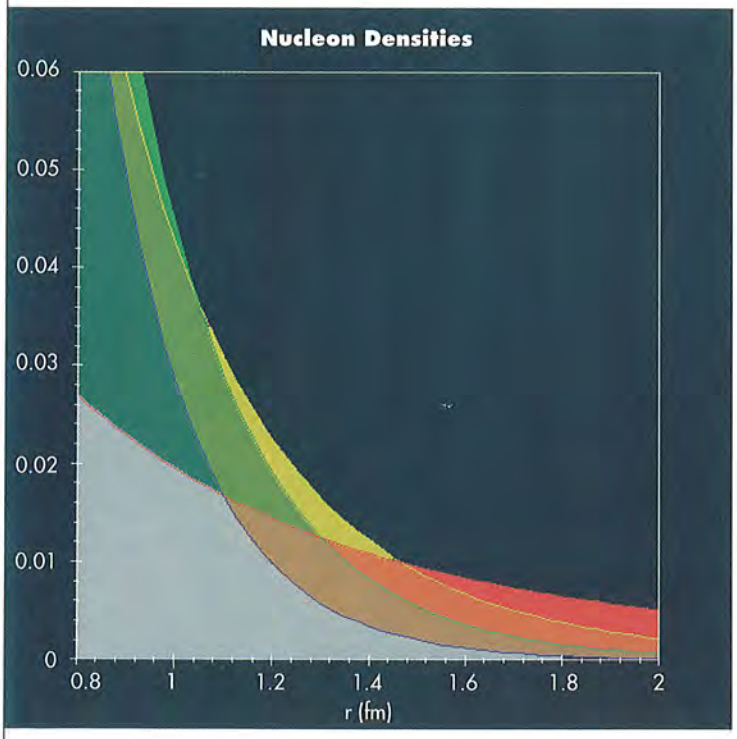
To determine the structure of the proton and neutron from the first-principle calculation of the fundamental strong interaction theory—quantum chromodynamics of quarks and gluons.

Computational Approach

The gauge field configurations are generated with the Monte Carlo algorithm, and the quark matrices are inverted with the conjugate gradient algorithm. Recently, we have developed a Padé-Z_2 method to estimate the fermion determinants with high precision. We employ this method in hybrid Monte Carlo updating for the gauge configurations. Our production program is parallelized on the T3E, and the data analysis is done on the C90.

Accomplishments

We have calculated various form factors of the nucleon. They include the electromagnetic, axial, pseudoscalar, scalar, and tensor form factors. From these form factors, one can deduce the shapes of the densities associated with the probing currents. As shown in the figure, the longest-range density (plotted in red) is the pseudoscalar density, which depicts the pion cloud distribution in the nucleon. The next one, plotted in yellow, is the scalar $\bar{s}$ s density, which depicts the $\bar{k}$ k meson cloud. The green one is the density of the electric charge in the proton, which reflects the vector meson cloud. Finally, the blue one is the axial-vector density, which shows the a_1 meson cloud distribution.



Probing current densities deduced from form factors of the nucleon.

Significance

These *ab initio* calculations from the fundamental theory of the strong interaction have revealed nucleon structures which were not achievable using the model approach. In fact, the calculation on the flavor-singlet axial coupling constant has resolved the "proton spin crisis" and made it in agreement with the high-energy experiment. Similarly, our calculation on the scalar density and the strangeness content in the nucleon has reconciled a long-standing puzzle associated with the pion nucleon sigma term. Future calculation of the orbital angular momentum and the gluon spin will predict how much the proton spin is divided in its components.

Publications

Dong, S. J., J.-F. Lagaë, and K.-F. Liu. 1995. *Phys. Rev. Lett.* 75:2096.

Dong, S. J., J.-F. Lagaë, and K.-F. Liu. 1996. *Phys. Rev. D* 54:5496.

Thron, C., S. J. Dong, K. F. Liu, and H. P. Ying. N.d. *Phys. Rev. D*, in press.

http://www.pa.uky.edu/~fu/liu/group.html

COMPUTATION OF MATERIALS PROPERTIES FROM FIRST PRINCIPLES

Steven G. Louie and Marvin L. Cohen,
University of California, Berkeley, and
Lawrence Berkeley National Laboratory

Research Objectives

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

Computational Techniques

Materials properties are computed using the density functional formalism by solving a set of self-consistent Schrodinger-like equations. Computations involve extensive determination and manipulation of the eigenvalues and eigenvectors of large matrices with dimensions up to several hundred thousand on the Cray C90 and T3E.

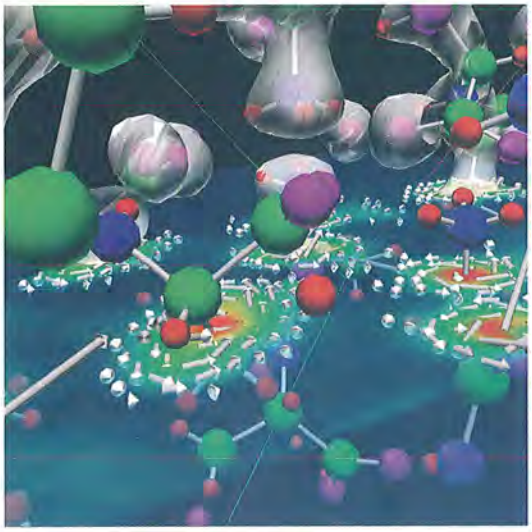
Accomplishments

First-principles calculations have been performed on a number of materials systems. A new theory was formulated and implemented, allowing the *ab initio* calculation of nuclear magnetic resonance (NMR) chemical shifts in solids and liquids for the very first time. Calculations on clusters explained the properties of nanocrystals and fullerene materials. Studies have been performed to predict the properties of materials under pressure.

Significance

NMR is a valuable tool in chemistry and physics. By measuring the screening of an applied magnetic field, NMR experiments help elucidate the structure of materials. Atoms with a different chemical environment screen an applied magnetic field differently, resulting in a "chemical shift." Previously, there was no rigorous theory for first-principles calculation of the chemical shifts in solids and liquids. Our development of a new method allows us to predict and understand the NMR chemical shifts of extended systems such as crystals, amorphous materials, liquids, or defects in solids. Our calculations resolved several important issues related to the nature of the NMR spectra of chemical-vapor-deposited (CVD) diamond and amorphous carbon. With this method, we are now investigating amino acid and peptide crystals, systems of importance in biology.

In a joint experimental and theoretical effort, we investigated what geochemists refer to as the "missing xenon" problem. The amount of Xe on earth is known to be significantly lower than in meteorites and the sun. A leading explanation has been that the earth's iron core might store the primordial Xe, owing to its high pressure and temperature. We showed that Xe has no tendency to react with Fe, even at pressures exceeding a million atmospheres. With this new result, geochemists and geophysicists now have to seek another explanation for the mystery of the missing xenon.



A look into an alanine crystal: carbon (green), hydrogen (red), oxygen (purple), and nitrogen (blue). The arrows show how the electrons flow when a magnetic field is applied perpendicular to the cutting plane.

Publications

Caldwell, W. A., J. H. Nguyen, B. G. Pfrommer, F. Mauri, S. G. Louie, and R. Jeanloz. 1997. Structure, bonding, and geochemistry of xenon at high pressures. *Science* 277:930.

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Mauri, F., B. G. Prommer, and S. G. Louie. 1997. *Ab initio* NMR chemical shift of diamond, chemical-vapor-deposited diamond, and amorphous carbon. *Phys. Rev. Lett.* 79:2340.

http://tiger.berkeley.edu/research/

EFFICIENT DATA ACCESS FOR HIGH-ENERGY AND NUCLEAR PHYSICS EXPERIMENTS

D. Olson, A. Shoshani, W. Johnston, and F. Wang,
Lawrence Berkeley National Laboratory
B. Gibbard, Brookhaven National Laboratory
D. Malon, Argonne National Laboratory

Research Objectives

The purpose of this project is to develop techniques and tools that will enable efficient access to the massive datasets of modern high-energy and nuclear physics (HENP) experiments, particularly for experiments at the Relativistic Heavy Ion Collider (RHIC) beginning in late 1999, in their search for the quark-gluon plasma (QGP). Access to these 100+ terabyte datasets by hundreds of scientists, in conjunction with carrying out the large-scale computations necessary to refine and reduce them to the essential physical properties buried within, is one of the forefront problems of high-performance computing today.

Computational Approach

The principal approach to this problem is to cast it in the form of an extremely large hierarchical collection of objects (some persistent and some transient) that experience has shown is very well matched to this event-based experimental data. Modern object-database technology allows us to address the issue of physical storage layout separately from the logical relationships between the objects. The primary issue for physical storage is to organize the data so that it is stored according to how it is accessed rather than by how it is generated. The NERSC T3E is used to simulate the relativistic heavy ion collisions that will occur at RHIC and produce a dataset with these characteristics for which expected access patterns can be studied. The newly installed HPSS system at NERSC enables us to address issues related to effectively coupling the required amount of high-performance computing cycles to these massive object databases.

Accomplishments

The NERSC T3E was used to calculate theoretical predictions of what may occur in the relativistic nuclear matter collisions at RHIC. These collisions will produce matter under conditions that have never before been produced in a laboratory. A method being employed to address the uncertainties is to calculate this matter under various initial conditions and then propagate it in time and space in order to see the effects in the detector data. The accompanying figure, an example of such a calculation performed on the T3E, shows the energy density within the nuclear matter for a time range spanning the duration of the collision.

Significance

The direct significance of this work is to enhance the capabilities of large-scale high-energy and nuclear physics experiments to achieve their full scientific potential in exploring new regions of the physical world.

Publications

Johnston, W. E., et al. 1997. High-speed distributed data handling for on-line instrumentation systems. *Proceedings of ACM/IEEE SC97: High Performance Networking and Computing.*

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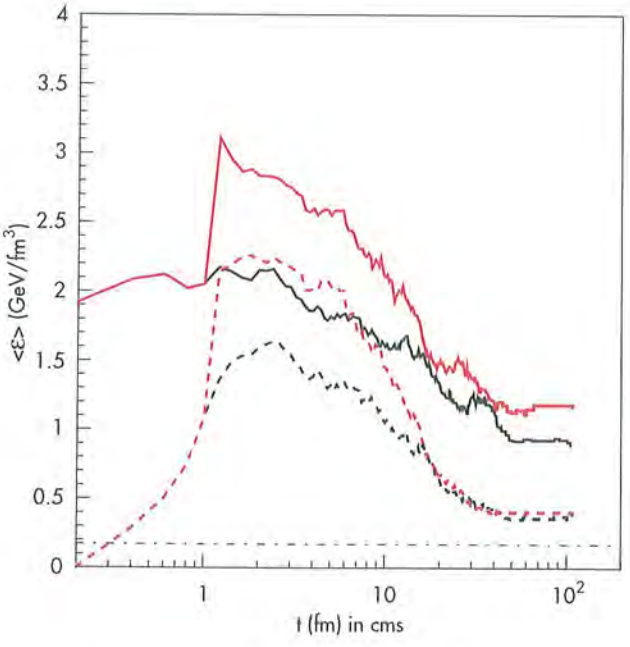


Energy density within nuclear matter for time range spanning duration of collision.

ANALYZING CLIMATE VARIABILITY WITH ENSEMBLES OF SIMULATIONS

Gerald Potter and Michael Wehner,
Lawrence Livermore National Laboratory

Research Objectives

It has long been known that the chaotic nature of the atmosphere causes the detailed long-term prediction of weather events to be impossible. However, climate—the average of weather—may be simulated by performing long-term integrations of weather and averaging the results. Using this technique, the details of the instantaneous simulated weather are not actually realized in the true climate system. However, given a realistic-enough model, the simulated events are realizable as possible states of the true system. By averaging over a long-enough period, simulated climate statistics may be generated that may be legitimately compared with observations of the true climate system.

Computational Approach

Recent advances in high-performance computing have revealed that the model average climate statistics also possess a degree of variability. This is borne out by several investigators who have performed ensembles of climate simulations where each realization differs only slightly in the initial conditions. Not surprisingly, the degree of predictability depends on the field in question, the length of the temporal averaging, the geographic location, and the season of the year.

Our principal tool for simulating the climate is the LLNL parallel atmospheric general circulation model (AGCM). This finite-difference model of the global atmosphere, based on the UCLA model, is parallelized using straightforward two-dimensional domain decomposition techniques. The code is highly portable across all leading distributed memory parallel computing architectures. Our best performance to date has been achieved on the 512-processor NERSC T3E.

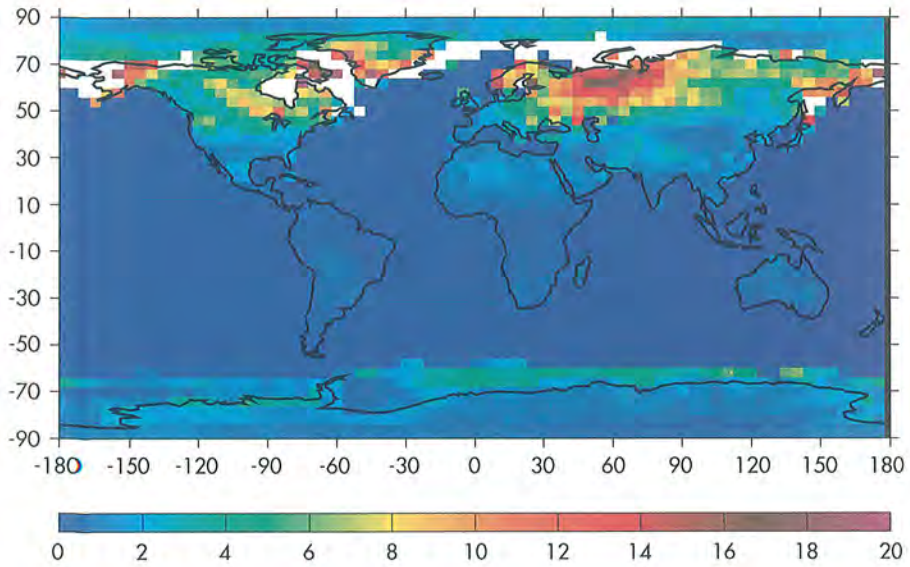
Accomplishments

We have previously completed an ensemble of 20 atmospheric simulations of the decade 1979-1988. Using standard statistical techniques, we related the variability of the model output and the tolerance and statistical certainty required on this output to calculate the required minimum ensemble size. The accompanying figure shows the number of realizations required to calculate the decadal averaged seasonal surface temperature to within 0.5 degrees Kelvin at 95% statistical certainty. As seen in this image, this ensemble size is relatively large despite a high degree of averaging. For shorter averaging periods, such as only a single season, the required size is significantly larger.

Significance

The implication for climate change prediction is serious. Long-term climate simulations tax the capabilities of even the most powerful computers. It is desirable that the resolution of global models substantially increases from that currently used in order to better simulate regional features. Comprehensive climate models also must include processes other than atmospheric circulation, such as ocean circulation, sea ice processes, biological processes, and atmospheric chemistry. These model improvements further increase the demand for computer resources. Our work now implies that single calculations are not sufficient to access certain aspects of the simulated climate, further increasing the computational burden.

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



The number of atmospheric general circulation model calculations required to compute the decadal averaged seasonal surface temperature to within 0.5° Kelvin at 95% statistical certainty.

COMPUTATIONAL ACCELERATOR PHYSICS: ADVANCED MODELING FOR NEXT-GENERATION ACCELERATOR APPLICATIONS

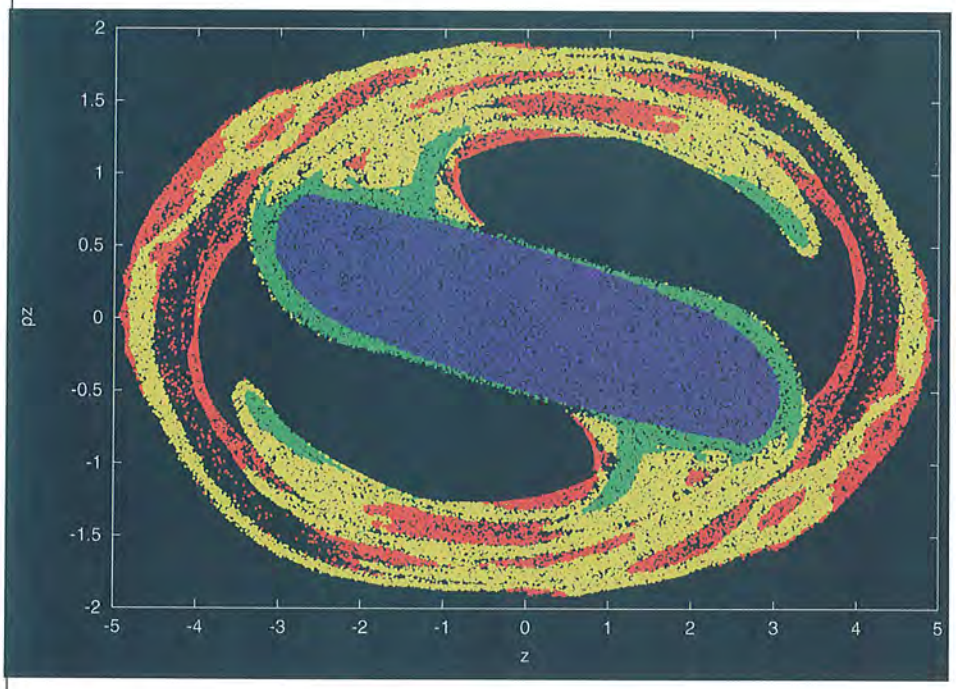
Robert D. Ryne, Los Alamos National Laboratory

Research Objectives

The next generation of particle accelerators will require a major advance in numerical modeling capability, due to extremely stringent beam control and beam loss requirements and the presence of highly complex three-dimensional accelerator components. The primary goal of this Grand Challenge is to develop an advanced, parallel modeling capability, based on High Performance Computing and Communications resources and state-of-the-art numerical methods and algorithms, that will enable the design, optimization, and numerical validation of future accelerators.

Computational Approach

A charged particle beam in a high-intensity accelerator is subject to strong linear and nonlinear, internal and external forces. It requires a careful treatment of both magnetic optical effects and space charge effects. The field of magnetic optics has matured greatly with the development of transfer matrix and Lie methods. Similarly, the simulation of space charge effects in plasmas has also matured with the development of the plasma particle-in-cell (PIC) approach and other methods. Our approach is to combine the best features of high-order magnetic optics simulation techniques with PIC simulation techniques in a framework optimized for parallel computations. To accomplish the fusion of these two separate fields, we are using modern split-operator symplectic integration algorithms. We are also optimizing the space charge algorithm, which is the most time-consuming part of high-current beam dynamics simulations, in order to achieve high performance on parallel platforms.



Longitudinal phase space of a 3D mismatched beam. The density varies by a factor of 10,000 from the core (blue) to the edge of the halo (red). The system being modeled is a spheroidal bunch, initially a stationary solution of the Vlasov/Poisson equations, which develops a halo due to improper matching into the beamline. The simulation used 25 million particles and a 256 x 256 x 256 grid for the Poisson solver. The figure shows the longitudinal phase space (z, pz) after the halo has formed. It contains approximately 100,000 particles color-coded according to density. In the blue region (the core), the density equals 1 at the center and 1/10 at the blue-green boundary. It decreases through the green, yellow, and red regions, and equals 1/10,000 at the edge of the red region. If we had simply plotted the same number of particles chosen randomly from the 25 million in the simulation, the halo would barely be visible and show almost no structure.

Accomplishments

This past year we developed a parallel version of the code LINAC, which is being used to support the Accelerator Production of Tritium (APT) project. This is now the primary code for performing large-scale beam halo simulations for the project. A primary accomplishment was a 5-fold increase in the performance of the space charge algorithm over our initial implementation.

In addition to LINAC, we developed a new code called IMPACT, which is based on split-operator techniques. IMPACT (Integrated-Map and Particle Accelerator Tracking code) has an especially accurate and efficient treatment of radio frequency accelerating gaps, obtained by numerical integration of the gap transfer map rather than integration of single particle trajectories. The code is especially useful for modeling superconducting proton linear accelerators, where there are only a few types of accelerating cavities.

A third code, called HALO, has been developed specifically for beam halo studies. Beam loss is known to be associated with the very low-density distribution of charge far from the beam core (the halo). This is a major issue for future high intensity LINACs, since the particle loss can lead to activation of accelerator components, thereby hindering or preventing hands-on maintenance. HALO, developed in collaboration with the University of Maryland, includes a new three-dimensional beam equilibrium model, which helps isolate beam halo growth mechanisms.

The huge amount of data in a high-resolution beam dynamics simulation, coupled with the fact that we are often interested in a very small fraction of the particles in the halo, necessitates the use of internal data analysis in our codes prior to storing simulation results. We have developed and implemented algorithms on the T3E that drastically reduce the amount of data needed to visualize the halo.

Significance

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

The societal impacts are related to both environmental and national security-related issues. Benefits to the environment are based on the proposed use of accelerators for nuclear waste transmutation and plutonium disposal. Benefits to national defense are based on the use of accelerators for tritium production and Science Based Stockpile Stewardship.

Economic impacts include both energy-related and industrial issues. Accelerator-driven fission energy production schemes have the potential to produce clean, safe energy without critical assemblies and in accord with non-proliferation concerns.

In the area of fundamental science, high-resolution accelerator modeling is crucial to the development of next-generation spallation neutron sources for materials science and biological science research, as well as the design of next-generation accelerators for high energy physics, including linear colliders.

Publications

Gluckstern, R., A. Fedotov, S. Kurennoy, and R. Ryne. N.d. Halos in beam bunches with self-consistent 6-dimensional distributions. *Phys. Rev. Lett.*, submitted.

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

LATTICE MODELS FOR PROTEIN FOLDING KINETICS

Daniel Rokhsar, University of California, Berkeley, and Lawrence Berkeley National Laboratory

Research Objectives

Our goal is the complete characterization of the folding pathways of proteins, which reach their unique folded state from an astronomically large number of possible conformations, and an understanding of their equilibrium phase diagrams.

Computational Approach

We use Monte Carlo and molecular dynamics techniques to directly simulate the equilibrium and kinetic properties of protein-like heteropolymers. These codes utilize the massively parallel processing capabilities of the T3E in two ways. First, our free-energy calculations are parallelized to allow for efficient determinations of the entire phase diagram of the polymer. Second, since each folding event is microscopically different, folding pathways must be characterized statistically; the ability to simulate tens of millions of folding events in parallel is critical to the success of this project.

Accomplishments

By direct evaluation of the free-energy surface of a model protein, we have demonstrated the existence of a third phase of proteins, the "molten globule." The molten globule is a distinct liquid-like state that appears in the phase diagram of proteins separated by first-order phase transitions from the unfolded and folded ("native") states.

For the first time, we have completely and explicitly characterized the folding pathway of a protein-like heteropolymer 48 residues long. Using a novel computational method that relies heavily on the parallel processing capabilities of the T3E, we unambiguously determined the ensemble of transition state conformations that govern the rate-limiting step of folding, and showed that folding proceeds through a molten-globule intermediate.

Significance

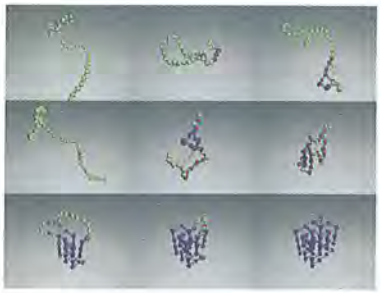
Protein folding is one of the great unsolved problems of modern biophysics. A better understanding of the protein folding problem has potential biological, biomedical, and industrial applications. An understanding of the mechanisms by which proteins naturally achieve their functional folded states can be expected to yield insights into the prediction of these folded structures directly from amino acid sequences, and to permit the design of medically useful proteins. The molten-globule state we have studied is implicated in the mechanisms of folding as well as the aggregation of improperly folded proteins, both of which have medical relevance; for example, the improper aggregation of proteins is responsible for several diseases, including Alzheimer's.

Publications

Pande, V. S., and D. S. Rokhsar. N.d. Is the molten globule a third phase of proteins? *Proceedings of the National Academy of Sciences of the U.S.A.*, in press.

Pande, V. S., A. Y. Grosberg, T. Tanaka, and D. S. Rokhsar. N.d. Protein folding pathways: is a "new view" needed? *Current Opinions in Structural Biology*, in press.

Pande, V. S., and D. S. Rokhsar. N.d. Transition states and intermediates in a lattice model for protein folding. *Nature: Structural Biology*, in preparation.



Monte Carlo simulation of a folding event. Each frame displays the average position of a 48-mer chain during a 10^4 iteration time window. The color of each bead represents the variance of the position of the bead during this time interval, with yellow/green indicating large fluctuations and blue indicating small fluctuations. The entire folding event takes 8 x 10^5 iterations.

SIMULATION OF GREENHOUSE-GAS-INDUCED CLIMATE CHANGE

Michael E. Schlesinger, Natasha Andronova, Eugene Rozanov, Vladimir Zubov, Wanqiu Wang, Ayman Ghanem, Sergey Malyshev, Fanglin Yang, Thomas Reichler, and Mozhi Tang, University of Illinois at Urbana-Champaign

Research Objectives

The objectives of our research are to simulate and understand past, present, and potential future climates and chemical compositions of the atmosphere.

Computational Approach

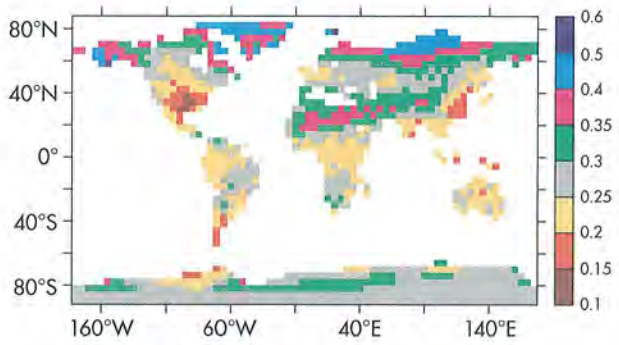
We employ finite-difference methods to solve in space and time the equations governing the large-scale motion of the atmosphere and ocean in spherical coordinates on the rotating earth, with parameterizations for the unresolved subgrid-scale processes. We use the Cray C-90 computer.

Accomplishments

With our atmospheric general circulation/mixed-layer ocean (AGC/MLO) model and our global ice-sheet/asthenosphere model, we simulated the onset of the last glacial climate 115,000 years ago. We used our AGC model to simulate and understand the observed tropical intraseasonal oscillation.

We performed simulations with the AGC/MLO model for the present climate; the equilibrium climate resulting from a doubling of the CO_2 concentration (2 x CO_2); and the equilibrium climates induced by the direct radiative forcing caused by the emission of sulfur dioxide (SO_2) gas, which is converted to sulfate aerosol in the atmosphere. We have performed two simulations for the worldwide emission of SO_2—one for the present emission rate and another for ten times this rate (10 x SO_4)—and seven simulations for regional 10 x SO_4 emissions—one each for Europe, North Africa, Russia, China, North America, and the Southern Hemisphere, and the seventh for all regions other than Europe. Using our simple climate/ocean model, we calculated trajectories of future global-mean surface-air temperature changes for the Intergovernmental Panel on Climate Change (IPCC) business-as-usual scenario and for two scenarios that stabilize the CO_2 concentration at 550 ppmv. We continued to develop and test our stratospheric-tropospheric general circulation/photochemical model and our coupled atmosphere/ocean general circulation model.

We developed a new hybrid numerical scheme for the transport of chemical species. From the observational temperature record, we estimated the climate sensitivity and sulfate-aerosol radiative forcing. We collaboratively developed an adaptive strategy for abating climate change, calculated the expected economic cost of protection or abandonment against sea-level rise in the United States, and calculated country-specific market impacts of climate change.



Geographical distribution of the difference in surface-air temperature between two scenarios that stabilize the CO_2 concentration at 550 ppmv for the year 2087, when the difference between the WRE (Wigley, Richels, Edmonds) and IPCC annual global-mean surface-air temperature changes reaches its maximum for a CO_2-doubling temperature sensitivity of 2.5°C.

Significance

Our studies will facilitate the determination of the economic and ecological impacts of anthropogenic influences on atmospheric composition and climate, thereby facilitating development of rational mitigation and adaptation policies.

Publications

Schlesinger, M. E., and M. Y. Verbitsky. 1996. Simulation of glacial onset with a coupled atmospheric general circulation/mixed-layer ocean-ice-sheet/asthenosphere model. *Palaeoclimates—Data and Modelling* 2:179-201.

Wang, W., and M. E. Schlesinger. N. d. The dependence on convection parameterization of the tropical intraseasonal oscillation simulated by the UIUC 11-layer atmospheric GCM. *J. Climate*, submitted.

Schlesinger, M. E., N. G. Andronova, A. Ghanem, S. Malyshev, E. Rozanov, W. Wang, and F. Yang. N. d. Geographical scenarios of greenhouse-gas and anthropogenic-sulfate-aerosol induced climate changes. In preparation. http://crga.atmos.uiuc.edu/public/CRG_Publications/index.html

http://crga.atmos.uiuc.edu/

SPARSE LINEAR ALGEBRA ALGORITHMS FOR MPPS

Horst D. Simon, Kesheng John Wu, Osni Marques, and Luis Bernardo, Lawrence Berkeley National Laboratory
Bernd Pfrommer, University of California, Berkeley
Hongyuan Zha, Pennsylvania State University

Research Objectives

Our goal is to develop a scalable parallel library to solve large sparse symmetric eigenproblems on distributed memory machines. Our research addresses several crucial issues such as robustness, scalability, and portability.

Computational Approach

A block-shifted and inverted Lanczos algorithm for sparse generalized eigenvalue problems is being implemented. Software components of this algorithm developed elsewhere are being integrated with newly developed software. Although our development platform is the Cray T3E at NERSC, the software will be developed in MPI and ported to other platforms.

Accomplishments

We ported and parallelized the scalar LANSO code by Beresford Parlett to run efficiently on the 512-processor Cray T3E at NERSC. We ported the new PLANSO code to a cluster of SMPs, where we studied the trade-off between shared memory (threads) and distributed memory (MPI) parallelism. We developed a new technique called "thick restart" and found that PLANSO runs consistently faster than competing software called PARPACK.

Scalable approximate inverse preconditioners based on the SPAI (sparse approximate inverse) approach by Barnard, Grote, and Huckle were investigated for their potential to speed up the Lanczos process. In collaboration with Steve Barnard at NASA Ames, the SPAI software was ported and tested successfully on the T3E. We believe this is the first preconditioner that can be scaled to 512 processors.

We investigated a number of applications of the Lanczos algorithm:

1. We applied the algorithm to large text retrieval using latent semantic indexing. In collaboration with the Web search engine Inktomi (HotBot), we used our algorithm to compute the first 5 singular values of a data matrix of 100,000 terms by 2,559,430 documents. To our knowledge this is the first time that the singular value decomposition of such a large matrix has been computed.

2. In collaboration with Don Vasco of the Berkeley Lab Earth Sciences Division, our algorithms were used to solve inverse problems arising in the study of the Earth's interior structure (see figure). The resulting matrices were of the order 1,500,000 by 200,000.

3. With the Cohen-Louie group at UC Berkeley, we considered the application of the new Lanczos algorithm to electronic structure calculations in materials science. In this case the direct application of the Lanczos code proved to be less effective than a conjugate-gradient minimization.

Significance

Scalable sparse linear algebra algorithms can provide efficient solutions to common problems in computational chemistry, physics, earth sciences, materials science, and information retrieval on a previously unknown scale. The software library under development will be easily portable to other platforms and emerging new architectures.

Publications

Pfrommer, B., S. Louie, and H. Simon. 1997. Conjugate gradient based electronic structure calculations on the Cray T3E and SGI PowerChallenge. *Proc. of the 8th SIAM Conference on Parallel Processing*, Minneapolis, March 1997.

Simon, H. D., and H. Zha. 1997. Low rank matrix approximation using the Lanczos bidiagonalization process. LBNL-40767. Submitted to *SIAM J. Scientific Computing*.

Barnard, S. T., L. Bernardo, and H. D. Simon. 1997. An MPI implementation of the SPAI preconditioner on the T3E. LBNL-40794. Submitted to *Int. J. of Supercomputer Applications*.

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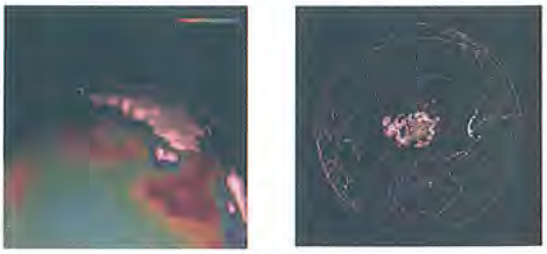


New images of deep geological structures were revealed when innovative algorithms and NERSC's Cray T3E were used to transform seismic data from around the world into models of the three-dimensional seismic structure of the earth's crust, mantle, and core. Velocity variations in the uppermost mantle are correlated with surface tectonics, while variations at greater depths coincide with regions of past and present subduction. (Don Vasco and Osni Marques, Berkeley Lab)

LATTICE QUANTUM CHROMODYNAMICS WITH APPLICATIONS TO THERMODYNAMICS OF HADRONIC MATTER AND PROPERTIES OF HADRONS

D. K. Sinclair, J.-F. Lagae, and G. T. Bodwin,
Argonne National Laboratory
J. B. Kogut, University of Illinois

Research Objectives

Our objectives are to determine the position and nature of the phase transition from hadronic matter to a quark-gluon plasma from lattice quantum chromodynamics (QCD), to determine properties of hadrons from lattice QCD, and to improve lattice QCD methodology.

Computational Approach

QCD is simulated on a discrete space-time lattice (lattice QCD) by formulating it as a molecular dynamics problem and solving its "time" evolution numerically. A stochastic driving term is applied periodically to ensure ergodicity and rapid progress through phase space. The Dirac operator which describes quark propagation is inverted numerically using a conjugate gradient method. These computations have been ported to the T3E using the natural parallelism associated with the lattice and the locality of its interactions.

Accomplishments

We have probed the chiral nature of the QCD phase transition at finite temperature by studying the screening lengths for mesonic excitations in the hadronic matter and plasma phases. This gave evidence that the flavor singlet axial current is not restored at this transition.

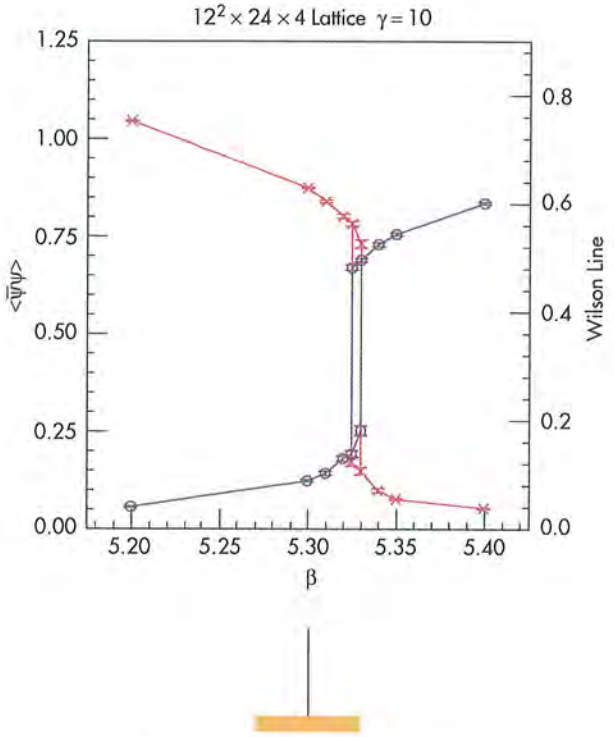
By adding a four-quark interaction to our lattice action, we have been able to study the lattice QCD phase transition for zero quark mass. This will give us direct access to the scaling properties at this transition, and ultimately the equation of state for hadronic matter and the quark-gluon plasma.

We developed a new class of lattice staggered quark actions which have less flavor symmetry breaking due to discretization errors.

Significance

The finite temperature phase transition is expected to be observed in relativistic heavy ion collider experiments. It is also important for the understanding of the early universe.

Improved actions allow the use of coarser lattices, thus reducing the computing requirements for simulations.



Order parameters near the finite temperature phase transition in lattice QCD with explicit 4-fermion couplings.

Publications

Kogut, J. B., J.-F. Lagae, and D. K. Sinclair. 1997. Topology, fermionic zero modes and flavor singlet correlators in finite temperature QCD. E-print hep-lat/9709067 and ANL-HEP-CP-97-4.
http://www-spires.slac.stanford.edu/spires/form/hepspif.html

J.-F. Lagae and D. K. Sinclair. 1997. Improving the staggered quark action to reduce flavour symmetry violations. E-print hep-lat/9709035.
http://www-spires.slac.stanford.edu/spires/form/hepspif.html

J. B. Kogut and D. K. Sinclair. 1997. QCD with chiral four fermion interactions. *Nuclear Physics (Proc. Suppl.)* 53:272.

COSMIC MICROWAVE BACKGROUND RADIATION DATA ANALYSIS

George Smoot and Julian Borrill,
Lawrence Berkeley National Laboratory
Andrew Jaffe, University of California, Berkeley

Research Objectives

To develop the novel computational techniques necessary to extract fundamental cosmological parameters from forthcoming cosmic microwave background (CMB) datasets.

Computational Approach

Central to our task is being able to locate and describe the maximum of the likelihood function of the cosmological parameters, given the data—here an N-pixel map—generated by any one of the forthcoming CMB observations. At present N is at most a few thousand, but this will increase to tens and hundreds of thousands with the MAXIMA and BOOMERANG balloon flights, and to about a million with the MAP and PLANCK satellite missions. Our present approach scales as N-squared in size and N-cubed in time, so a supercomputer like the T3E is essential to our work. However, even the T3E will be unable to handle the largest datasets; we must therefore develop alternative algorithms, either with better scaling properties or able to successively analyze subsets of the overall dataset.

Accomplishments

Our project received funding in September 1997. In the two months since then we have completed the development of the quadratic estimator formalism for performing a rapid search for the maximum of the likelihood function, and have implemented it on the T3E both in serial and in parallel (using the LAPACK and ScaLAPACK libraries respectively). We are currently working to demonstrate the ability of the parallel code to analyze at least the first generation MAXIMA/BOOMERANG data. To this end we are now developing simulated datasets, comprising the signal from a known underlying theory and a model of the instrument noise and sky foregrounds associated with each experiment.

Significance

The Cosmic Microwave Background provides a picture of the universe as it was a mere 100,000 years after the Big Bang. As the earliest possible photon image available to us, it is our most powerful discriminant between different cosmological models. The unprecedentedly detailed CMB datasets obtained in the next 10 years will allow us to determine the fundamental cosmological parameters—in many cases currently known to no better than a factor of 2—to the 1% level.

Publications

Bond, J. R., A. H. Jaffe, and L. Knox. 1997. Estimating the power spectrum of the cosmic microwave background. *Phys. Rev. D*, submitted.
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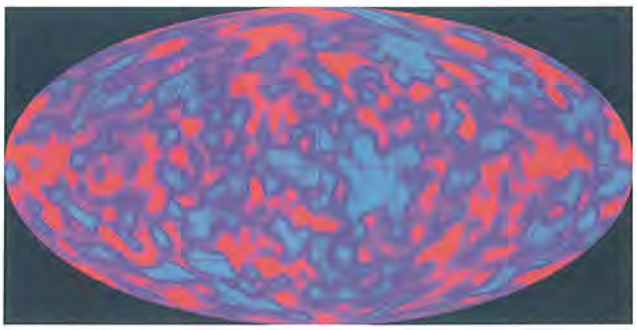
Smoot, G. 1997. The cosmic microwave background anisotropy experiments.
http://xxx.lanl.gov/ps/astro-ph/9705135

http://aether.lbl.gov/
http://cfpa.berkeley.edu/group/cmbanalysis/



Cosmic microwave background fluctuation map.

WEAK MATRIX ELEMENTS WITH DOMAIN WALL QUARKS

Amarjit Soni, Thomas Blum, and Matthew Wingate,
Brookhaven National Laboratory

Research Objectives

We want to set up a comprehensive framework for using lattice gauge methods with "domain wall quarks" (DWQ) for the calculation of weak matrix elements.

Computational Approach

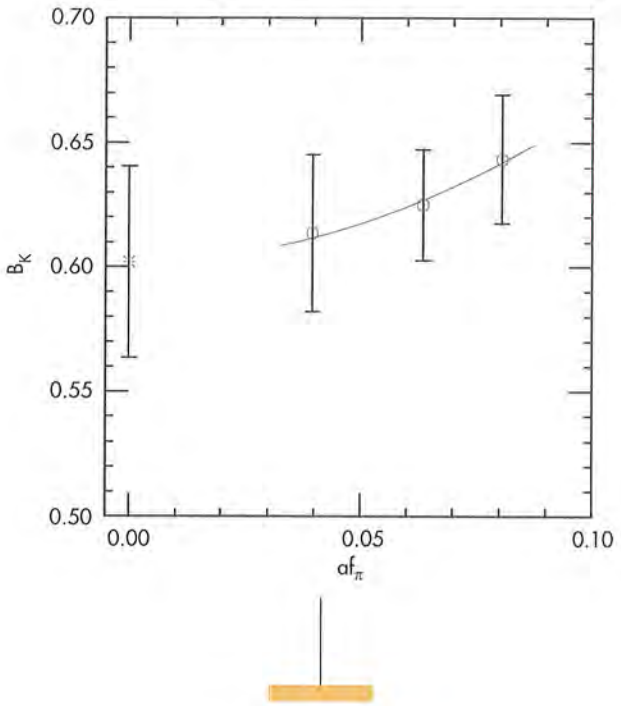
The basic ingredient in the method is a calculation of the quark propagator. The novel element in our method is that it requires introduction of a fictitious fifth dimension. The T3E-600 and T3E-900 at NERSC have been used for these computations.

Accomplishments

We have demonstrated that DWQ start to exhibit the crucial symmetries of the continuum theory (chiral symmetries) with a modest extent in the fifth dimension, i.e., even when the number of lattice sites in the extra dimension is as few as about 10. In the work finished so far, we have obtained a number of key results, including a calculation of the important matrix element B_K. 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

The significance of this work is that it 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 underway. Further progress with DWQ could enable us to test for clues for the new physics that lies beyond the Standard Model.



The kaon B parameter.

Publications

Blum, T., and A. Soni. 1997. QCD with domain wall quarks. *Phys. Rev. D* 56:174.
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http://ojps.aip.org/prlo/top.html

G. Malcolm Stocks, Oak Ridge National Laboratory
Bruce N. Harmon, Ames Laboratory
Michael Weinert, Brookhaven National Laboratory

Research Objectives

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

Computational Approach

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

Accomplishments

This year our codes have been ported to the Cray T3E. All of the codes are specifically designed to take advantage of the massively parallel architecture, and one of our codes (LSMS) achieves the highest Mflops performance of any code currently running on the machine.

The fully relaxed structure of a clean Si(111) surface has been well established. However, the electronic structures of the surface states and phase transitions between the 7x7 and 1x1 phases have not been studied due to the large unit cell needed for the ab initio calculation. The enormous computing power of the Cray T3E has allowed us to attack these problems using *ab initio* plane-wave pseudopotential methods and Car-Parrinello molecular dynamics.

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, remanance) of magnets and microstructure.

Publications

Chetty, N., and M. Weinert. 1997. Stacking faults in magnesium. *Phys. Rev. B* 56:10844-10851.

Faulkner, J. S., Y. Wang, and G. M. Stocks. 1997. Coulomb energies in alloys. *Phys. Rev. B* 55:7492.

M. Alatalo, M. Weinert, and R. E. Watson. N.d. Stability of Zr-Al alloys. *Phys. Rev. B*, in press.

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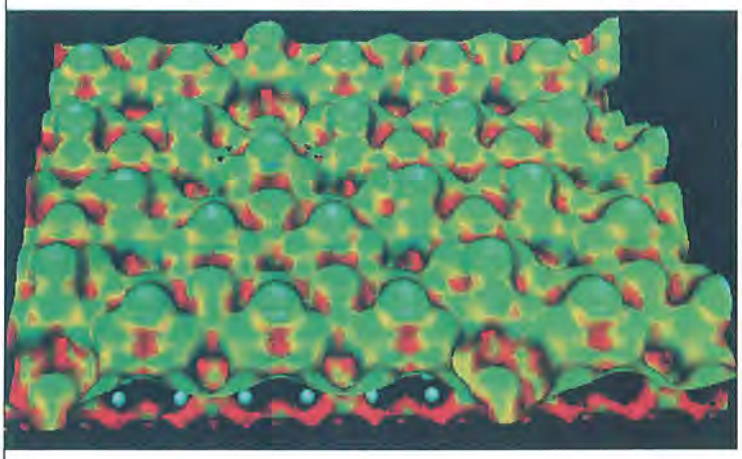


As computer chip designers put more and more components onto a single chip, they need to understand the microscopic electronic structure of the chip surface, which can only be obtained accurately through large-scale quantum simulations on supercomputers. This plot shows the isovalue surface for the total charge density of the DAS(7x7) reconstruction of the Silicon(111) surface. The different colors show the different gradients of the surface. This 498-atom simulation was performed on 128- and 256-processor runs on NERSC's T3E-900. (Zhong-Yi Lu, Dave Turner, Cai-Zhuang Wang, Kai-Ming Ho, Iowa State University/Ames Laboratory; Andrew Canning, NERSC; Malcolm Stocks, Oak Ridge National Laboratory).

Michael R. Strayer, David J. Dean, and
Anthony Mezzacappa, Oak Ridge National Laboratory

Research Objectives

To implement and develop nuclear structure calculations, including modern Monte Carlo techniques, for solving the shell model problem. To solve the core collapse supernova problem. To develop next-generation radiation transport and radiation hydrodynamics codes for computational astrophysics.

Computational Approach

During the past several years, an alternative method for the exact solution of the shell model, based on auxiliary field Monte Carlo techniques, has been developed. The resulting problem becomes one of many-dimensional quadrature, which is carried out by Metropolis sampling. These calculations are compute-intensive and are ideally suited to take advantage of developments in parallel computing (C90/J90/T3E).

Two sets of astrophysics simulations were conducted on the C90 and J90: (1) one-dimensional simulations of core collapse supernovae using a transport code, BOLTZTRAN, that solves the neutrino Boltzmann kinetic equations; and (2) two-dimensional simulations using one-dimensional multigroup flux-limited diffusion neutrino transport and two-dimensional piecewise parabolic method (PPM) hydrodynamics.

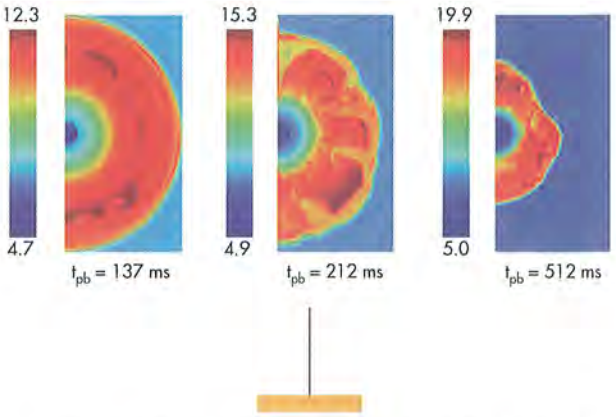
Accomplishments

We began a series of multi-major oscillator shell calculations (the largest ever attempted) to investigate the properties of extremely neutron-rich nuclei. Some of these systems play a role in r-process nucleosynthesis. We have also investigated nuclear transitions that determine the electron capture rates in iron-region nuclei. These nuclei play an important role in the precollapse phase of the supernova.

A detailed comparison was made between Boltzmann neutrino transport and multigroup flux-limited diffusion, focusing on key quantities that are central to the neutrino shock reheating mechanism about which all current supernova modeling revolves. The increased heating is promising and will be fully explored this year.

Significance

The accurate description of nuclear structure remains an important and challenging many-body problem. New experiments are studying nuclei at extreme temperatures, angular momentum, and/or neutron/proton balance; such data will increase dramatically with operation of radioactive beam facilities including the ORNL Holifield facility. These experimental investigations will allow us to explore nuclei that are weakly bound and have large spatial dimension. Clearly a substantial theoretical and numerical effort is required to develop and further our understanding of nuclei far from stability. The theory group at ORNL continues to maintain an active and leading role in this effort.



Two-dimensional entropy plots showing the evolution of neutrino-driven convection beneath the supernova shock wave in our 15 solar mass model, at 137, 212, and 512 ms after core bounce.

Publications

Mezzacappa, A., A. Calder, S. Bruenn, J. Blondin, M. Guidry, M. Strayer, and S. Umar. N. d. An investigation of neutrino-driven convection and the core-collapse supernova mechanism using multigroup neutrino transport. *ApJ*, in press.

Mezzacappa, A., A. Calder, S. Bruenn, J. Blondin, M. Guidry, M. Strayer, and S. Umar. N. d. The interplay between proto-neutron star convection and neutrino transport in core-collapse supernovae. *ApJ*, in press.

Radha, P. B., D. J. Dean, S. E. Koonin, K. Langanke, and P. Vogel. N. d. Gamow-Teller strength distributions in fp-shell nuclei. *Phys. Rev. C*, in press.

http://csep1.phy.ornl.gov/boltz/translate/doe_hpcc_gc/doe_hpcc_gc.html
http://csep2.phy.ornl.gov/theory_group/people/dean/nersc/dean.html
http://csep2.phy.ornl.gov/theory_group/people/mezz/mezz.html

THE ORDER OF THE HIGH-TEMPERATURE QUANTUM CHROMODYNAMICS PHASE TRANSITION

Doug Toussaint, University of Arizona

Research Objectives

Theory predicts that at temperatures of order 150 MeV there will be a phase transition in which protons and neutrons effectively "melt" into their constituents. Temperatures this high probably occurred in the very early universe and will be created in collisions of heavy ions at the Relativistic Heavy Ion Collider (RHIC) under construction at Brookhaven National Laboratory. This transition is expected to be a second-order transition in the same universality class as the O4 spin model. However, recent studies by the Japanese Lattice QCD (JLQCD), Bielefeld, and MIMD Lattice Computation (MILC) collaborations have failed to find the expected O4 scaling behavior. This leaves open the question of the order of the phase transition—perhaps it is really a first-order transition at small-enough quark masses. Our research objective is to check this possibility to a higher accuracy than previous tests.

Computational Approach

We use the standard "refreshed molecular dynamics" method to generate sample configurations for the QCD gluon fields at high temperature. Thermodynamic quantities such as the order parameter and free energy are monitored as a function of a fictitious "simulation time". Although this simulation time is not the same as real time, behavior of the system as a function of simulation time can be used as an indicator of the type of transition. The code is the MILC collaboration's QCD code, which runs on a variety of multiple-instruction, multiple data (MIMD) machines, in this case on the NERSC T3E.

Accomplishments

We have run Monte Carlo simulations of the system on a larger spatial volume (L=24) than previous tests, using starting configurations in the hot and cold phase. This is a standard technique for testing for first-order transitions. If the transition is first order, and you have adjusted the temperature near enough to the phase transition, large systems will be metastable in the phase where they start. In contrast, for higher-order transitions, observables in the two time histories will evolve together.

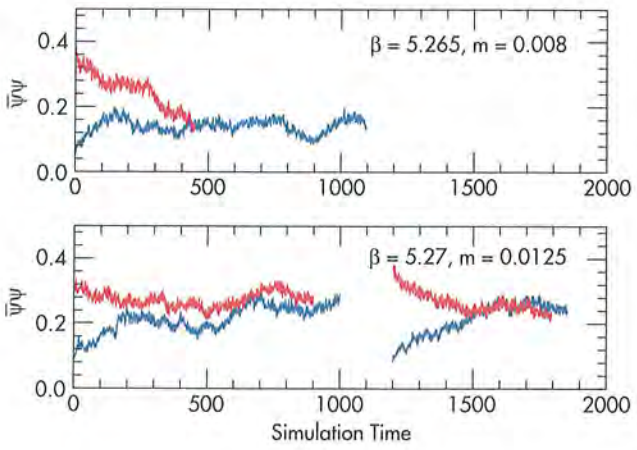
For two values of the quark mass, we found hot and cold starts evolving to the same final values, so this simulation favors a second-order transition. Previous studies have found that results are strongly dependent on the spatial size of the system being simulated. These simulations use a spatial size 1.5 times as large as previous tests, as well as a quark mass which is slightly closer to the real-world value. These results will be analyzed together with a set of runs spanning a range of temperatures to see if the expected scaling forms are seen with these quark masses.

Publications

Bernard, C., T. Blum, T. A. DeGrand, C. DeTar, S. Gottlieb, U. M. Heller, J. Hetrick, L. Karkkainnen, K. Rummukainen, R. Sugar, D. Toussaint, and M. Wingate. 1997. MILC studies of high-temperature QCD—A progress report. QCD on Parallel Machines Workshop, Tsukuba, Japan. http://www.physics.arizona.edu/~doug/tsukuba_thermo_proc.ps

Bernard, C., T. Blum, C. E. DeTar, S. Gottlieb, U. M. Heller, J. E. Hetrick, B. Jegerlehner, K. Rummukainen, R. L. Sugar, D. Toussaint, and M. Wingate. 1997. Critical behavior at the chiral phase transition. Lattice-97 Conference, Edinburgh. http://www.physics.arizona.edu/~doug/lat97_detar.ps

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



Time histories of the order parameter for hot and cold starts with a quark mass of 0.05*T and 0.032*T, with two separate starts for the larger quark mass. The temperature in these runs has been adjusted to be right at the peaks in the susceptibilities.

ADVANCED COMPUTING FOR GEOPHYSICAL INVERSE PROBLEMS

D. W. Vasco, Lane R. Johnson, and E. Majer,
Lawrence Berkeley National Laboratory

Research Objectives

In this project we are using several million seismic travel times and massively parallel computing to produce the first three-dimensional image of the structure of the entire Earth (crust, mantle, outer core, and inner core). In addition, we simultaneously estimate the topography of the internal boundaries of the Earth, such as the core-mantle boundary. Our results indicate intriguing coherent structure in the lowermost region of the outer core which may be related to the convection process. This structure has never been imaged before, and the facilities at NERSC are allowing us to obtain a rigorous inversion of the seismic data.

Computational Approach

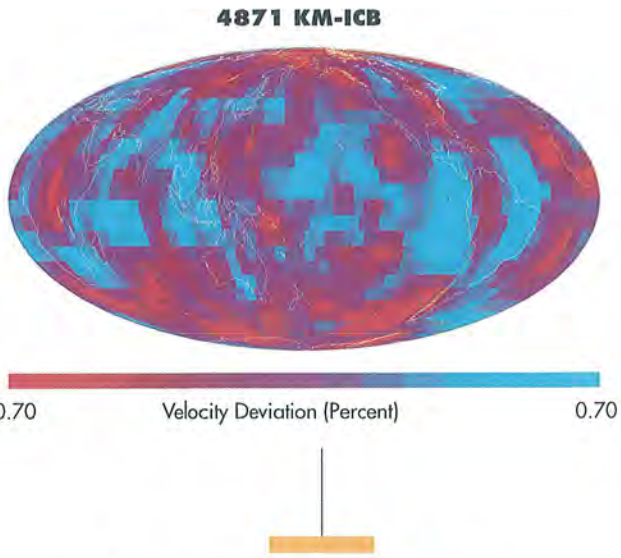
We are using an iterative Lanczos algorithm to image the Earth's interior. A critical element of the algorithm is a matrix-vector multiply which is done in parallel on NERSC's T3E.

Accomplishments

We have completed work on our first three-dimensional image of the structure of the entire Earth. The results are described in a paper in press in the *Journal of Geophysical Research*. An additional paper, submitted to *Science*, examines an intriguing structure in the Earth's fluid outer core which is symmetric around the equator (see figure). We are writing up the results of a Lanczos recursion approach which is a significant improvement on conventional imaging methods because it enables us to calculate the spatial resolution of the Earth's structure as well as its uncertainty. Current work involves a much more detailed inversion which makes the problem 4 times larger but allows us to estimate fine-scale three-dimensional structures.

Significance

The advent of plate tectonics has brought about an increased interest in the lateral variations of the Earth's material properties. The three-dimensional distribution of density, temperature, and the compressional (P) and shear (S) velocities within the Earth have a direct relationship to its dynamics. Therefore, fundamental issues related to convection within our planet, such as earthquake generation, resource distribution (petroleum and minerals), and environmental issues, may be answered by studies of the aspherical Earth structure. For example, we image the outer core, the region in which the Earth's magnetic field is generated. Recent three-dimensional numerical models of convection in the core have generated renewed interest in this region. Our results indicate a symmetric structure in the fluid outer core which is compatible with this convection modeling.



Map of the seismic velocity variations at the bottom of the Earth's outer core. Red signifies slower seismic velocities, and blue signifies faster velocities.

Publications

Vasco, D. W., Peterson, J. E., and Majer, E. L. N. d. Resolving seismic anisotropy: Sparse matrix methods for geophysical inverse problems. *Geophysics* (in press).

Vasco, D. W., and Johnson, L. R. N. d. Whole Earth structure estimated from seismic arrival times. *J. Geophys. Res.* (in press).

Vasco, D. W., and Johnson, L. R. N. d. The seismological signature of core dynamics? *Science* (submitted).

CLIMATE CHANGE SIMULATIONS WITH INCREASING GREENHOUSE GASES AND SULFATE AEROSOLS

Warren M. Washington and Gerald A. Meehl,
National Center for Atmospheric Research

Research Objectives

To investigate the effect of greenhouse gas increase and sulfate aerosols on global warming.

Computational Approach

This climate model has three major components: an atmospheric spectral model, an ocean model with a 1 degree horizontal grid and 20 vertical levels, and a sea ice component including dynamics and thermodynamics.

Accomplishments

We conducted several global climate change experiments with a coupled climate model that includes the effects of increasing CO_2 and the radiative cooling effects of sulfate aerosols. The greenhouse gas increase causes general global warming; however, the sulfate aerosols cause less warming and even regional cooling, which yields climate change patterns closer to those observed.

We configured a global coupled ocean-atmosphere general circulation model without flux correction and integrated it into a set of 75-year sensitivity experiments that included increasing CO_2 concentrations and the direct and indirect efforts of anthropogenic sulfate aerosols. Sulfate aerosol forcing increased from zero to present-day estimates in the first 30 years of the integrations, while equivalent CO_2 forcing increased by 1% per year relative to the control experiment, similar to the rate of increase of observed greenhouse gas forcing over the period 1960-1990. Annual mean averages around year 30, analogous to present-day conditions, indicate better agreement with recent observed geographic and zonal mean temperature anomaly patterns in the sulfate aerosol experiments and less warming in northern summer than in winter.

Sulfate aerosols were then increased following the internationally agreed scenario, while CO_2 continued to increase at 1% per year. Averages around year 70, analogous to conditions roughly 40 years in the future, indicate warming almost everywhere in the troposphere over the globe as the CO_2 forcing overwhelms the negative radiative forcing from the sulfate aerosols. There is also a weakening of the south Asian monsoon in the sulfate aerosol experiments. Results of the sulfate aerosol experiments show qualitative agreement on the patterns of the temperature changes, both geographic and zonal, with the magnitude of the changes being a function of the size of the radiation forcing. Increased cloud reflectance and indirect sulfate aerosol experiments were also conducted.

Significance

One of the most significant issues that society has to face is climate change associated with man-made emissions of carbon dioxide and sulfate aerosols. Modern climate models are an important tool for studying possible impacts.

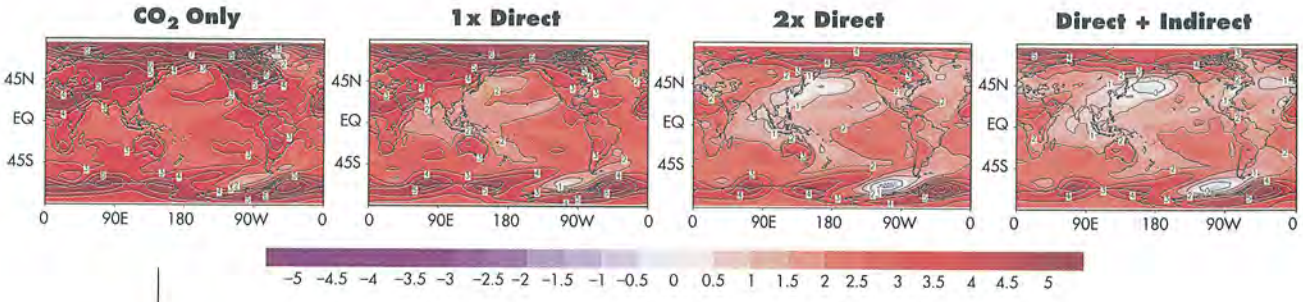
Publications

Washington, W. M., and G. A. Meehl. 1996. High latitude climate change in a global coupled ocean-atmosphere-sea ice model with increased atmospheric CO_2. *J. Geophys. Res.* 101:12,795.

Meehl, G. A., and W. M. Washington. 1996. El Niño-like climate change in a model with increased atmospheric CO_2 concentrations. *Nature* 382:56.

Meehl, G. A.,1997. Modification of surface fluxes from component models in global coupled models. *J. Climate* 10:2811.

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



This figure shows the surface air temperature difference between a control experiment, labeled "CO_2 Only," and three experiments in which the carbon dioxide is increased by 1% per year, which takes into account roughly all of the other increases in greenhouse gases. The warming (red areas) and cooling (blue areas) correspond to estimated changes at the mid-21st century. The three alternative experiments have the additional effect of sulfate aerosols, which can cool regions where there is high industrial activity. One of the sulfate effects, termed "Direct," is generation of haze, which can reflect solar radiation. Because of uncertainties, two "Direct" experiments were conducted, one with the approximate effect and another with twice the effect. The final experiment, "Direct + Indirect," adds changes in the brightness of clouds due to sulfate aerosols, which are also highly uncertain. These experiments will be repeated with improved climate models and intercompared with observations and other climate modeling efforts.

TERNARY TRANSITION METAL ALUMINIDE ALLOY FORMATION

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

Research Objectives

To understand and predict the stability and properties of metallic alloys.

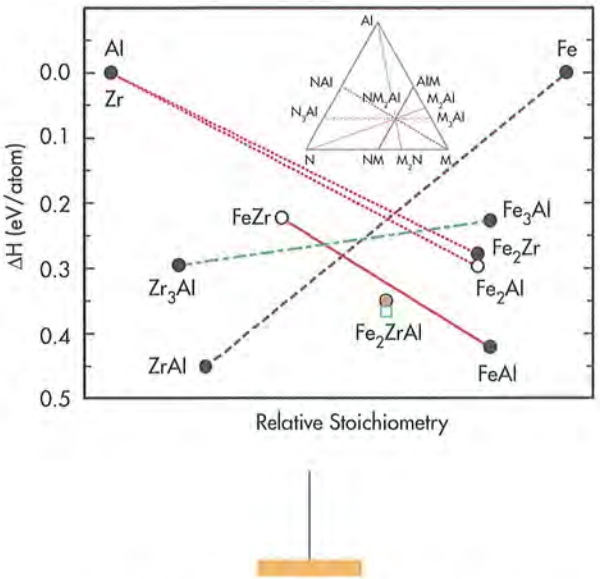
Computational Approach

First-principles local density calculations, using the full-potential linearized augmented Slater-type orbital (FLASTO) method, provide a means of obtaining the heats of formation of competing alloy phases, both for observed and unobserved structures. In this approach, the electronic structure problem is cast into a set of effective one-particle equations that must be solved self-consistently. The resulting single-particle wave functions are expanded in a set of Slater-type orbitals in the interstitial, augmented by numerical solutions of the effective potential in spheres surrounding each atom. To get a consistent set of heats of formation, all the structural parameters (volume, c/a ratios, internal atomic positions, etc.) need to be optimized. The large number of calculations needed to adequately investigate the competing alloy compositions, different crystal structures, and structural parameters were done on the cluster of Cray J90s at NERSC.

Accomplishments

The bonding of aluminum with the transition metals is of scientific and technological concern. Despite this interest, the properties of ternary aluminides have received relatively little theoretical attention. Almost 50 ternary transition metal aluminides have been reported in the ordered antiphase Heusler BiF_3 structure, representing roughly half of the observed ordered ternaries. To investigate the possible occurrence of other aluminides in this structure, the heats of formation of 38 ordered M_2NAl ternaries, most not reported to occur, have been calculated. While all but one are stable relative to the elemental metals, the test for ternary stability requires comparison of the ternary heat with competing two- and three-phase mixtures of binary phases.

As an example of the competition among different phases, the heats of formation of the ordered Fe_2ZrAl alloy (red filled circle) and various two-phase mixtures are compared in the accompanying figure. (The corresponding lines connecting binary phases in the ternary triangle are shown in the inset.) Although the ordered ternary is predicted to be stable relative to the two-phase mixtures, a three-phase mixture of FeAl-Fe_2Zr-$ZrAl_2$ (square) is even more binding and will suppress the Fe_2ZrAl alloy. Similar investigations for the other 37 alloy systems have been done.



Heats of formation of the ordered Fe_2ZrAl alloy compared with various two-phase mixtures.

Significance

Of the BiF_3 ternaries hitherto unreported, 9 are estimated to occur, while 18 are found to be unstable. The advantage of having theoretical predictions of the stability of the alloys is the possibility of discerning which of the unreported phases should not occur, as opposed to those that are yet to be observed. The pattern of occurrence obtained from experiments and calculations, taken together, suggests that on the order of another 20 compounds beyond those predicted here might exist. Thus, this important ordered phase is more pervasive than previously suggested by experiment.

Publications

Watson, R. E., M. Weinert, and M. Alatalo. N. d. Ternary transition metal aluminide alloy formation: The BiF_3 structure. *Phys. Rev. B*, in press.

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

MAGNETOHYDRODYNAMICS COMPUTATIONS ON AN UNSTRUCTURED MESH

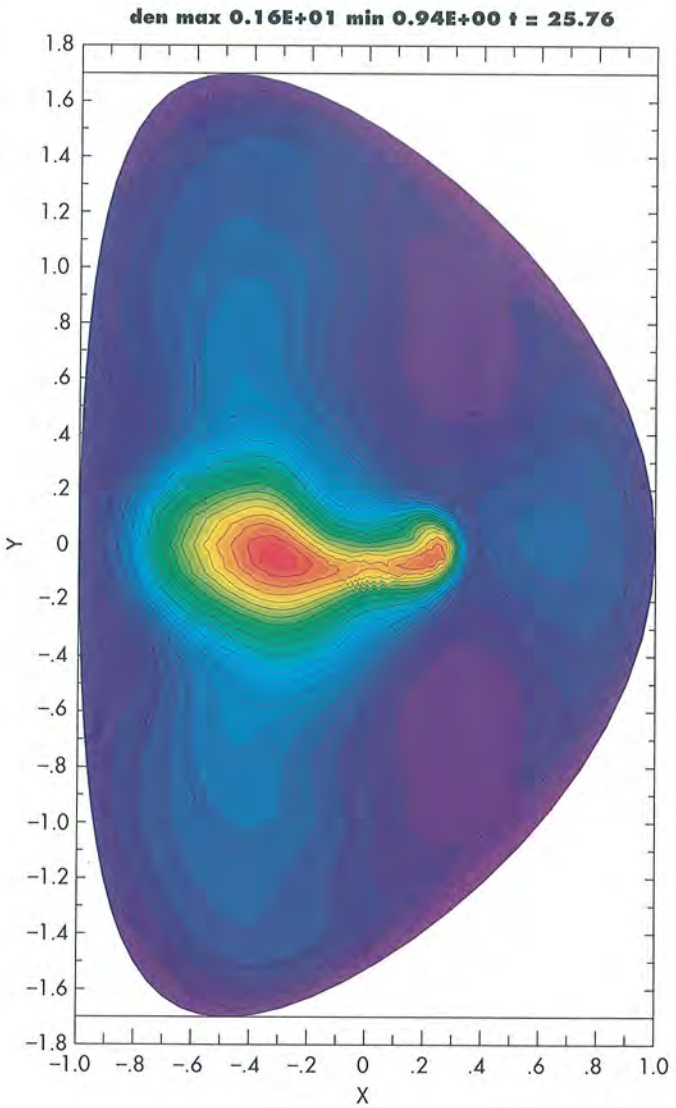
H. Weitzner and H. R. Strauss, New York University

Research Objectives

Develop and apply unstructured mesh numerical methods for magnetohydrodynamics (MHD) simulations.

Computational Approach

The MHD equations are discretized using finite element or finite volume methods on a two-dimensional unstructured mesh of triangular and quadrilateral cells. The mesh generation and discretization routines are packaged as a C++ class library, which encapsulates and hides the finite element code from the calling program, written in FORTRAN. Discretization in the third spatial dimension is on a regular mesh using either finite difference or spectral methods. Codes have been run on the NERSC C-90. A parallel version is under development.



Accomplishments

The MH3D++ code has been improved and is being used in applications. The code is an unstructured mesh version of the Princeton Plasma Physics Laboratory MH3D code, which calls the unstructured mesh class library. Pellet simulations are initialized with stable MHD equilibria. Introducing the pellet produces an unbalanced force, which causes the pellet to move outward (to the right), as well as spreading out along the magnetic field, until a new equilibrium is reached.

Significance

An unstructured mesh provides important advantages over conventional numerical approaches. It allows the mesh to conform to complicated boundary shapes, permits the mesh to be aligned with the magnetic field, and permits high resolution near important features. These advantages allow three-dimensional MHD simulations in magnetic field configurations with complex geometry, such as tokamaks with divertors. The pellet simulations are important for tokamak fueling, particularly for the proposed International Thermonuclear Experimental Reactor (ITER).

Publications

Strauss, H. R. 1996. Edge-localized mode simulations in divertor tokamaks. *Phys. Plasmas* 3:1.

Park, W., Z. Chang, E. Fredrickson, G. Y. Fu, N. Pomphrey, H. R. Strauss, and L. E. Sugiyama. 1996. 3D simulation studies of tokamak plasmas using MHD and extended-MHD models. F1-CN-64/D2-2, Sixteenth IAEA Fusion Energy Conference, Montreal.

http://math.nyu.edu/mfdd/

Penetration of a fuel pellet, localized in three dimensions, into a tokamak.

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