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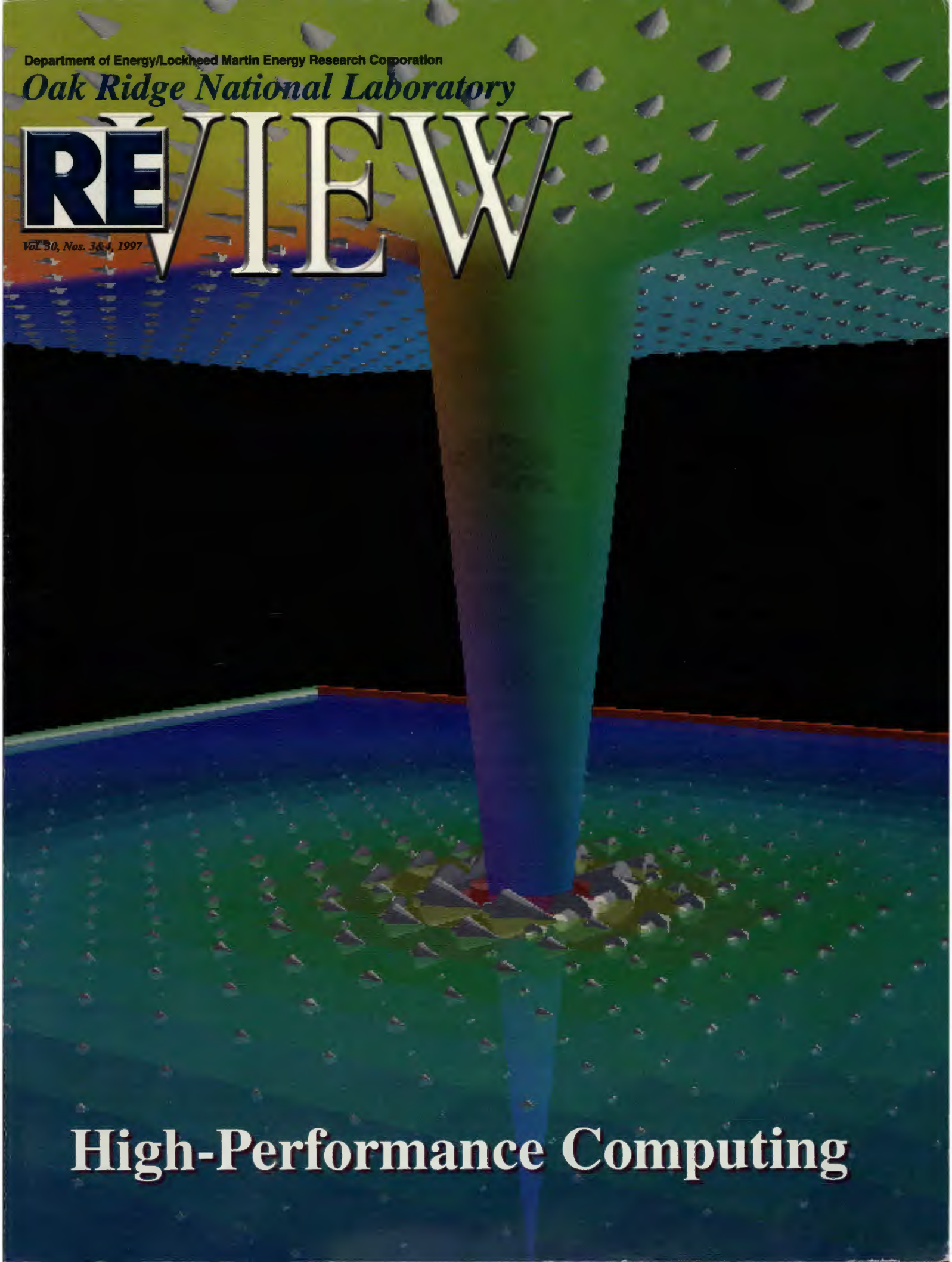
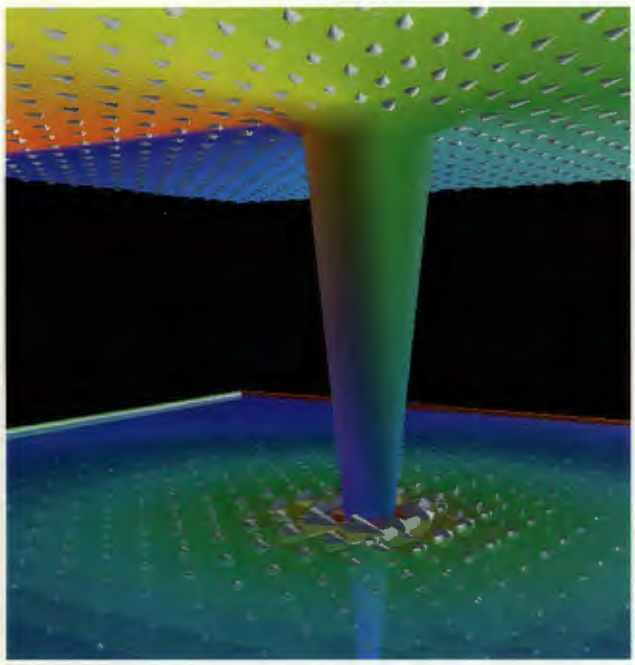


High-Performance Computing



COVER CAPTION

Colorful visualizations are among the most intriguing products of high-performance computing, including the efforts at ORNL that are featured in this special issue. The cover image, dubbed the "blue tornado," shows the vortex state in a superconductor. The vortex state arises when a magnetic field, which is deleterious to superconductivity, penetrates a superconductor by creating normal (nonsuperconducting) regions. Although the existence of the vortex state was suggested from a phenomenological theory and confirmed by experiment in the 1950s, it had not been studied from the full microscopic theory of superconductivity. Such a study was made possible by use of the Intel Paragon XP/S 5 and XP/S 35 supercomputers shortly after they arrived at ORNL. The illustration shows how the various quantities that describe the vortex state vary in the neighborhood of a superconducting vortex. The solution is for a two-dimensional regular periodic lattice relevant to high-temperature superconductors such as yttrium-barium-copper oxide. On the lower surface, circulating currents are indicated by arrows while the color encodes the degree to which the magnetic field has penetrated the superconductor. The upper surface shows the variation of the superconducting order parameter. This quantity, which is a complex number, is represented by its magnitude and phase. The height of the upper surface represents the size (magnitude) of the order parameter while the color encodes the phase, which varies from zero (blue) to two-pi (red) as the vortex is encircled. The inverted cone shows the core of the vortex where the magnitude of the order parameter plummets to zero and superconductivity is lost, and where the magnetic field reaches its maximum (red) value. This work was performed by Paul Miller, a research student of Professor B. L. Gyorffy of Bristol University in the United Kingdom, during a visit to ORNL to work with Malcolm Stocks of ORNL's Metals and Ceramics Division.

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Oak Ridge National Laboratory

REVIEW

Volume 30, Numbers 3 & 4, 1997

FEATURES

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in energy production and end-use technologies; biological and environmental science and technology; advanced materials synthesis, processing, and characterization; and the physical sciences including neutron-based science and technology.

Foreword

This issue of the *ORNL Review* highlights many important computational science activities at Oak Ridge National Laboratory. The articles describe both the computational infrastructure that is in place to support breakthrough computational science, as well as significant accomplishments in science made through computation.

Some articles illustrate that computation is becoming an equal partner with theory and experimentation in the advancement of science.

Rich Sincovec, former director of ORNL's Computer Science and Mathematics Division, starts off the issue with a discussion of the future of high-performance computing.

Ken Kliewer describes the Center for Computational Sciences, which is the focal point for computational science at ORNL, as well as one of the leading computational centers in the world. The future direction of computing is toward widely distributed networked computing capabilities. The connection between Oak Ridge and Sandia national laboratories to link two powerful computers allows scientists to address major problems such as predicting global climate change, as described by Kliewer. Bill Shelton and Malcolm Stocks show how this link helps scientists better understand the magnetic structure of magnetic alloys.

Algorithms, tools, and software to facilitate the use of benchmarking and performance evaluation of high-performance computers are described by Ed D'Azevedo et al. This and other articles in this issue stress the importance of interdisciplinary teams of mathematicians, computer scientists, and computational scientists working together to advance science through computation. The successful scenario has the application needs driving the algorithmic, tool, and software activities. Results of such collaborations support the thesis that each order of magnitude increase in computing power is accompanied by an order of magnitude increase in efficiency, thanks to improved algorithms. This synergism between increased computational power and improved algorithms is fundamentally important because extra computing power is quickly consumed in an attack on problems previously considered intractable.

Tools and software components that enable a broader spectrum of users to more easily use advanced computing resources are especially important. They enable scientists to spend their time gaining scientific insight from the computations rather than bogged down in the details of using the computing infrastructure. Parallel virtual machine (PVM) software originally developed at ORNL has had a significant impact on heterogeneous network computing, and its broad availability has virtually guaranteed portability of applications based on PVM. Tools that emulate shared memory, such as the Distributed Object Network Input/Output (DONIO) Library, not only make distributed memory computers easier to use but often lead to better performance. Software components such as ScaLAPACK, QMRPACK, and sparse linear algebra facilitate the development of applications for high-performance computers, as described in this issue.

Large computations typically produce large output data sets that require visualization to understand the results. As the volume of data generated by computations, sensors, or other means continues to grow, new approaches to understanding the data have become mandatory. Ray Flanery et al. discuss the role of visualization along with future directions that promise to enhance interactions between humans and computers. Ross Toedte and Dianne Wooten write about ORNL's scientific visualization services and successful use of visualizations to glean scientific insights.

Arthur Kohl discusses the use of ORNL-developed CUMULVS to simulate and influence the outcome of scientific experiments. Computer simulations of materials are discussed in Shelton and Stocks' article. Osman Yaşar explores the use of a parallelized computer code to design and analyze more efficient, pollution-minimized engines. Bill Butler et al. examine the potential of giant magnetoresistance for improving electronic data storage systems. Srdan Simunovic et al. discuss car crash modeling and analyses of the performance of lightweight materials to accelerate their use in automotive applications. B. Radhakrishnan et al. show that computer simulations shed light on material microstructure. Laura Toran et al. describe the use of high-performance computing to understand and facilitate cleanup or containment strategies for contaminated groundwater sites. The existence of a new "hexatic" phase between solid and liquid is shown through computations by Mark Mostoller et al. Edge dislocations in silicon are explored by Ted Kaplan et al. Ed Uberbacher describes the important role that computation has had in the Human Genome Project and its expected significant role in the future.

Another article on our scientific computing covers DOE 2000 efforts at ORNL in which electron microscopes are operated remotely for research projects and electronic notebooks are used by scientists across the nation to record, share, and search information on instrument use and experimental results. The final article by Kimberly Barnes et al. focuses on ORNL research in adapting computer technologies to allow geographically dispersed decision makers to respond quickly in a collaborative environment to better manage disasters.

—Thomas Zacharia, director, ORNL's Computer Science and Mathematics Division

The Future of High-Performance Computing

Rich Sincovec relaxes outside Building 6025, headquarters for ORNL's Computer Science and Mathematics Division. *Photograph by Tom Cerniglio.*

By Richard F. Sincovec

The World Wide Web, the graphical part of the Internet, has created a ne environment for research and communication. Today most users employ search for and view information from remote databases. The infrastructu includes algorithms, tools, and software to utilize fully the potential of th computational science, is in its infancy. However, it is expected to grow r enhanced capabilities become available for use or retrieval of remote an program libraries and databases, for remote and distributed execution, a remote and distributed visualization activities.

Browsers, including those compatible with Sun Microsystems' Java programming language, have become the norm for accessing information on the Web. Given current trends in Web use and the rapidity with which advances are realized, it is tempting to envisage a world in which the Web is the universal medium for computing. In such a world, applications would not be constructed from scratch or even built using standard software libraries; instead they would be put together using prefabricated components available through the Web. For example, Java, which has an object-oriented approach, permits software components to be easily constructed and used together to create complete applications. These may be operated in either a stand-alone mode or as applets (mini-programs written in Java) that can be run over the Web to enable "programming in the large." Likewise, multimedia interfaces will evolve that will provide the user access to "a global meta-computer" that will enable access to the computing resources required without the need to worry about where or how the work is done. Problem-solving environments (PSEs) are created by using these technologies in concert with each other.

Problem-Solving Environments

Funding is now available from several U.S. agencies to support the design and development of PSEs. A PSE is a computing environment that will provide all the computational and informational resources needed to solve problems within a specific domain. Some examples of questions that a PSE might address are "How do I design a new material with specified properties?" "How do I remediate a specific contaminated site?" and "What investment should I make now?" For each problem domain, there is a separate PSE. Some non-Web-based PSEs already exist; however, future PSEs are likely to use software that becomes available on the Web.

A multimedia user interface represents a PSE to the user. The interface will present a coherent view of the problem domain and hide the intrinsic details of the underlying computing infrastructure. PSE will use the language of the target class of problems and avoid, to the extent possible, information that requires specialized knowledge of the underlying computer hardware or software. PSE will provide a system that is closer to the scientist's problem than to general-purpose parallel hardware and systems software while still providing a complete environment for defining and solving problems in the problem domain.

The PSE multimedia interface will provide the scientist with a set of tools for exploring all aspects of the problem. PSE will also provide a visual editor for creating new applications or modifying existing applications using software available c tools will enable m ing codes and facili of codes developed working in the prob will have features t researcher to includ methods, to easily i solution methods, a select solution met

The PSE multim also permit the scie progress of the com extended problem-s review them easily. will provide the use to use visualization or new breakthroug understand the resu be further enhanced jects at ORNL in el and videoconferenc provide improved c

PSEs will not o efficient use of exis computing resource more important, wi enhance scientists' enabling them to by consuming comput their work so that t on the scientific asp will be free to spen analyzing results ra problems for the co ment. PSE facilitat use of software dev thereby enabling ra new and enhanced

PSE will also enable collaborative problem solving with scientists at other locations. Collaborative activities can include interactive visualization and remote steering of experiments through distributed applications by multiple collaborators. PSE might also involve resources other than computing resources, such as specialized scientific instruments coupled with appropriate collaborative and control capabilities. Interaction with the virtual environment can be expected to involve new mechanisms for interaction between humans and computers.

Overall, PSEs will have the potential to create a framework that is all things to all people: they solve simple or complex problems, support rapid prototyping or detailed analysis, and are useful in introductory computer education or at the frontiers of science.

What Is Required to Develop a PSE?

Current projects at ORNL and within other organizations in software components and tools provide the foundation for creating PSEs. Recent work in fault tolerance and task migration is essential for a robust PSE. Current projects are also exploring how to integrate different tools and program components at the proper level of abstraction so that the resulting PSE is both sufficiently flexible and easy to use.

PSEs require computer networks that possess adequate speed and bandwidth. Minimal network latency and maximum network reliability are also essential, as are security and authentication mechanisms that are uniform throughout the virtual computing environment. Finally, as free-market computing becomes more dominant, accounting mechanisms with audit trails will be necessary for proper user billing and fraud prevention. Ultimately, computing resources will be paid for as they are used, and they will be universally accessible.

Seamless Computing Environment

The development of PSEs using the Web depends on the development of an underlying seamless computing environment (SCE). SCE provides the middle ware between PSEs and library routines, databases, and other resources that are available on the Web. SCE assigns, coordinates, and schedules the resources required by PSE. Specifically, SCE addresses such functions as job compilation, submission, scheduling, task migration, data management, and monitoring.

Using the SCE interface, the user specifies the job to be performed, along with required resources. The interface acts as an intelligent agent that interprets the user input to assign computing resources, identify storage requirements, and determine database needs, all within constraints imposed by the user with respect to cost and problem completion. The intelligent agent may choose to pass the job to more distant agents. Those agents then interact with local agents to assign or perform the work. The user will be able to specify unique requirements, such as computer architecture, including parallel computers with a specified number of processors, specific domain-dependent databases, and the maximum cost the user is willing to pay to solve the problem. The interface will provide information on progress and resources being consumed while the job is being executed.

SCE, which has agents that are programmed to optimize the use of distributed resources, will provide more efficient use of existing computing resources, including workstations and high-performance computers. More importantly, new scheduling environments will enable computations to be performed where they can be done most effectively, in a manner transparent to

Sincovec surveys the ORNL campus near the Swan Pond, part of the view for many computer scientists at the laboratory.

the user. The distributed nature of SCE provides fault-tolerant capabilities.

Computing, visualization, and mass storage systems that make up the distributed computing environment must be linked in a seamless manner so that a single application can use the power of multiple computers, use data from more than one mass storage system, store results on more than one mass storage system, and link visualization resources so users can view the results using desktop virtual reality environments.

SCE must provide a secure and robust distributed computing infrastructure that has scalable shared files, global authentication, and access to resources at multiple Web sites. PSE and SCE will most likely be based on object-oriented methodologies.

Economic Model for PSEs Based on SCE

Within PSE, the scientist specifies a problem to be solved, the resources required, and the maximum amount of money available to solve the problem within a specified time. When PSE submits its requirements to SCE, SCE assigns the problem requirements to an intelligent software agent (ISA) that attempts to solve the problem within the specified cost and time constraints. If the job cannot be done locally, the ISA passes the requirements on to remote ISAs (RISAs). RISAs interact with other ISAs in bidding to perform the work. The local ISA selects the RISA that submits the lowest bid to perform the work in the specified time frame. Upon completing the job, the ISA that runs the job charges the scientist for the resources used. If the job uses third-party software, ISA charges the user and remits the fee to the bank account of the software owner.

In one vision of the future, a nomadic computing environment would enable you to go anywhere and use everything. You would have a persistent electronic presence—that is, always "me" online. You would also be able to expect 100% network availability, ubiquitous wireless access, and ultrahigh bandwidth nets for research.

Outlook

When will it happen? Soon! The Center for Computational Sciences is currently laying the groundwork for an SCE. ORNL and other government laboratories are working on various projects that provide the fundamental building blocks. Computer hardware and software vendors are providing new products that directly support the development of PSEs and SCEs. Computer scientists and applied mathematicians are developing the concepts, tools, and algorithms. The funding agencies are creating programs that support the design and development of PSEs. Because of the rapid rate of technology development in computing and networking, you will not have to wait very long. **ornl**

A Research Agenda for the Internet

Exploiting the power of the Internet through the use of PSEs and SCEs requires a broad research agenda to help create

- ❑ multimedia user interfaces (MMUIs) that support the problem and computing domain;
- ❑ a scheduling environment to enable the most effective performance of computations at a location transparent to the user;
- ❑ a secure and robust distributed computing infrastructure that features security and authentication mechanisms that are uniform throughout the accessible environment and that enable user access to resources at multiple sites;
- ❑ storage and search tools to find applicable resources, including codes, documents, and data in multimedia databases;
- ❑ new programming paradigms, languages, compilers, and mapping strategies;
- ❑ machine and software abstractions;
- ❑ scalable shared file system and transparent access to remote databases;
- ❑ code reusability coupled with tools that enhance reuse and enable a layered approach to application development;
- ❑ tools to support code development, testing, and validation in the proposed environment;
- ❑ domain-specific environments, including hierarchy of object-oriented abstractions;
- ❑ repository research, including indexing, storage, search, security against viruses, and some insurance of portability;
- ❑ remote collaboration tools, including computational steering tools; and
- ❑ accounting mechanisms and audit trails.

BIOGRAPHICAL SKETCH

RICHARD F. SINCOVEC was director of ORNL's Computer Science and Mathematics Division until he left for San Antonio, Texas, in August 1997. He received M.S. and Ph.D. degrees in applied mathematics from Iowa State University. Before joining ORNL in 1991, he had been director of NASA's Research Institute for Advanced Computer Science in Ames, California. He also has been professor and chairman of the Computer Science Department at the University of Colorado at Colorado Springs, manager of the Numerical Analysis Group at Boeing Computer Services, professor of computer science and mathematics at Kansas State University, and a senior research mathematician at Exxon Production Research. He has also been affiliated with the Software Engineering Institute of Carnegie-Mellon University, Lawrence Livermore Laboratory, and Hewlett-Packard. He is the coauthor of five books that cover topics in software engineering, Ada, Modula-2, data structures, and reusable software components. He is a member of the Association for Computing Machinery and the Society for Industrial and Applied Mathematics (SIAM), and he is editor-in-chief of the *SIAM Review*.

The Center for Computational Sciences:
High-Performance Computing Comes to ORNL

Ken Kliewer points to Sandia National Laboratories (SNL), whose Intel Paragon is connected with ORNL's Intel Paragons by a high-speed network. The high-performance computers are communicating with each other and running calculations together in parallel to solve complex problems that cannot be solved by one Paragon alone. *Photograph by Tom Cerniglio.*

By Kenneth Kliewer

ORNL's Center for Computational Sciences is one of the world's premier computational science centers. Its facilities include parallel Intel Paragon computers having 200 gigaflops of computing power and a data storage system exceeding 100 terabytes in capacity. The Center's focus is the solution of Grand Challenge-level problems, requiring extensive expertise in the development of a broad range of parallel application codes and algorithms. The Center has taken an innovative step into the "computing of the future" arena by linking its huge Paragons with a Paragon at Sandia National Laboratories through state-of-the-art networks. This extraordinarily powerful "distributed computer" makes possible solutions of problems too complex to be solved at either site alone.

Computers became a visible part of the national technical scene in the 1950s. Thereafter, improvements came rapidly as both hardware and software—systems, strategies, and concepts—evolved and matured. On through the 1970s, improvements and innovations were dramatic, with corresponding advances in performance.

Throughout this period, the basic computer remained the same. The heart of the machine was the central processing unit (CPU) which, as programmed by the user, performed the desired calculations or processes step by step in time—that is, sequentially. But then, with a mighty nudge from Mother Nature, a new perspective emerged.

The subsequent discussion is simplified with the introduction of a measure of speed for computers: FLOPS, which stands for FLoating-point OPerations per Second. For our purposes here, it is appropriate to think of FLOPS as "arithmetic operations per second."

While CPUs were moving through the kiloflops class to megaflops—from thousands to millions of mathematical operations per second—it was clear that Mother Nature had imposed a limit. When computing, CPUs operate through sequences of electrical signals, but these signals cannot move arbitrarily quickly. Their motion is limited by the speed with which light (or electrical signals) can travel, which is fixed by natural law. However, the expectations of computer users and the computing requirements associated with demanding problems knew no such limits.

The Parallel Solution

Thus emerged a new strategy: Put multiple CPUs into a single computer and have all of them work together simultaneously to solve problems. This procedure is now known as parallel computing. Machines providing the highest level of performance today are all parallel computers, not sequential machines.

Within the world of parallel computing, there are two fundamentally different ways of handling machine memory. One way is to ensure that all CPUs are in direct contact with the entire machine memory, a configuration called shared memory. An alternative is for each CPU to have its own share of the total system memory. In this arrangement, any CPU that requires information stored in the memory of another must send a message requesting this information. The requested information is then supplied through a response message. This configuration, referred to as distributed memory, involves sophisticated strategies for "message passing." One message-passing arrangement is shown in Fig. 1.

Distributed memory machines currently provide the highest performance, but the ease of programming shared memory machines has compelled a concerted, largely U.S. effort to develop ever higher-performance machines of this type. ORNL has made seminal contributions to message-passing strategies, as discussed in the article "Algorithms, Tools, and Software Aid Use of High-Performance Computers," starting on p. 38.

U.S. Computing Initiative

How did CCS become one of the world's premier computational centers? The imaginative federal High-Performance Computing and Communications (HPCC) Initiative opened the door for CCS, and a successful proposal from ORNL to the Department of Energy's Office of Scientific Computing [OSC, now the Mathematical, Information, and Computational Sciences (MICS) Division] was the first step. The proposal established ORNL's CCS as a DOE High-Performance Computing Research Center (HPCRC) and the Intel Supercomputer Systems Division (SSD), later called the Scalable Systems Division, with its message-passing, parallel Paragon computers, as the major computer supplier.

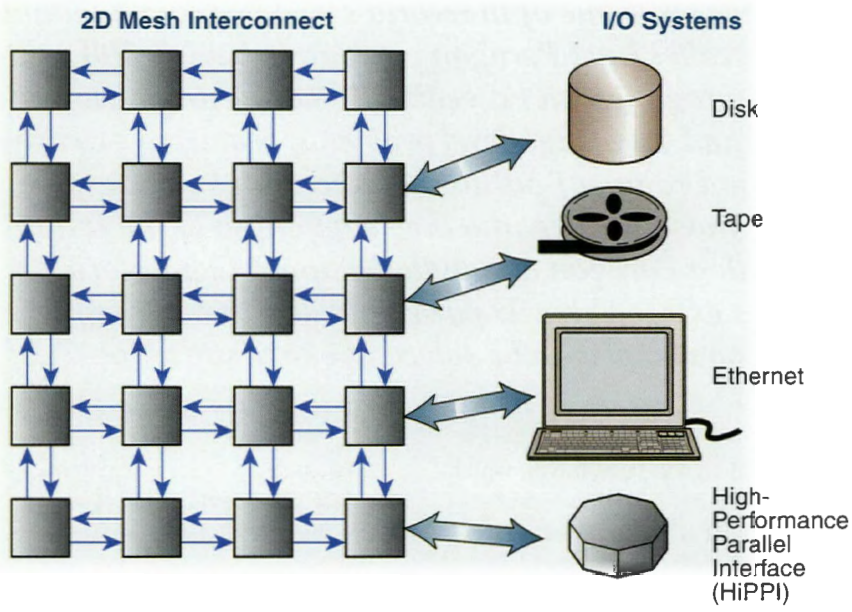


Fig. 1. The interconnect architecture of the Intel Paragon is an example of a message-passing system. The squares represent nodes connected in a two-dimensional mesh. Each node contains memory and two or more CPUs, one for message passing and the others for computing. Message-passing paths are indicated by arrows. Typical input/output (I/O) systems and devices are shown on the right.

However, CCS's technical path to its current Intel Paragon XP/S 150 centerpiece (see photograph at right) had a different origin: The first machine was the 32-processor Kendall Square Research KSR-1 computer, delivered in September 1991. This shared memory machine was truly innovative at that time. But the defining HPCC event was a cooperative research and development agreement (CRADA) between Intel SSD and ORNL. In September 1992, this CRADA brought to CCS the first of the Intel Paragons, a 66-node XP/S 5 with the general purpose (GP) architecture (i.e., two CPUs per node, one for computing and the other for message passing, as depicted in Fig. 1). The architecture of this and subsequent Paragons was the two-dimensional mesh shown in Fig. 1. (The number following "XP/S" in the names of Intel machines is a measure of the peak computing speed of the overall machine in billions of FLOPS, or gigaflops.)

Building from this CRADA, ORNL and Intel SSD signed a contract in June 1992 that culminated in the Paragon XP/S 150, but this machine was preceded by a smaller machine, planned initially to be part of CCS only until the arrival of the XP/S 150. The smaller machine, the Paragon XP/S 35, also with GP architecture, had 512 nodes with 16 million bytes [megabytes (MB)] of memory per node; it was also delivered in September 1992. In the same month, our Kendall Square machine was expanded to a 64-processor KSR-1. This Kendall Square machine was an important component of our computing capabilities until August 1997.

Using the XP/S 35 as our computing "workhorse," we had achieved an initial goal: we could solve very large-scale and formidable problems, often called Grand Challenges. Also, we could utilize to great advantage the excellent computational environment we had assembled. The small XP/S 5 was a machine for code development, initiating users into the realities of parallel computing, and system and computational experiments. The XP/S 35 was reserved for those who had demonstrated the requisite level of expertise and were prepared for major computational projects. To preserve this highly effective arrangement and to extend our computing capabilities, we renegotiated the contract with Intel SSD in early 1994 to make the XP/S 35 a permanent CCS machine and to increase its memory to 32 MB per node. Preserving this hierarchical machine arrangement has been a major factor in the success of CCS.

At this point, Intel modified the structure of its forefront Paragon nodes to the multi-processor (MP) form—three processors per node, two for computing and one for message passing. This is the architecture of the XP/S 150: 1024 MP nodes, each with at least 64 MB of memory, with mesh connectivity as is illustrated in Fig. 1. As part of the aforementioned CRADA, we began receiving an MP node machine in May 1994, thereby providing our users an opportunity to familiarize themselves with and develop strategies for more effectively using the soon-to-be available XP/S 150.

Our initial plan was fully implemented on January 4, 1995, when Intel delivered the Intel Paragon XP/S 150 to CCS following successful completion of an arduous set of acceptance tests. Now we have a computer that can do 150 billion mathematical operations per second. But the capabilities in high-performance computing and scientific expectations are escalating rapidly. Accordingly, we are currently discussing with DOE the purchase of a

Ken Kliewer and Buddy Bland check operations of the Intel Paragon XP/S 150, a parallel supercomputer at ORNL. *Photograph by Curtis Boles.*

machine with power reaching into trillions of mathematical operations per second (teraflops).

Our current computational environment (shown in Fig. 2) has made possible a striking array of scientific successes, a number of which are described in other articles in this issue. The accomplishments of CCS also point clearly to our sensitivity to what is expected of us through the HPCC initiative. Foremost among these expectations were

- bringing immature parallel systems to production-level capabilities,
- making meaningful progress in solving Grand Challenge problems, and
- accelerating the use of high-performance systems by the U.S. industrial sector.

The results achieved using the CCS machines and the ever-improving machine reliability make clear our success with the first two expectations. Our successes with the third expectation are described in the article "Industrial-Strength Computing: ORNL's Computational Center for Industrial Innovation," starting on p. 16.

CCS Users and the User System

The major fraction of our computational resources is provided to Grand Challenge groups selected by DOE-MICS through a competitive process. These groups, whose members are located around the country, include high-energy physicists working on quantum chromodynamics, groundwater transport and remediation investigators, materials scientists focusing on studies emphasizing fundamental principles, and computational chemistry modelers addressing pollution chemistry. An additional major user is the DOE Computer Hardware, Advanced Mathematics, Model Physics (CHAMMP) program, in which complex models of the atmosphere and ocean are developed and used with the goal of understanding global climate change over extended periods of time.

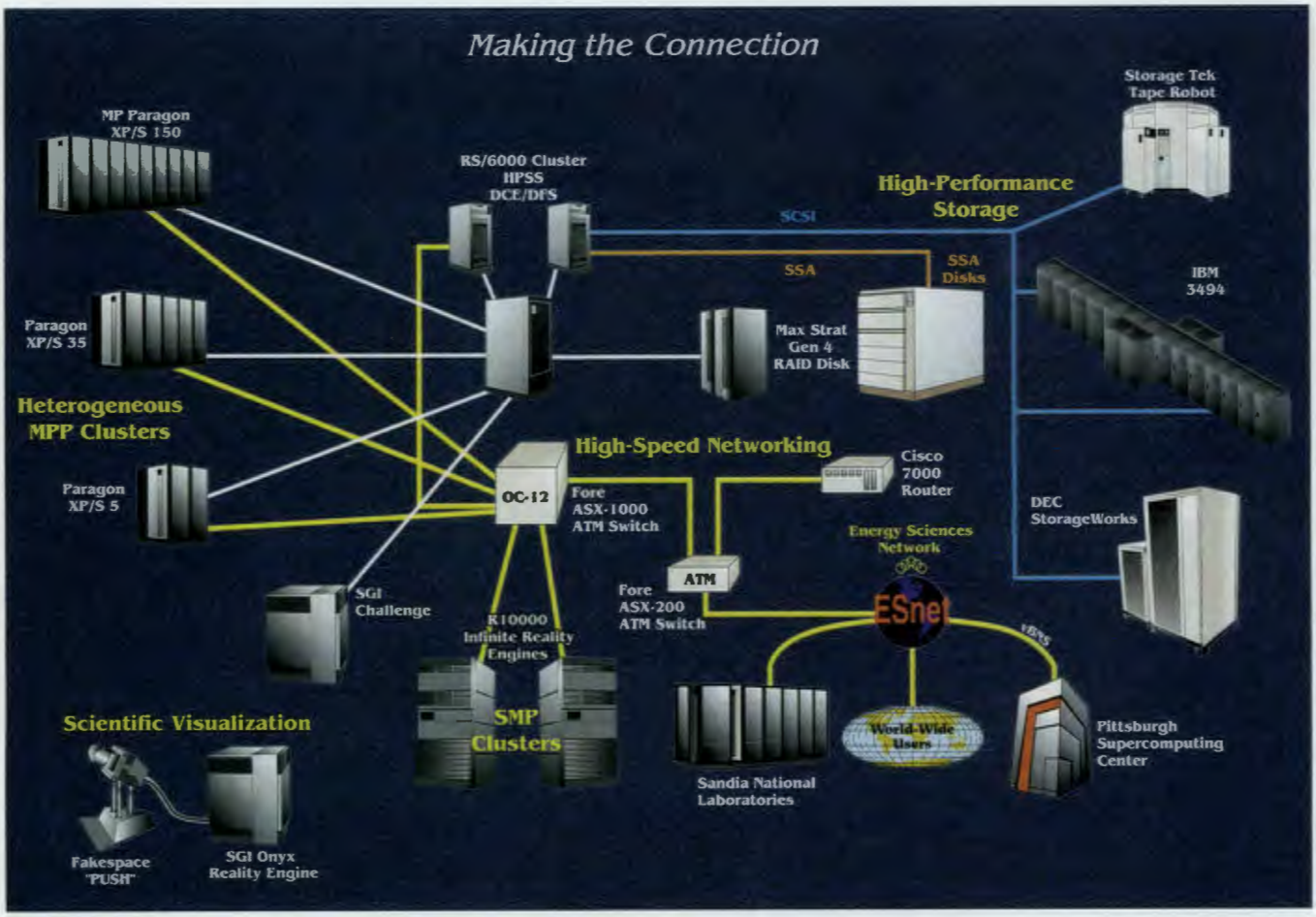


Fig. 2. The current CCS computational environment.

A share of CCS computing resources is provided to the CCS director, with the Computational Center for Industrial Innovation (CCII) using the most. ORNL also benefits from CCS resources allocated to internally funded Laboratory Directed Research and Development proposals and to others through a competitive proposal process. We also encourage innovative tests of parallel computing strategies and benchmarking and provide resources to individuals and groups working in these areas.

Most of our users employ FORTRAN in their calculations, but we also have other languages available, including C, C++, and High Performance FORTRAN (HPF). A large number of codes have been written for the Paragon, many of which were developed at ORNL for specific research problems. Others, like Dyna-3D and KIVA-3, are well-known codes from the sequential world that have been written into parallel form for the Paragons. Several of these codes are described in articles in this issue.

We provide a User Services group to assist users with debugging, coding, and eliminating possible machine and algorithm problems; to handle questions related to accounts and scheduling; and to organize educational courses to train users to become effective parallel programmers. An irreplaceable component of CCS is the VizLab, which provides an array of scientific visualization systems and services for our users. The capabilities and accomplishments of the VizLab are described in the article "Scientific Visualization at ORNL," starting on p. 21.

Data Storage

The impression that may have been imparted to this point is that the only consideration in establishing our computational environment was processor power. Not so. Of equal, or some may say, more importance are data storage and access systems.

Powerful computers generate vast quantities of data, and there must be systems in place to obtain, store, and catalog all of these data. Further, those systems must be able to provide rapidly and precisely all these data upon request. And all of these tasks must be done with absolute reliability.

Working collaboratively with the DOE Atmospheric Radiation Measurement (ARM) Program, we have assembled an extraordinary storage system. Currently using NSL-UniTree software, the CCS/ARM storage system is a state-of-the-art client/server file storage system. Principal components include

- a Storage Tek 4410 tape robot, updated with advanced tape drives and with a capacity of about 30 trillion bytes (TB);
- nearly 2 TB of disk storage; and
- a pair of IBM 3494 tape robots, the storage system centerpiece, each having about a 50 TB capacity. One has eight high-performance tape drives, and the other has four.

As may be clear from the specifics here, data storage systems are generally hierarchical. From the computer memory, data will normally flow into disk storage, providing high-speed access, and then, ordinarily, into slower-speed but higher-capacity tape storage environments.

Although the storage system software is currently NSL-UniTree, the future looks very different. CCS, together with Sandia National Laboratories, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and IBM Global Government Industry, has been developing a software system having far higher capability, the High-Performance Storage System (HPSS). HPSS is indeed the storage system of the future, providing data transfer rates extending into the multigigabit-per-second range. An advantage of HPSS is that it is network centered. That is, the control network can be distinct from the data transfer network, allowing the data to be transferred at network speeds rather than be slowed by having to flow through the memory of a control device. A possible configuration is sketched in Fig. 3.

While NSL-UniTree is sequential, HPSS is parallel. Thus, data from a single data file or multiple data files can be transferred into or out of the storage system through multiple channels simultaneously. Having these parallel capabilities is essential for many high-performance computing environments. Effective use of our multiple tape-drive and Redundant Array of Inexpensive Disks (RAID) storage systems requires these parallel capabilities, as does our research with medical records and medical image archives.

Experiments with HPSS are under way in our computer room. Following extensive stress testing of this system, HPSS became our production storage system software in 1997. We are also very pleased that HPSS, now an IBM product, received a 1997 R&D 100 Award from *R&D* magazine.

Networks

Essential to all of our computing are networks that provide for quick and efficient movement of information. CCS uses many different types of networking hardware to provide access to our machines as well as to the CCS/ARM storage system. Within our computer center, High-Performance Parallel Interface (HiPPI) networks provide 800 megabit-per-second (Mb/s) connections among our Paragon systems and the CCS/ARM storage system.

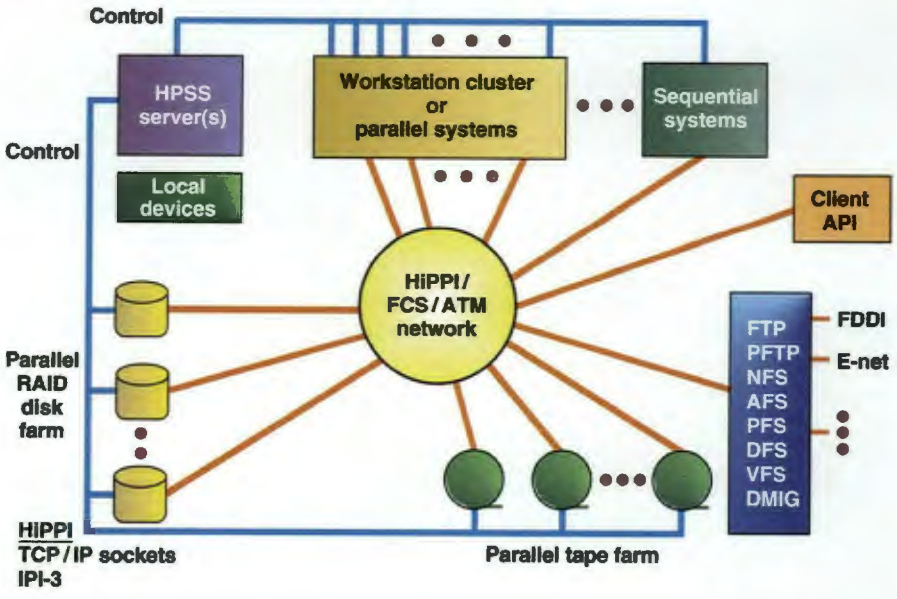


Fig. 3. The innovative data storage configuration made possible by the High-Performance Storage System (HPSS) software. Note that the control network and the data-transfer network are logically distinct. Also, HPSS permits parallel data transfers to and from disks and tapes.

Connectivity between the computer center and our ORNL CCS users occurs through both fiber distributed data interface (FDDI at 100 Mb/s) and Ethernet (10 Mb/s). CCS's principal connection to the outside world occurs through the Energy Sciences Network (ESnet), the DOE Energy Research branch of the Internet where very important innovations and additions are taking place. General connectivity through ESnet, currently at the speed denoted T3, or 45 Mb/s, will reach 622 Mb/s in 1998.

ORNL-Sandia Connection

As we emphasized earlier, the building blocks of a lightning-fast parallel supercomputer are small computers linked together that simultaneously solve pieces of a complex problem. So, most computing experts agree that the next logical step in high-performance computing is to link these fast parallel supercomputers together. But what if two of the world's fastest computers are separated by hundreds or even thousands of miles? Then the challenge becomes finding a way to connect them through a very-high-speed network to ensure the combined power made possible by this connection.

Scientists from CCS and Sandia National Laboratories (SNL) are demonstrating the effectiveness of such an arrangement (see Fig. 4). These two laboratories possess a striking level of computer power, making such a connection noteworthy.

The basic idea is to link the three large Intel Paragons (an 1840-compute-processor XP/S 140 at SNL and the 2048-compute-processor XP/S 150 plus the 512-compute-processor XP/S 35 in the CCS) over a high-speed asynchronous transfer mode (ATM) network, to solve problems too large for one machine alone—extraordinarily

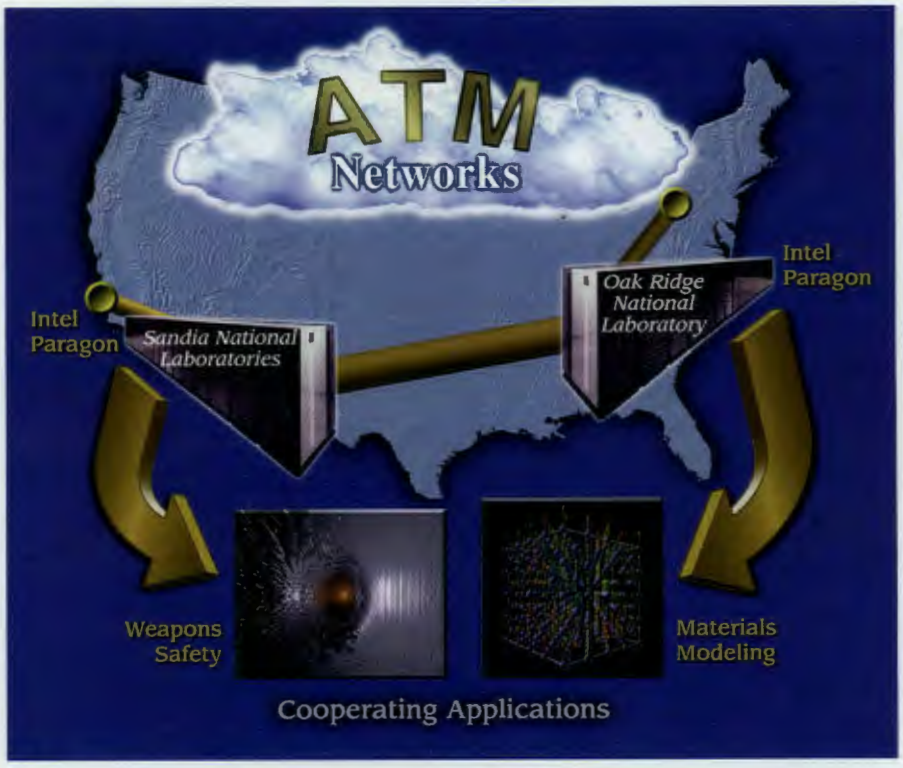


Fig. 4. Through high-speed ATM networks, Intel Paragons at SNL and ORNL will work together to solve complex problems related to national security, materials modeling, and global climate change, among others.

formidable problems relevant to both ORNL and SNL. By extending computational parallelism into the network and surmounting an extensive array of technical hurdles on this path to distributed high-speed computing, the researchers are also making important contributions to the technology.

To use this distributed computing power effectively requires codes developed with the ORNL-SNL communication time in mind. One example is a materials science code written by ORNL researchers to model the magnetic structure of complex magnetic alloys. Another is a global change code that couples the ORNL code modeling the atmosphere with the Los Alamos National Laboratory code modeling the ocean to provide a superior climate simulation over extended times. Additional codes that address national security are also being prepared.

To enable the Paragon computers to work together, ATM boards were specially designed and built for them by the small company GigaNet, with support from SNL. The excellence of these boards, which recently received an R&D 100 Award, was initially demonstrated through high-performance links connecting the SNL, ORNL, and Intel booths at the Supercomputing '95 exhibition in San Diego.

Our work is focused on ensuring compatibility among codes, operating systems, ATM, and communications software (PVM and MPI). We are also seeing a fascinating array of performance challenges that must be overcome in order to meet scientific goals. Significant questions concerning network connections and network availability are being addressed.

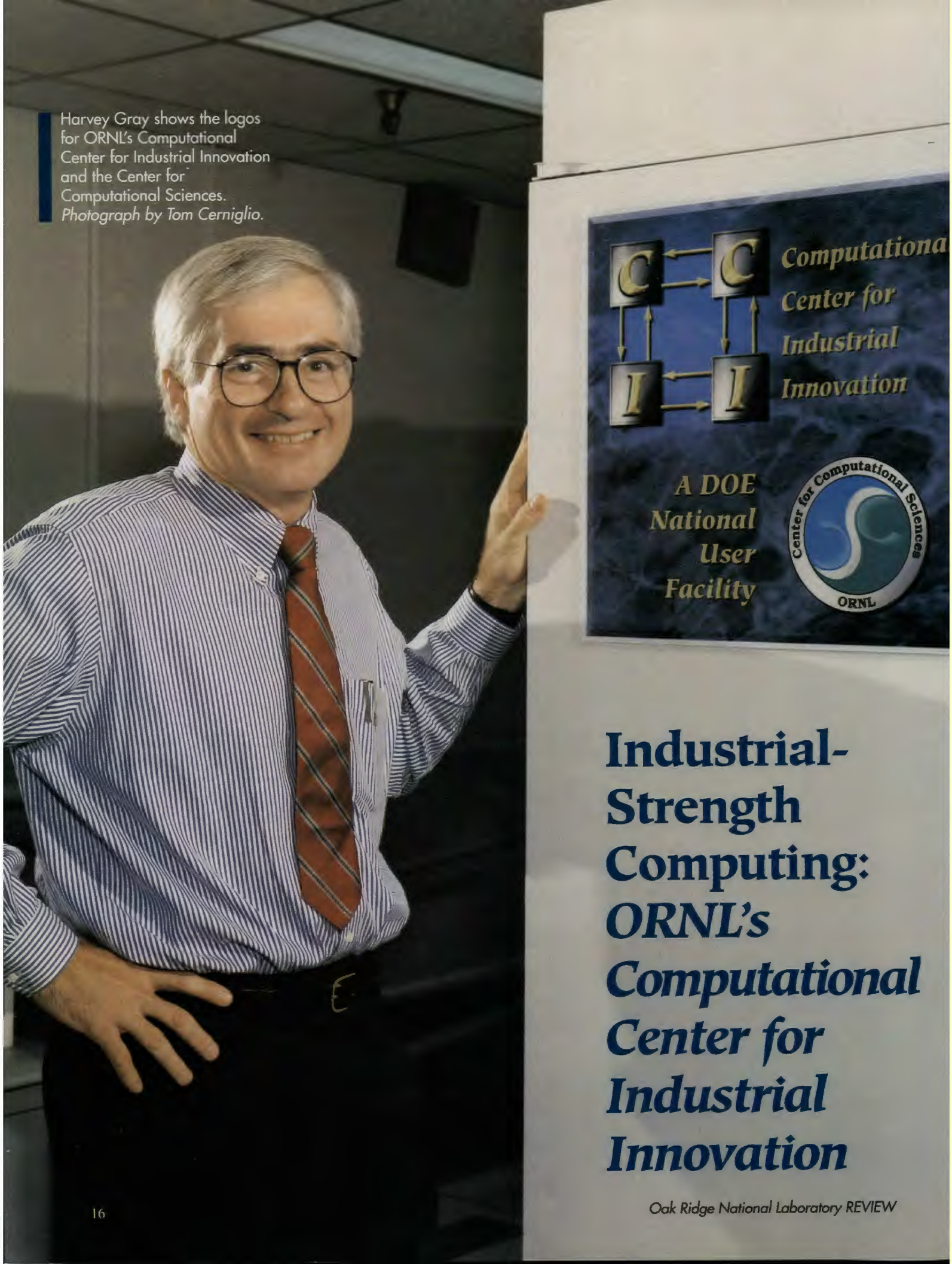
We do want to emphasize again that our objective with the ORNL-SNL connection is to solve major problems. We are not simply doing a connectivity demonstration.

The work being done through CCS is state-of-the-art. The GigaNet ATM boards operate at the speed designated OC-12, or 622 Mb/s. Using an ATM board on each of the XP/S 150 and XP/S 35 supercomputers in the CCS computer center, we were doing experiments at this speed. However, our connections to SNL at this point are no faster than OC-3, or 155 Mb/s. We anticipate having access to SNL over networks providing OC-12 connectivity in 1998. Our goal of OC-48, 2.56 gigabits per second, was achieved through use of four GigaNet boards in parallel at each site. This networking capability permits a huge step in the sizes of the materials science and national security problems that we can solve, as well as open avenues to effective distributed computing with far larger machines than we are currently using.

In conclusion, the Laboratory's CCS has emerged as one of the world's leading computational science centers. The scientific emphases in CCS are applications and the solution of large-scale, complex problems. It is, however, the technical expertise embodied in the powerful computing environment established in CCS that has made these applications successes possible. This expertise and the innovative spirit in CCS and at SNL have been key features in extending the capabilities and impact of distributed computing through the networked ORNL-SNL system. **ornl**

BIOGRAPHICAL SKETCH

KENNETH L. KLIEWER, director of the Center for Computational Sciences (CCS) at ORNL, is a theoretical physicist. Computing and computational science have been at the center of his career. He has a Ph.D. degree in physics from the University of Illinois at Urbana-Champaign. In addition to the CCS directorship, he is the leader of the ORNL High-Performance Storage System (HPSS) development team and a member of the HPSS Executive Committee. Prior to joining ORNL in 1992, he was dean of the School of Science, assistant vice-president for research, and professor of physics at Purdue University. He came to Purdue from Argonne National Laboratory, where he was Associate Laboratory Director for Physical Research. His research interests include surface physics, optical physics, and electrochemistry. He is a fellow of the American Physical Society.



Harvey Gray shows the logos for ORNL's Computational Center for Industrial Innovation and the Center for Computational Sciences. *Photograph by Tom Cerniglio.*

Industrial-Strength Computing: *ORNL's Computational Center for Industrial Innovation*

By W. Harvey Gray

DOE's Computational Center for Industrial Innovation at ORNL is helping researchers from American industrial firms, governmental agencies, and universities harness parallel computing to solve complex industrial problems. Using powerful parallel computing codes and machines at ORNL, researchers are simulating advanced aircraft, aluminum production processes, collisions of lightweight automobiles, internal combustion processes, and the buildup of ice on airplane wings. The results of this cost-effective approach to research should aid the design and manufacture of safer, more efficient products.

For some industrial firms, a new or improved product or process is not possible without solving complex problems. Sometimes these solutions can be obtained only by writing computer codes that run on parallel computers built from many nodes. To enter the esoteric world of codes, nodes, and other aspects of high-performance computing, industrial firms often require the aid of appropriate computer experts. Such expertise could help many companies become more competitive in the world marketplace and manufacture safer, more efficient products.

Providing support and assistance to U.S. industry to smooth its path into high-performance computing is a prime expectation of ORNL's Center for Computational Sciences (CCS). To help meet this expectation, CCS launched the Computational Center for Industrial Innovation (CCII). This DOE national user facility, established in August 1994, hosts ORNL-industry collaborations in projects featuring high-performance computing. Thanks to our computational capabilities, CCII users are solving challenging, industrially relevant problems—problems that have previously eluded solution because of insufficient computational power or inadequate software availability.

A number of user agreements have been signed with a variety of businesses, software vendors, universities, and other federal agencies. Since the inauguration of CCII, users who have taken advantage of the substantial computational environment afforded by CCS include Reynolds Metals, Lockheed Martin Skunk Works, SENES Inc., Computational Mechanics Corp., Eastman Chemical, Samsung Advanced Institute of Technology, the Department of Transportation, UES Inc., and Tennessee State University in Nashville.

Consider these ORNL-industry collaborations that illustrate CCII's impact.

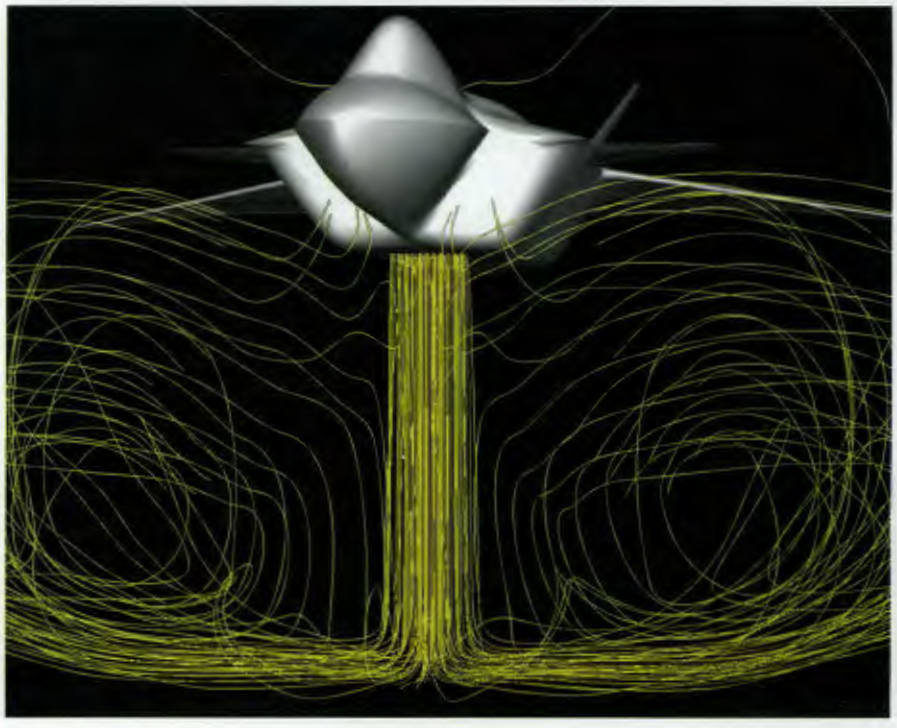


Fig. 1. Image of an advanced short takeoff and vertical landing fighter aircraft simulated by Lockheed Martin Skunk Works' scientists using computers available at the Computational Center for Industrial Innovation at ORNL. The yellow strings are particle traces of the exhaust from thruster jets during a simulated landing.

Aircraft Simulation

Advanced military aircraft are being designed to take off and land quickly, avoiding the need for long runways. To explore the aerodynamic properties of generic "advanced short takeoff and vertical landing" fighter aircraft, Lockheed Martin Skunk Works scientists are using CCII facilities. Large, complex three-dimensional models of this type of aircraft are simulated using sophisticated computational fluid dynamics codes. Shortened takeoff distances and vertical landings for these aircraft are made possible by using additional jet outlets under the aircraft's fuselage and wings to provide a large vertical thrust. Investigating the design parameters of this aircraft using conventional experimental techniques is difficult and expensive. By using the high-performance computational facilities of CCS, Skunk Works scientists can rapidly and accurately simulate many aircraft systems and flight envelopes while reducing the number of costly physical experiments that must be performed (see Fig. 1).

Modeling Aluminum Production Processes

Reynolds Metals scientists are using CCII facilities to model industrial magnetohydrodynamic processes in which a magnetic field interacts with a conducting fluid. These processes are widely used in the aluminum industry for stirring, confining, and controlling liquid metal before and during casting operations. In addition, after the aluminum solidifies, inductive heating devices are frequently used both in the rolling of the aluminum ingots into strips and in the final heat treatment of the strips. Accurate modeling of these processes is important for both control of the existing manufacturing processes and design of future enabling technologies. This modeling, however, is computationally intense because of the strong coupling among various physical phenomena, such as heat transfer, electromagnetism, and fluid flow. Differences in magnitude between the size of the processes (typically meters) and the scale of change of the parameters that must be modeled (often millimeters) further complicate the calculations. Preliminary modeling of these complex industrial processes has been achieved by using the powerful Intel Paragon computers in CCS.

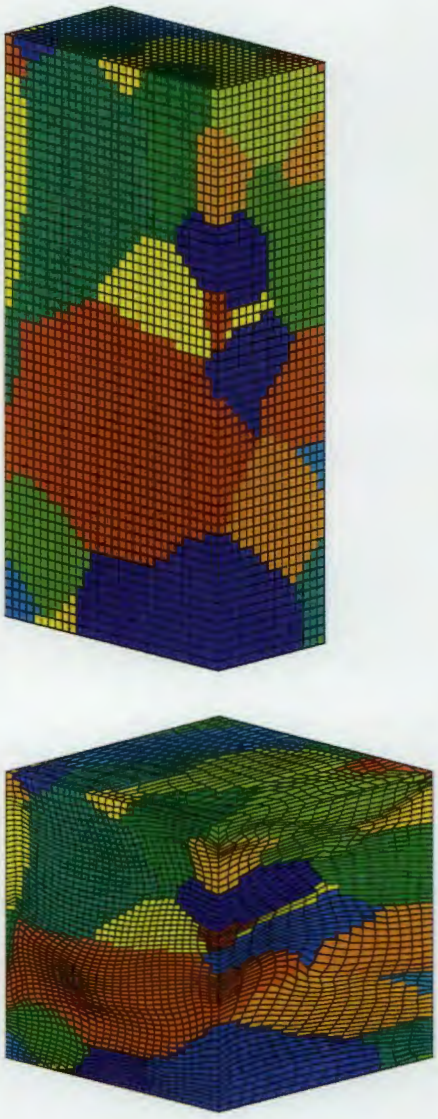


Fig. 2. This colorful image shows how the polycrystalline microstructure of aluminum changes during deformation. By modeling the nonuniform deformation of metals using a parallel supercomputer, scientists can obtain information on how to optimize processing conditions to obtain desired microstructures—and properties.

Modeling microstructural changes that accompany the deformation processing of aluminum is another important area in which Reynolds Metals and ORNL scientists are collaborating. Bulk deformation processes, such as rolling, extrusion, and forging, are routinely used in the aluminum industry to form, shape, and modify the strength of aluminum products. Of particular interest to researchers modeling these processes is the subtle change in crystal texture during deformation.

By using the Intel Paragon computers in CCS, researchers can model the micro-mechanical changes within an aluminum product and integrate them into a continuum framework to enable a simulation of bulk deformation processes that accurately reflects the metal's prior deformation history. A hybrid finite element analysis formulation, coupled with a model for crystalline plasticity theory, is used to simulate the texture change during the metal's plastic deformation. Preliminary results from the models of several deformation processes (see Fig. 2) agree with micrographs of aluminum products undergoing deformation.

Car Performance Simulation

An important national goal in transportation is to design an automobile that travels three times farther on a tank of fuel than the average car today, yet emits virtually no pollutants. Leaner, cleaner cars now being designed would be made of materials lighter than the steels used today—materials such as aluminum, magnesium, and plastic composites. One safety question of great interest is whether a properly designed car made of these lighter materials would be as resistant to damage in a collision as vehicles made of steel. Using CCS computers at CCII to simulate automobile performance involving cars made of various materials, scientists are addressing questions related to vehicle safety, fuel efficiency, and emissions.

Researchers at the U.S. Department of Transportation are collaborating with ORNL researchers to evaluate simulation capabilities for automobile performance modeling using high-performance parallel computers; to evaluate new algorithms and material models for advanced structural materials being developed at ORNL; and to evaluate biomechanical simulation of the effects of safety systems, such as air bags, on human models during automobile collisions. (This activity is discussed in more detail in the article "Analysis of Material Performance in Automotive Applications" by Srdan Simunovic, Gus Aramayo, and Thomas Zacharia, starting on p. 100.) Several different collision scenarios are being modeled to explore and optimize vehicle simulations. These simulations use a massively parallel, finite element analysis program. The program calculates vehicle accelerations, velocities, deformations, and forces, taking into consideration variables such as different materials, impact interactions, complex constraints, and spot welds. The results of this collaborative research will produce accurate vehicle and material models that can be used to evaluate the performance of lightweight materials in vehicles with respect to safety and fuel efficiency.

Modeling Internal Combustion Engines

ORNL scientists and collaborators are developing better computational tools for modeling the complex physical processes in internal combustion engines. These tools will help the automobile and power generation industries design engines with improved fuel efficiency and lower emissions of harmful combustion by-products. CCII users are exploring internal combustion engine simulation using models developed for the KIVA computer program. KIVA is a computer model that analyzes the coupled fluid dynamics, fuel spray dynamics, combustion and pollution formation reactions, and heat transfer in an engine cylinder. It is a widely used analysis tool within the industry. (KIVA is discussed in more detail in the article "Computational Engine Modeling" by Osman Yaşar, starting on p. 116.) By applying the processing power of the Intel Paragon XP/S 150, more realistic engine models that take into account the physics of the process can be developed to explore operational regimes that may reduce emissions of nitrogen oxides. Researchers from Samsung Advanced Institute of Technology investigated computational engine modeling after being taught general parallel computational techniques during their three-month stay at CCII in the spring of 1996.

Modeling Airplane Ice Deposits

The accumulation of ice on wings has been considered a contributing cause of several crashes of commuter airplanes. Ice accretion on airfoils (surfaces of a wing, propeller blade, or rudder, whose shape and orientation control stability, direction, lift, thrust, or propulsion) is being studied by CCII users at Tennessee State University (TSU), who have been using CCS facilities to apply high-performance computing techniques to several areas of their research. TSU researchers are developing and extending a coupled computational fluid dynamics, heat transfer, and mass transfer model that simulates the air flow around an airfoil under conditions that are conducive to the formation and buildup of ice deposits. Improving models of ice buildup on airfoils may help researchers determine design and operational parameters that reduce the adverse aerodynamic effects caused by the ice.

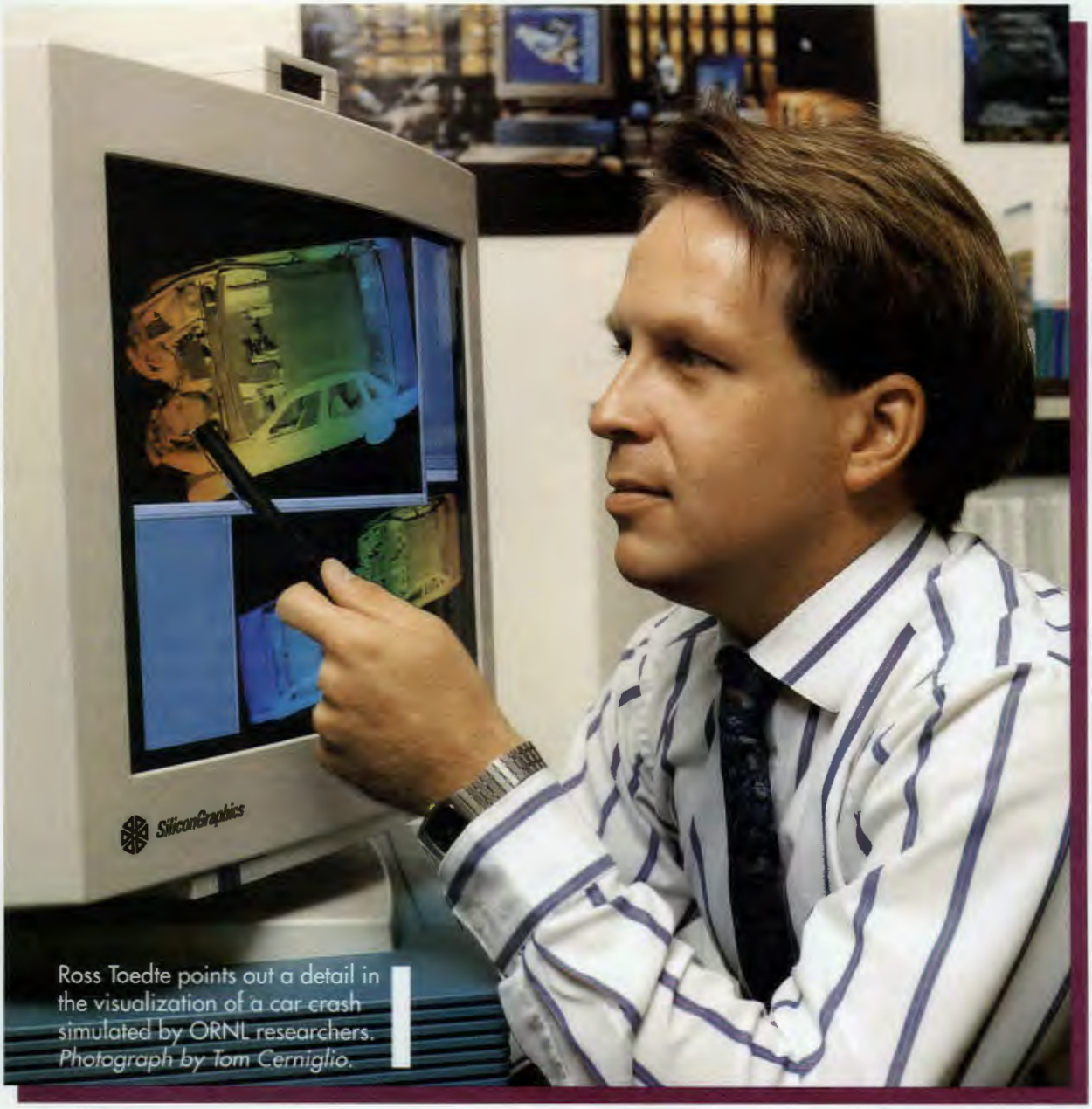
Conclusion

Other projects under way at CCII involve computational chemistry, materials processing and design, engineering design, nuclear reactor modeling, and manufacturing strategies. Additional companies are joining the center, and still more, upon learning of CCII capabilities and accomplishments, are considering membership. By calling upon the capabilities and systems provided by CCS to help open doors to industry, CCII is helping to meet an important need of U.S. industry—computational tools and skills for economically designing safer and more efficient new products, improving the competitiveness of American industry in the world marketplace. **ornl**

BIOGRAPHICAL SKETCH

W. HARVEY GRAY, then director of the Computational Center for Industrial Innovation (CCII) at ORNL and now deputy director of the National Security Program Office for Lockheed Martin Corporation's DOE plants in Oak Ridge, is a mechanical engineer who has a Ph.D. degree from Vanderbilt University. He has held a variety of positions at ORNL since joining the staff in 1974. His position in the Center for Computational Sciences involved managing CCII, the Department of Energy's national user facility that serves as the focal point for industrial partnerships with ORNL in the critical area of high-performance computing. Prior to accepting this position, he was a group leader in the Computing and Telecommunications Division, where he led projects in computer-aided manufacturing, electronic medical records, and computer-aided engineering data exchange. In addition, he represented ORNL on the CAM-I Next Generation Manufacturing Systems project and on several DOE complex-wide computer-aided design, manufacturing, and engineering committees. Earlier, as a member of the Laboratory's research staff, he used high-performance computing to design and develop advanced superconducting magnets for fusion projects.

Scientific Visualization at ORNL



Ross Toedte points out a detail in the visualization of a car crash simulated by ORNL researchers. *Photograph by Tom Cerniglio.*

Interpreting the world around us as visual images is an activity humans have been engaged in throughout history. Even our cave-wall pictures tell a story. Visualization of the physical world is one manifestation of this activity. The ultimate goal of science is insight into physical phenomena, and visualization serves to tell this story. It enhances the verification of expected results and highlights the unexpected. Similarly, as Richard Hamming, senior lecturer at the Naval Postgraduate School, stated so succinctly, "The purpose of computing is insight, not numbers." In addition, the ability to share information visually is the most effective way people can communicate. The role of the Center for Computational Sciences Visualization Laboratory at ORNL is to enhance insight through the use of visualization and virtual (immersive) techniques as well as state-of-the-art software and hardware.

By Ross Toedte and Dianne Wooten

In 1990, the Visualization Lab at ORNL (see the *Review*, Vol. 23, No. 2, 1990), dubbed the VizLab, was formed to help ORNL researchers develop scientific visualizations of their data and results of their calculations. The VizLab then was part of the Graphics Development Section of Martin Marietta Energy Systems, Inc. Our primary mission was to acquire and demonstrate visualization technology, educate ORNL users, and provide proof-of-principle visualizations for researchers to justify the use of such technology in their own work. Visualization was promoted as a tool for science.

In 1994, ORNL's Center for Computational Sciences (CCS), which is part of what is now Lockheed Martin Energy Research Corporation, absorbed the Visualization Lab because of the unique fit between its ongoing computational science interests and the VizLab's capabilities. With the mission of ORNL in mind, the VizLab now focuses on being a key participant in the scientific discovery process. By providing state-of-the-art visualization hardware, software, and techniques, the VizLab partners with scientists to augment their investigations. This focus has enabled the VizLab to contribute to ORNL's awareness of the importance of visualization. In addition, researchers from most ORNL divisions have taken advantage of the VizLab's resources to produce significant results.

Through CCS we have had the opportunity to work on numerous ORNL projects in areas such as materials science, groundwater remediation, car crash safety, and nanotechnology. One such project was with Malcolm Stocks of the Metals and Ceramics Division, who conducted a study of the magnetic properties of alloys. The VizLab was able to visualize a lattice of copper and nickel atoms with vectors attached to each atom (see back cover). Each vector represented the magnitude and direction of the atom's magnetic moment. As these vectors changed over time, an animation was created that was useful in helping researchers understand the unique magnetic behavior of the alloy.

Visualization's Role in Scientific Discovery

The roots of computer-based visualization and virtual (immersive) reality can be traced to such pioneers as Ivan Sutherland in the 1960s. Sutherland, viewed by many as the father of computer graphics, cofounded Evans and Sutherland Computer Corporation. His research contributed early to the development of military flight simulators. Since that time, visualization has had an ever more pronounced effect on scientific discovery at research institutions around the world. (For examples of discoveries in which ORNL visualizations played a role, see Figs. 1, 2, and 3.) From its early use in simulating terrain navigation, visualization has affected the very scientific method it serves. Computer-assisted visualization has become commonplace and has been used advantageously in nearly every type of research. Now, we hardly consider how this silicon and software-based technology has changed the process in which it is embedded. Examples of visualization can be readily found in microscopy, earth sciences, materials science, and every discipline in between. Today, the interpretation of visual results often determines whether an experiment is continued, terminated, or modified and restarted.

This fundamental change in the experimental process has occurred only partly because of the availability of computing technology. Another important contributing factor has been the rapid reduction of computer prices, which has encouraged researchers to use computers to integrate with or even replace more traditional equipment in their labs. Recent reductions in federal research funding have aroused increased interest in purchasing low-priced, graphics-capable computers for experimental laboratories.

Essential Tool for High-Performance Computing Environments

Visualization has been intimately linked to high-performance computing since its advent in the 1970s. Whether they employ large monolithic processors, vector processors, massively parallel processors, or combinations thereof, high-performance computing engines have one consistent trait—lots of data. A 1989 report funded by the National Science Foundation entitled *Visualization in Scientific Computing* states, "The human brain cannot interpret gigabytes of data each day, so much information goes to waste." Since the publication of that report and because of continued advances in computer performance, it is reasonable to replace the prefix "giga" with higher-order prefixes such as "tera" or even "peta." Future advances along the computational power curve will undoubtedly result in even larger data volumes, necessitating increased reliance on new visualization and multisensory techniques for interpretation.

Visualization is critical to the operation of these computing environments in a manner that is effective for researchers. Visualization has a role not only in understanding the results of a computer simulation once it has concluded but also in viewing

the results as they are produced. If the results are not desirable, it may be necessary to change the simulation parameters while the simulation is running. This ability to change parameters is called "computational steering." The technique was first exhibited at the 1989 SIGGRAPH computer graphics conference in Boston. Simulations running on computers in Illinois were changed on the fly with input from a terminal on site at the conference.

Elements of Visualization

When a scientist comes to us for help in presenting data, we first determine how the visualization is going to be used. The technique we recommend depends partly on whether the visualization is to be used as part of a presentation or as an analysis tool. A very-high-quality static image or video animation is more costly to generate, but it may be better suited for use in a conference or as part of a presentation for future funding of a project. A simple, inexpensive image or animation may be the best solution for a researcher who needs to analyze data from multiple computer simulations. We also ask a prospective user to identify, if possible, the most important phenomenon he or she wants to observe or show. We can then tune the visualization to highlight that aspect of the science.

Consider a materials science problem of finding the area of the highest density of electrical charges within a three-dimensional (3D) volume. One way to simplify the process of looking into a volume is to break the problem down into a series of two-dimensional (2D) slices running along one of the axes of the volume. Each slice of the volume shows the charge density as a color contour map within that slice. The original volume can be represented by an outline of a rectangular box. The series of images generated by visualizing a perspective view of this box with each of the slices correctly oriented within the box produces an animation.

Another method of visualizing data in three dimensions is to generate isosurfaces. An isosurface is a surface generated by connecting all data in the volume that have the same value. In groundwater contamination modeling, a 3D volume of concentrations can be simplified by generating isosurfaces of different contaminant concentrations

Numerous visualization techniques are now available, ranging from simple

Dianne Wooten uses the VizLab's video capabilities to show molecular dynamics results from a project with researchers Don Noid and Bobby Sumpter of the Chemical and Analytical Sciences Division. *Photograph by Tom Cerniglio.*

x/y graphs to complex virtual reality environments. Images produced using 3D bar charts, contour plots, isosurfaces, molecular models, 2D cutting planes for 3D volumetric data, vector flow fields, and particle tracing can greatly enhance the understanding of science. We choose the best technique for presenting as much data as possible in an image without confusing or distorting the original data. In addition, annotation is important for clarifying what the scientist is trying to communicate. Just as a "picture is worth a thousand words," so is a picture worth millions of numbers.

VizLab Infrastructure and Capabilities

Once you have decided what you want to visualize and how to convey your meaning to your intended audience, you have to consider how to achieve your end product. Visualization is an activity that is highly leveraged by hardware and software. The availability of different software tools and the appropriateness of computing hardware are the keys to effective visualization. CCS has made significant investments in both of these areas in the quest to create a flexible visualization environment adaptable to the needs of ORNL and any of its affiliate organizations involved in computational science. These investments can be categorized as modeling, rendering, and animation on the software side; the principal hardware components include graphics generation, networking, and storage equipment. These elements do not make up the entire visualization infrastructure of CCS. However, they represent most of the major functional categories of a CCS visualization infrastructure that has successfully helped facilitate collaborative computational science activities involving ORNL, other national laboratories, universities, and industrial centers.

Modeling for visualization is not to be confused with modeling a physical process. The goal of the former is to meaningfully represent data produced by the latter using any of a variety of software packages.

One way of classifying these packages is by the maximum spatial dimensionality of the data representations they can produce. The packages mentioned in this article are not the only solutions, but we have proven to ourselves that they are well suited to particular visualization needs. Interactive Data Language (IDL) is an excellent package for looking at one-dimensional (e.g., *x/y* charts) and 2D data (images). IDL also has an animation capability for revealing how particular data change over time. Advanced Visual Systems (AVS) is another package that can be used for these types of data, but it is rather lean in its annotation capability. Where AVS really shines is in its flexibility in combining different visual cues into a complex but cohesive visualization application that can handle time-transient data. On the high end, we use the Wavefront Advanced Visualizer package to import complex 3D models (e.g., car bodies or manufactured parts) or to build from scratch models that are compositions of large numbers of simple geometric primitives such as triangles, polygons, and hexahedra.

Rendering is the process of creating a realistic view of a 3D scene for projection onto a 2D computer screen. To do this effectively, all factors that affect a particular view of the world should be considered, including surface smoothness, light intensities, perspective, and reflectance. AVS has a rudimentary rendering capability, but it ignores some ingredients of realistic scenes, such as shadows. Wavefront Advanced Visualizer has an excellent renderer for creating photo-realistic scenes. The tradeoff, of course, is that rendering a complex scene with this degree of realism takes longer—up to half a day on a mid-range workstation.

Ensuring that the visualization end product meets but does not exceed the need is critical for precisely this reason. A rough-cut visualization of airflow over a wireframe model of an aircraft wing is quite sufficient for on-screen inspection by a team of researchers working in close physical proximity. Save the half-day renderings for audiences at conferences and meetings with program sponsors. At these venues, the important technical points have been identified in advance, possibly through visualization. The degree of visualization "polish" needed for these purposes typically goes beyond that needed during scientific exploration.

Animation enables the use of physical time to look at a particular data parameter. Animation of a time-transient 3D problem is, for this reason, considered to be four-dimensional visualization. Often the animation parameter is the time step or iteration of the simulation that produced the data, but any data parameter can be suitable. For example, geologic core sample data could be animated as a function of the depth of the sample, possibly isolating a particular mineral in a slice of the core sample in a manner difficult to produce using other techniques, such as isosurfacing.

We employ a number of animation tools in the VizLab for handling various animation file formats. Hardware support of graphics varies greatly from workstation to workstation. The graphics engines used in the CCS VizLab range from single-processor Macintoshes to high-performance multiprocessor Silicon Graphics workstations. A number of our workstations have specialized chip

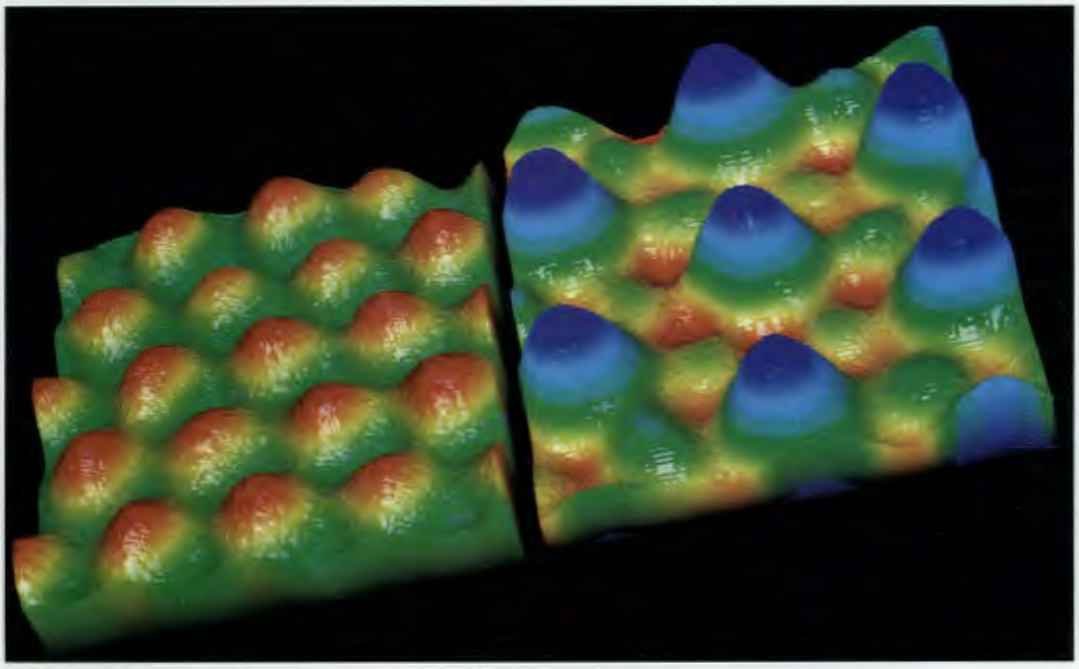


Fig. 1. Joe Carpinelli (Ph.D., May 1997), a physics student under the direction of University of Tennessee–ORNL Distinguished Scientist Ward Plummer, documented the first glimpse into how a charge density wave is formed at the surface of a crystal. Carpinelli explains that a temperature change can sometimes induce a crystal to lower its symmetry. "The electrons rearrange themselves to form something of a wave," he says. He used VizLab resources to enhance a visualization of such phenomena to produce this image, which appeared on the cover of the May 1996 issue of *Nature* magazine.

sets for expediting graphics processing. For example, hardware *z*-buffering is used for fast rendering of 3D scenes. By subdividing or "slicing" a scene along its depth, or *z*-axis, and determining which slices the object intersects, resolution of hidden objects becomes easier, simplifying a scene prior to rendering.

Texture mapping, a hallmark of virtual reality environments, is useful for making 3D scenes geometrically simple without sacrificing apparent realism. The objects are wrapped with digital images to give them a more varied and natural look. Often, these images can be produced procedurally to create a particular pattern. Let's say you wanted to model an orange. You can geometrically model it as a simple smooth sphere. It becomes realistic only when you drape it with a digital image of a fine-grained, semi-random pattern of hues ranging from orange to brown. These hues mimic the minute ridges and valleys of the orange peel.

The VizLab works as an integral piece of the CCS computational science infrastructure, creating implications for networking and storage to provide the speed and storage capacity needed for the problems being solved by CCS and its collaborators. Currently, we use fiberoptic-based networking on our higher-end machines to achieve data transfers an order of magnitude beyond Ethernet speed. We anticipate an investment in more advanced networking technologies to boost this nearly another order of magnitude. A total of 60 gigabytes of local disk storage is used to handle a wide range of data requirements.

We have several novel hardware devices that also deserve mention. Stereo viewing is essential for depicting 3D scenes realistically. Simulation of humans' natural ability to focus their eyes independently on objects to achieve a sense of depth is handled in two ways in the VizLab. In 1995, we acquired a high-resolution desktop stereo display. Called the Fakespace PUSH, this device has two 1280- by 1024-pixel 1-inch cathode-ray-tube displays, which the user looks at through a flexible face piece that resembles a SCUBA mask. The optics are mounted on an articulated tripod stand. PUSH's optics head moves independently from this tripod. The user moves virtually through a scene by pushing, pulling, and twisting the optics head while looking at the displays. Simpler but less natural stereo viewing is done by using shutter glasses. These glasses alternately restrict viewing to one or the other lens. The shuttering is synchronized to the graphics board of the computer via infrared light that pulses at a frequency of 60 Hz. On the positive side, these glasses are inexpensive and feel like regular glasses on your head. The downside is the mismatch between physical motion and virtual motion—that is, movement through the scene is facilitated by hand motion rather than head motion.

Tool for Public Communication

At its most basic, visualization is intended to facilitate understanding and communication, both of which are concepts intimately tied to education. It naturally follows that visualization is an invaluable tool for communication at all education levels. VizLab visualizations have been used in high school and university science education courses to facilitate education in computer science, visualization, and various other science disciplines. In recent years, the Saturday Academy for Computing and Mathematics (SACAM) program at ORNL enabled high school students from across the state to experience the Laboratory on a personal level. One of the SACAM technical seminars focused on the use of high-performance computing and visualization to address real-world problems. A half-day course introduced the students to scientific problems and ways to model them, visualize the results of the computational models, and interpret the resulting visualizations to gain understanding. The benefits these young adults obtained from the course are multiple. They included a greater appreciation of math and science, realization of the role interpersonal communication plays in a complex working environment, and exposure to new and exciting technologies.Conveying to the general public the complex nature of research activities at laboratories like ORNL is very difficult. Many of these research activities potentially have direct effects on society. However, many people have problems grasping the societal implications of these activities. Insufficient communication of the ramifications of this work breeds misunderstanding.

Visualization is a natural and effective way of remedying this problem. Take, for example, the VizLab's role in ORNL's computational nanotechnology effort. Nanotechnology involves research in the physical properties of objects miniaturized to a scale of thousands of atoms. Through visualization, it becomes obvious how different customized molecular structures can be useful in medicine, communications, and environmental applications. This enhanced communication can help create a sense of partnership between research organizations and the public.

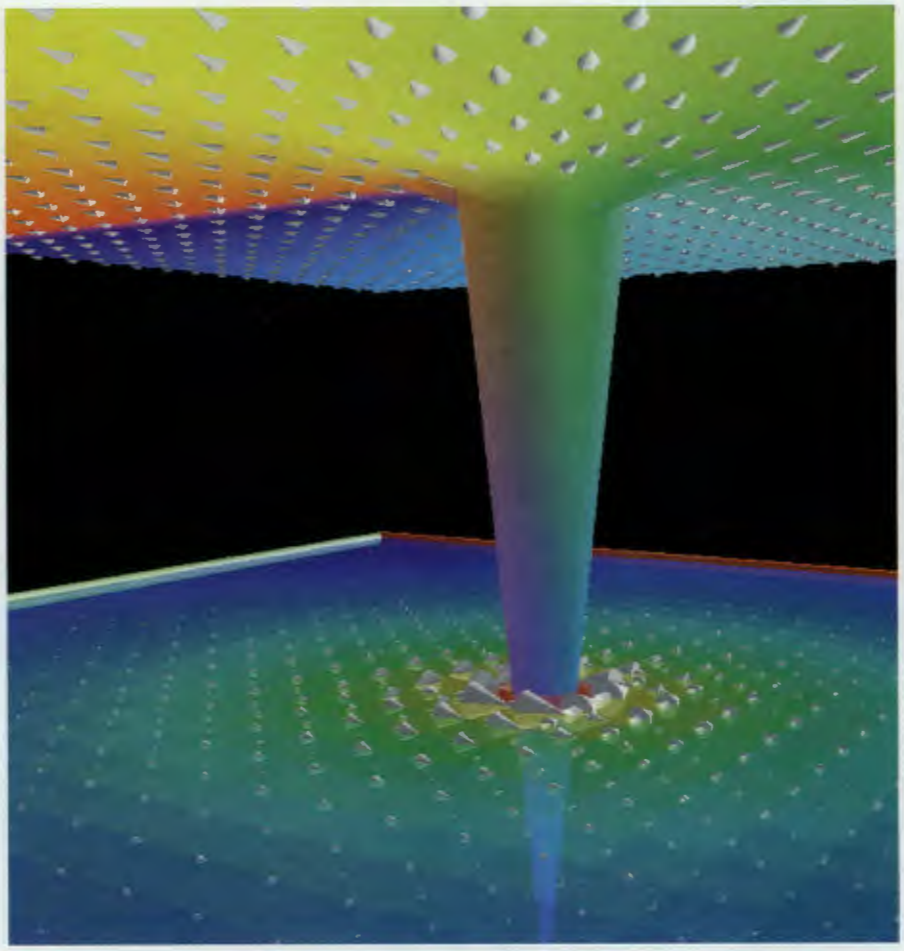


Fig. 2. This visualization, dubbed the "blue tornado," represents the results of calculations by visiting scientist Paul Miller concerning the vortex state which arises when a magnetic field penetrates a superconductor by creating normal, nonsuperconducting regions (see cover).

Visualization and the Entertainment Industry

Toy Story, the full-length computer-animated movie produced by Pixar, recently made its way from the box office to the corner video store. With this event, more people are being exposed to the leading edge of Hollywood's computer prowess, which has blossomed into a special effects industry that has helped rescue California's

ailing economy. Few people realize, however, that Hollywood is a leading source of computer graphics research. This research, in turn, migrates into commercial packages including those for visualization.

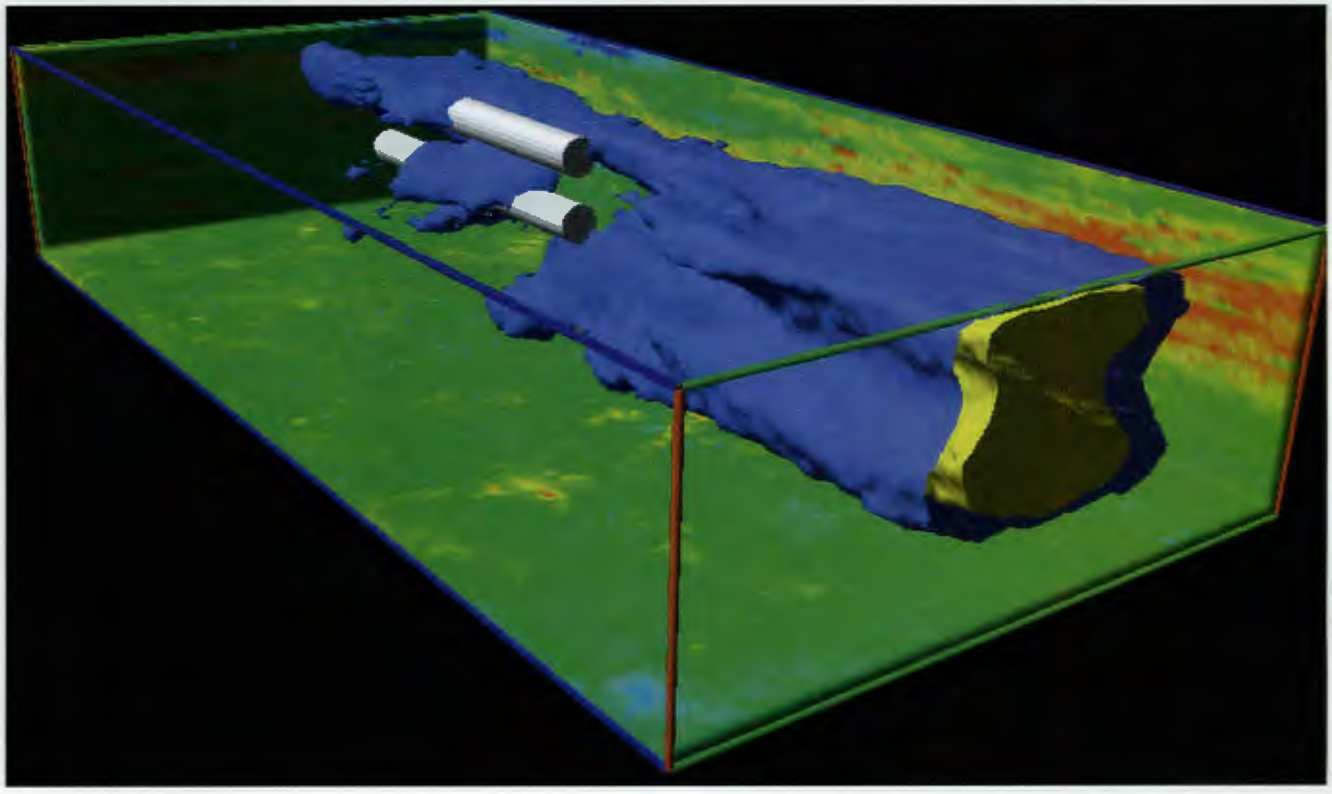
In the mid-1980s, computer graphics artists working for movie producer George Lucas at Lucasfilm were instrumental in the development of fast hidden-surface and shading algorithms. Particle flow models developed in the early 1990s were initially used to simulate natural waterfalls. These same algorithms have found many practical applications, such as in automobile manufacturing and fluid-flow modeling. The RenderMan rendering language, developed by Pixar and now available in commercial off-the-shelf products, is responsible for the realism seen in individual frames of *Toy Story* and past Pixar productions. Industrial Light and Magic is the LucasArts subsidiary responsible for blockbuster special effects seen in the past 15 years in movies such as *Star Wars*, *The Abyss*, and *The Mask*. *Star Wars* took 3D modeling to a new level with its highly detailed depictions of spacecraft and space travel. *The Abyss* provided a new approach to 3D morphology; the "virtual" star of the show was an alien pseudopod, seemingly composed entirely of sculpted water.

Because of its innovative chip designs, Silicon Graphics has been a driving force in the computer hardware market since the early 1980s. These designs are the platform of choice for the entertainment companies previously mentioned. Whether chip design precedes or follows societal demand for new forms of entertainment is debatable and probably unresolvable. As for visualization and virtual reality, it takes little mental effort to imagine the impacts of these technologies on the scientific research community. Moreover, as you watch these effects unfold in the movies or on television, you can envision applications that have significant implications for society. For example, imagine a driving simulator so immersive that it could affect human behavior in addition to helping measure it. Current technology makes possible the Iowa Driving Simulator at the University of Iowa. The simulator uses state-of-the-art graphics along with audio and a motion platform to examine a range of engineering and safety issues relevant to designers of cars and highway systems.

Immersive Reality

Immersive reality, also known as virtual reality, can be viewed as an

Fig. 3. This simulation, by G. Mahinthakumar of CCS, on the Intel Paragon shows the impact of heterogeneity on pump-and-treat remediation of contaminated groundwater.



extension of visualization. A tool for understanding high-volume and complex technical data, it involves the visual sense and often requires high-performance graphics. However, immersive reality differs from visualization because it appeals to more than just the visual sense to enhance understanding. It delivers realistic stimuli to the senses—especially sight, hearing, and touch—and minimizes overall system latency.

Immersive reality was originally developed by the military as a way to give personnel experience in varied, high-stress environments without exposing them to potential harm. More recently, it has been used as a way to experience theoretical circumstances and proposed products prior to their manufacture.

Specialized input/output hardware, some unique to immersive reality, has evolved for working in simulated worlds. Head-mounted displays (HMDs) are used to deliver stereo views of a 3D scene to the user. Navigation, pointing, and selection are handled by various hand-oriented input devices. Both HMDs and hand input devices use embedded positioning devices known as trackers to communicate location to the computer. The computer generates views of the 3D scene that are appropriate for the tracked position and actions.

Sound is useful as both an input and output medium. Although several systems exist for receiving and interpreting voice commands for the computer, each has a practical vocabulary limitation of several hundred words. The systems must be programmed to understand the speech nuances of the user, such as accent, pronunciation, and tempo. Directional sound can be simulated by replicating a sound across several speakers and varying the amplitude between speakers.

A recent development in immersive reality is the availability of haptic, or touch, devices. These devices simulate the sense of feel through various means. The most effective of these uses a motorized, articulated arm. By varying the resistance of one or more degrees of freedom of the arm, you can simulate properties such as gravity and kinetic energy.

Future Directions

Our foremost near-term goal is the development of visualization as an element of seamless computing environments. Interfaces that transparently enable derivation of meaning from and control of computing processes is critical to visualization's role as a research tool. We are continuing to investigate and integrate new products into our lab for immersive exploration of scientific worlds. We are also interested in exploring Web-based technologies, especially those that fully support 3D. Java and VRML have particularly interesting features for distributing visualization and immersive reality applications. Lastly, we are keenly interested in robust software that can be integrated with our visualization tools. The value of these tools will be measured by the extent to which they enable our collaborators to dynamically modify the worlds they see and the way they see them. Ultimately, our future research will be driven by the tools that offer the greatest contribution to the evolving cycle of scientific discovery through visualization of computational and experimental results. ornl

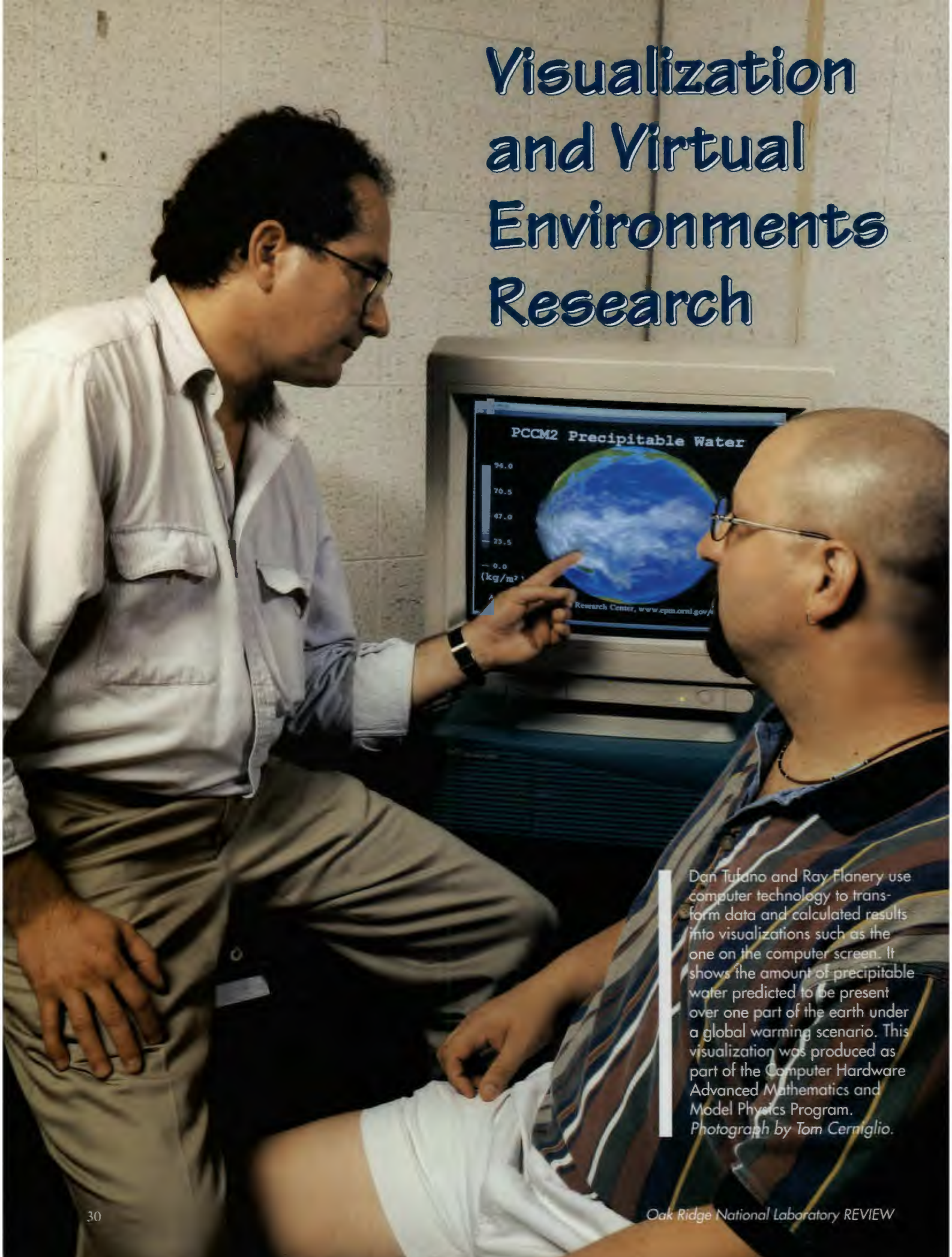
Dianne Wooten analyzes visualizations of atomic-scale interactions in important materials. *Photograph by Tom Cerniglio.*

BIOGRAPHICAL SKETCHES

ROSS J. TOEDTE is the visualization manager for ORNL's Center for Computational Sciences (CCS). His current activities include development of advanced graphics techniques for computational science, graphics systems integration, and visualization education. He has a B.S. degree in computer science from Southern Illinois University and has done work for an M.S. degree in computer science at the University of Tennessee at Knoxville. He has held a variety of positions at ORNL since joining the staff in 1981. His current position involves managing the CCS Visualization Lab (VizLab). In addition to the CCS staff, the VizLab serves affiliates of the Computational Center for Industrial Innovation, Partnerships in Computer Science (PICS) partners, and the ORNL research community. Before taking his current position, he was a computing specialist in the Computing and Telecommunications Division (C&TD). He has worked as a visualization practitioner and promoter since cofounding the visualization lab in C&TD in 1989. As a member of the Graphics Development Section from 1983 to 1989, he was involved in a wide range of graphics activities including corporate graphics device support and mainframe graphics consulting. He has also worked as a computing analyst in on-line and database systems. His professional interests include virtual reality, scientific visualization, animation, and video technology.

DIANNE WOOTEN is a computing specialist in CCS specializing in scientific visualization. She has a B.S. degree in mathematics from Tennessee Technological University and an M.S. degree in computer science from the University of Tennessee at Knoxville. At the CCS Visualization Lab, she provides visualizations in the form of prints, overheads, animations (on computers and on video), and virtual reality. Her interests include developing Web technologies and working with ORNL scientists to provide scientific insight through visualization. Prior to this current commitment, she worked in system support capacity, maintaining and developing computer codes used for computer graphics. She has worked with a number of ORNL scientists over the years, providing visualizations of their scientific data for analysis and for presentation materials. Most recently, she has developed Web-based applications that provide multiplatform accessibility to corporate data.

Visualization and Virtual Environments Research



Dan Tufano and Ray Flanery use computer technology to transform data and calculated results into visualizations such as the one on the computer screen. It shows the amount of precipitable water predicted to be present over one part of the earth under a global warming scenario. This visualization was produced as part of the Computer Hardware Advanced Mathematics and Model Physics Program. *Photograph by Tom Cerniglio.*

By Raymond E. Flanery, Jr., Nancy W. Grady, Joel W. Reed, and Daniel R. Tufano

Visualization and virtual environments research at ORNL is being spearheaded by the Advanced Visualization Research Center in ORNL's Computer Science and Mathematics Division. Previous research has included visualization for climate modeling, seismic modeling, and melting simulations, as well as visual interfaces for data mining. Current and future research areas include three-dimensional medical imaging, Web-based visualization, and multimodal interfaces for virtual environments.

Nancy Grady and Joel Reed discuss the results presented in a visualization (shown on the screen) of interest to the gas and oil industry. Produced as part of the Gas and Oil National Information Infrastructure Project, this visualization reveals subsurface structure based on measurements of the energy of acoustic waves passed through underground rock formations. *Photograph by Tom Cerniglio.*

Until recently, there were two kinds of scientists: theorists and experimentalists. But science is entering a new era in which research is classified in three ways: theory, experiment, and computer simulation. With the maturation of simulation as a full partner in the research enterprise comes an increasing need for visual communication techniques between the computer and the researcher. The Advanced Visualization Research Center (AVRC) in ORNL's Computer Science and Mathematics Division (CSMD) seeks to address this need. The Grand Challenge class of simulations strains the limit of hardware and software because of its computational intensity—the large size of the data sets involved and the large bandwidth needed for data transfer. Further, the increasing complexity of the data sets requires more sophisticated techniques for optimal human perception. With these research needs in mind, CSMD created AVRC.

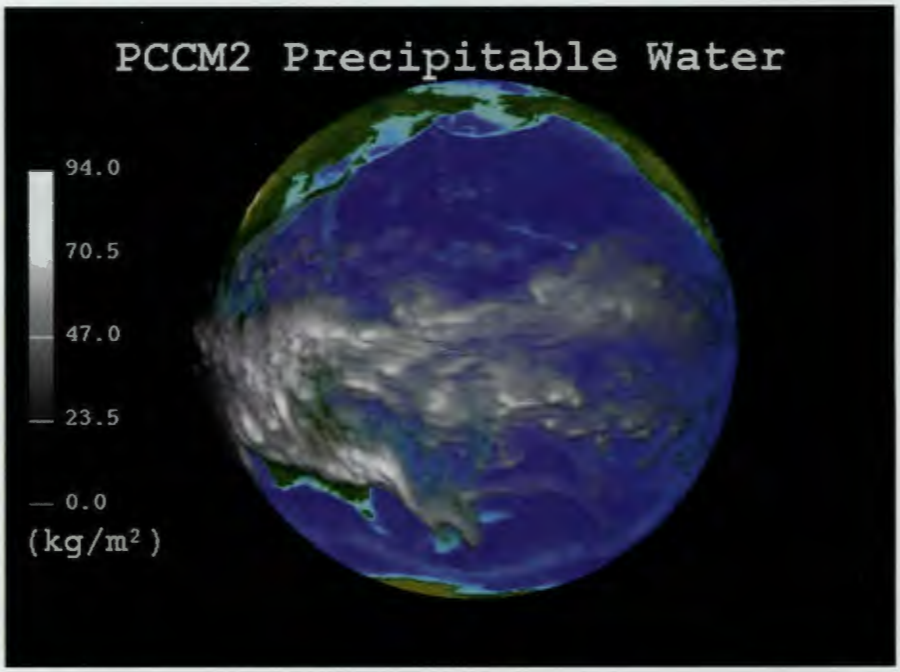


Fig. 1. View of precipitable water in the atmosphere, generated using the commercial visualization package AVS. The distribution of precipitable water is a key to important climatic trends such as drought, heavy rainfall, and destructive storms. See additional images on the back cover.

Large Data Sets

One of the first issues to be addressed was the handling of large data sets. ORNL is a participant in the Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP) Program with Argonne National Laboratory (ANL) and the National Center for Atmospheric Research (NCAR). This DOE program seeks to rapidly advance the science of climate prediction over decade and longer time scales, linking the emerging technologies in high-performance computing to the development of computationally efficient and numerically accurate climate prediction models. At full resolution, this project will generate 72 terabytes (TB) of data for a single 100-year climate simulation. This level of data creation has necessitated the development of techniques to use disk space as memory, and tape storage as others use disks, to make sufficient resources available for visualization of this data. Figure 1 shows a view of precipitable water in the atmosphere generated using the commercial visualization package AVS; the distribution of precipitable water is a key to important climatic trends such as drought, heavy rainfall, and destructive storms. This single frame required extracting the surface pressure and three-dimensional (3D) moisture fields from the approximately 60 variables stored during each step of the climate model. These variables are then used to calculate precipitable water at each step. A texture mesh with varying transparency is then superimposed on the globe to visually represent the precipitable water. (For video representations, see *http://www.epm.ornl.gov/vis/avrc.html* for three different mpeg videos of calculations of precipitable water from nine days to two months.) Modules were created within the AVS package to accept data being fed from the simulation running on the Intel Paragon XP/S 150 at ORNL's Center for Computational Science and processing data at the rate of one frame per simulation CPU hour to create movies.

Parallel Algorithms

A second project took a different approach to the visual analysis of large data sets. The Gas and Oil National Information Infrastructure project was a multilaboratory effort to develop the infrastructure technologies, such as computational steering, remote collaborative tools, and data distributed visualization, that are important to both the gas and oil industry and to DOE. As part of this project, supercomputers at four national laboratories—Livermore, Los Alamos, Oak Ridge, and Sandia—were used to produce a

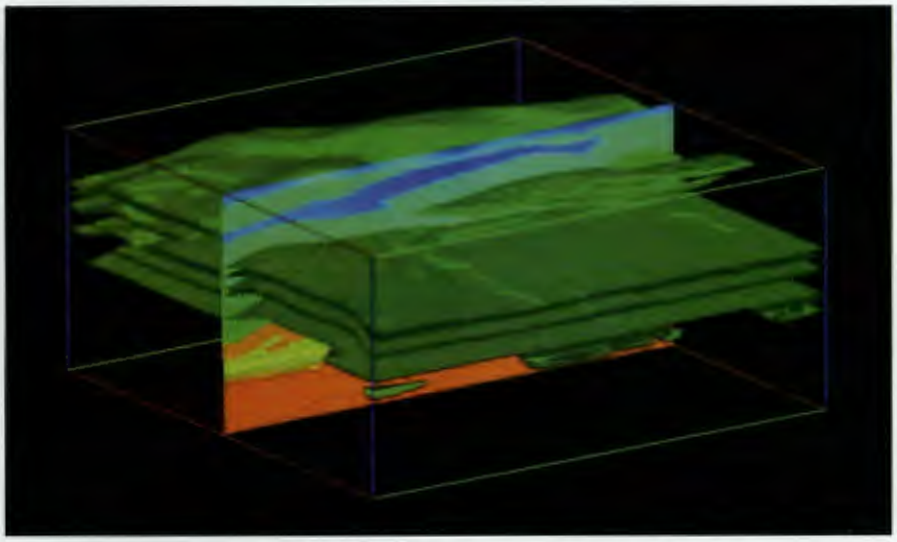


Fig. 2. This visualization reveals subsurface structure, using measurements of the energy of acoustic waves passed through and reflected by underground rock formations.

consistent data set containing synthetic seismic data. The idea was to create a visualization that reveals subsurface structure using measurements of the energy of acoustic waves passed through and reflected by underground rock formations. To facilitate processing of this 2- to 4-TB data set housed at the National Storage Laboratory at Livermore, data-parallel visualization techniques were developed to spread the computational load for isosurfaces (surfaces of constant velocity, indicating subsurface structure) within these data across a cluster of processors. The data were divided into slabs (groups of bytes), and the marching-cubes-based isosurface algorithm was used to process the data in parallel. Marching cubes is a contouring algorithm that creates surfaces of constant scalar value in three dimensions [W. E. Lorensen and H. E. Cline, "Marching Cubes: A High Resolution 3D Surface Construction Algorithm," *Computer Graphics* 21(3): 163–69, July 1987]. The results were reunited for rendering on the host visualization machine. Figure 2 shows the subsurfaces generated from this synthetic seismic data.

In Situ Vitrification

In situ vitrification (ISV) was developed by DOE's Pacific Northwest National Laboratory (PNNL) to stabilize radioactively contaminated soils in place. An electrical current is used to melt radioactive waste in underground soil, forming a leach-resistant glassy material. AVRC has developed codes that allow researchers to track the melt front during an ISV experiment. The code uses such information as temperature profiles (measured by a set of thermocouples), as well as the temperature and position of four graphite rods used to deliver the electrical energy. The final melt shape predicted by these codes matched extremely well the final shape of the solid, as measured after the experiment. The codes employ techniques from statistical analysis,

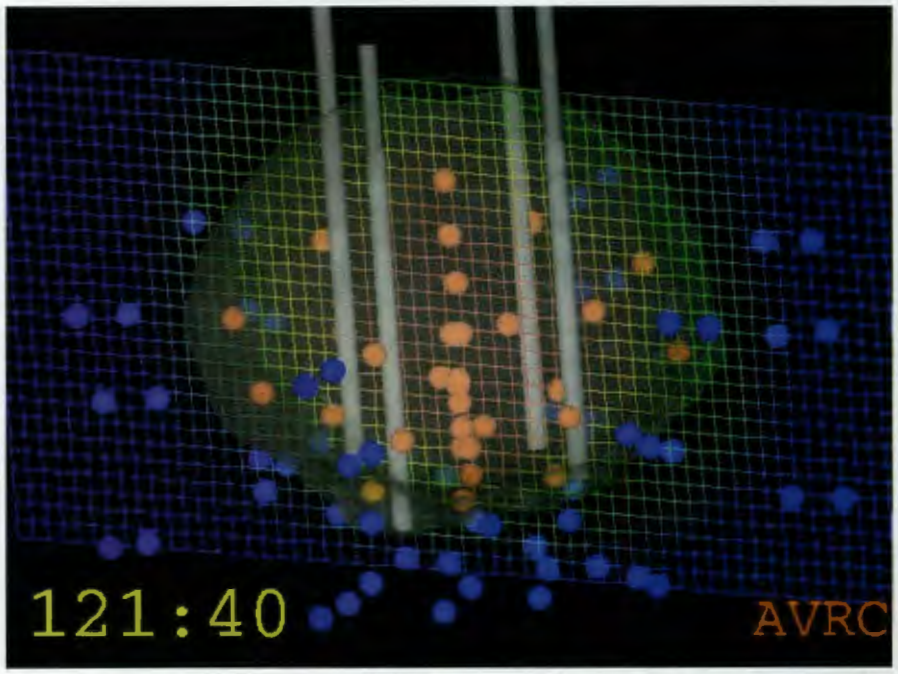


Fig. 3. Visual representation of data to predict final melt shape after an in situ vitrification experiment to seal waste in the ground. Shown are a set of spheres for each thermocouple for measuring temperature profiles (colored for temperature), cylinders showing the position at each time step of four graphite rods delivering electrical energy, and a surface showing the melt front.

numerical analysis, and visualization to take this spatially sparse set (about 90 values per time step) of temperature history at more than 8000 time steps. For each time step the temperature distribution is approximated throughout a $64 \times 64 \times 64$ volume with an isosurface representing the melt front in the soil, as shown in Fig. 3. The data are visually represented as a set of spheres for each thermocouple (colored for temperature), cylinders showing the position at each time step of the graphite rods, and a surface showing the melt front. The researcher can then interact with this visual representation of data either by rotating the image or by selecting a viewing position interactively and observing the development of the melt front over time as an animation.

Mathematical Algorithms for Surface Rendering

The entertainment industry is becoming one of the leading users of computers, as a medium for creating their art; in fact, the special effects industry is transforming computer visualization. The computer provides a great deal of flexibility for rendering and doing precise drawings, making it very easy to make changes. A highly visible modeling effort involving the definition of a mesh to describe a face and the manipulation of this mesh to animate facial features is evident in the movie *Toy Story*. At ORNL a current exploratory project in computational forensics is seeking to develop the tools to automate the facial recognition process. The idea is to use the computer to reconstruct the face of a mutilated or decaying body based upon skull measurements in the hope of identifying an unknown victim and possibly the killer.

Ed Uberbacher, head of ORNL's Computational Biosciences Section, Richard Mural of the Life Sciences Division, and Reinhold Mann, director of the Life Sciences Division, have created a database of facial tissue-thickness data using measurements from magnetic resonance imaging scans of living volunteers. Researchers in ORNL's Informatics Group are developing neural network techniques to predict skin thickness at a number of marker points on a human skull. Instead of basing the reconstruction on only a dozen or so points, they used the computer to plot thousands of points, so the surfaces of the face would be mathematically based on the shape of the entire skull, not just a few landmark points directly below the skin. Researchers in the Visual and Information Sciences Group use these points to generate a mesh for the skin surface and then to smooth, color, and texture-map this surface for realism, as shown in Fig. 4. This approach is being used to support experimental perception research being done to understand the critical factors for facial recognition, a project being explored within the Human Systems Research Group. This interdisciplinary team hopes to create a prototype of the process used to automate the generation of facial features, which the user could control mathematically, thus improving the chances of a reconstructed face being recognized.

Fig. 4. ORNL researchers can reconstruct the appearance of the probable face predicted from a number of marker points on the skull, using a neural net trained on measurements from recent MRI scans of living volunteers. As shown here, these points are used to generate a mesh for the skin surface, which is then smoothed, colored, and texture-mapped for realism to improve the chances that the victim will be identified.

Visual Interface for Time Series Data Analysis

Visual analysis of time series data becomes very difficult as large quantities of data are generated. Statistical techniques developed by George Ostrouchov, Darryl Downing, Max Morris, and Val Fedorov, all of the Statistics Group, can be used to extract useful or interesting information from data sets too large for normal browsing. A researcher cannot effectively monitor large data streams and pick out regions of interest. To allow automated monitoring and subsequent user browsing of interesting regions, a visual interface was created which incorporates statistical filters to "score" the data, store the data around the region of interest into an underlying database, and present the user with a

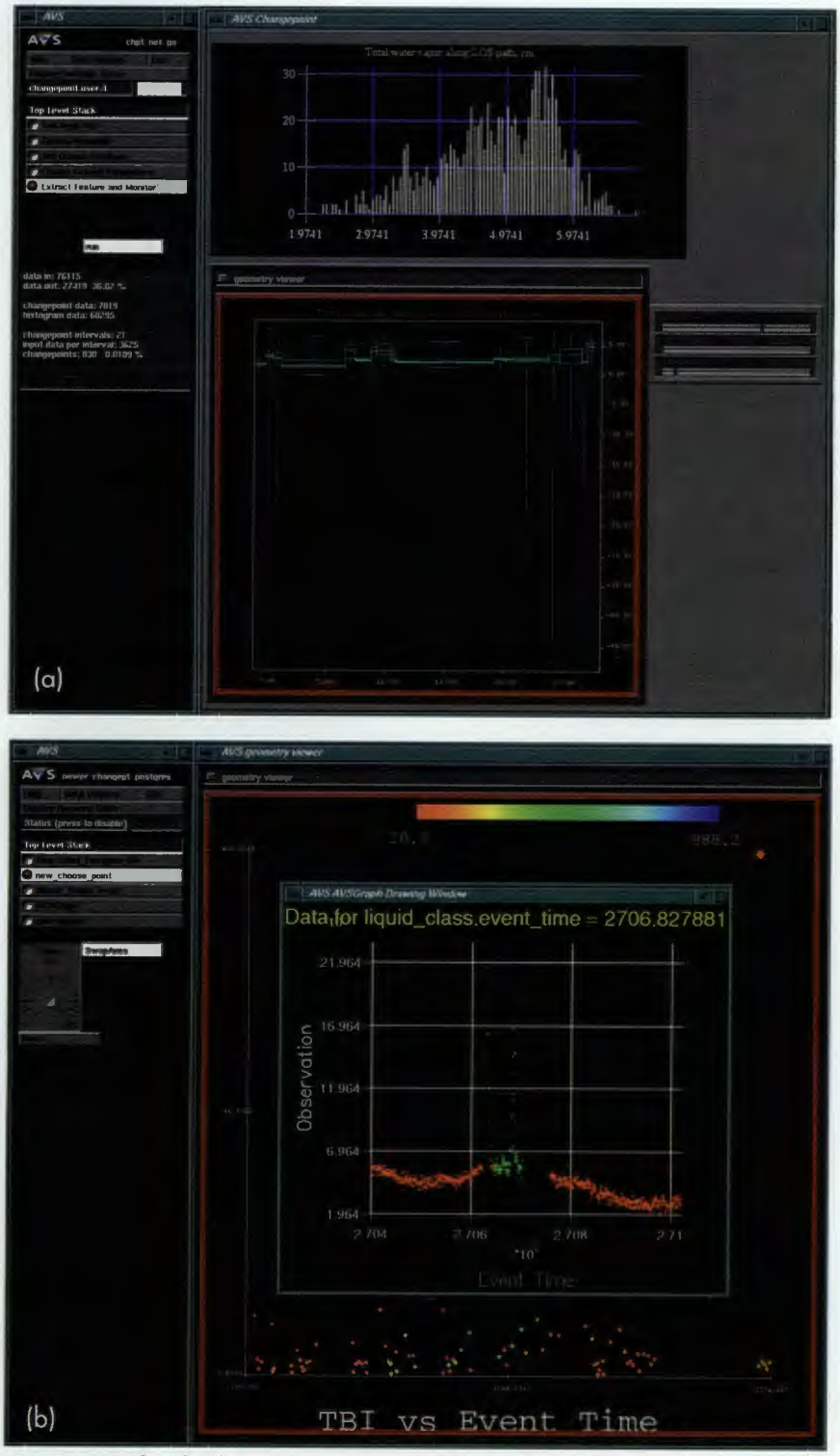


Fig. 5. (a) The displayed histogram and box plots of the raw data sections allow the user to examine the filtered data. (b) Pop-up window displays original raw data for researchers trying to understand more fully the data described in the meta-data display.

graphical interface to the scoring metadata.

The system begins by reading the raw data in intervals, applying the feature extractor to these chunks of data, and writing a representation of the filtered data to the database. During this process, as shown in Fig. 5(a), a histogram and box plots of the raw data sections are displayed, allowing the user to tailor parameters to better reduce or filter the resulting data representation.

In the visualization and analysis phase, the power of scientific visualization is used to discover unusual or interesting features of the original large data set in an easily comprehensible yet compact format. Through the visual interface the user displays one of the filtered representations of the original data. The system generates the necessary query language commands to the database system to load the appropriate filtered data.

As the user peruses the filtered data representation, the user can select a particularly interesting trend or point that appears to be worth more detailed examination. The system, via query language commands, retrieves location information about the corresponding original raw data values. The original raw data for the selection is loaded and displayed on a pop-up window, as shown in Fig. 5(b). This type of automated visual interface is important when researchers need to analyze quickly large amounts of data to determine the regions that should be examined.

Web-Based Visualization

One newly emerging visual medium is the Internet's World Wide Web. The Web has exploded in the past two years as an information exchange medium. Currently, this medium is dominated by the display of text-based information and simple graphics. A number of

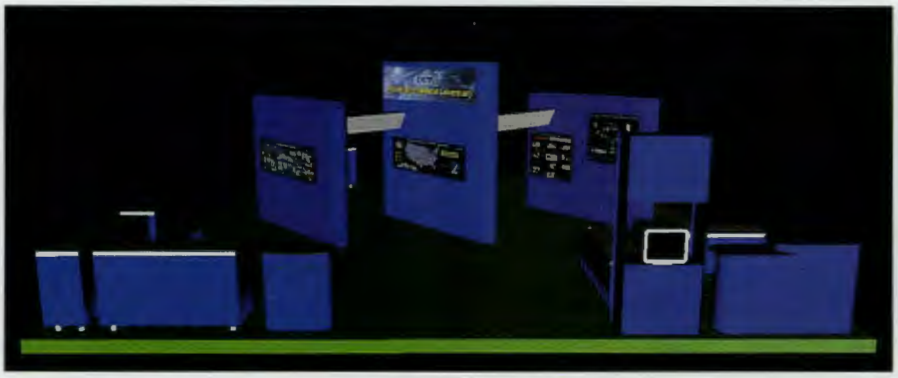


Fig. 6. A prototype of a 3D space was developed at ORNL and shown at both the Supercomputing '95 and Supercomputing '96 conferences. The booths at the conferences were created from computer-assisted drafting tools and imported into a drawing package that translated it into Virtual Reality Modeling Language. The links for additional information on any of the posters, demonstrations, and systems were inserted by hand to connect to available Web pages.

researchers are developing new capabilities that would allow them to present information within 3D spaces that can be navigated and manipulated. The Virtual Reality Modeling Language (VRML) was designed for the presen-tation of 3D worlds on the Web. It allows the visitor to interact with and manipulate the objects contained in the virtual environment. Using VRML 2.0, a 3D environment was prototyped for ORNL's participation in the Supercomputing '96 conference. Models of the objects in ORNL's booth were created using computer-assisted drafting tools, translated into VRML 2.0, and then combined to create the virtual booth shown in Fig. 6. Each poster in the scene has a behavior attached to it. When the poster is activated (by a mouse click), it highlights itself and then plays an audio file describing itself. Tools for developing 3D displays are evolving rapidly. This world may be seen at *http://www.epm.ornl.gov/sc96*. Although VRML is now largely used to display 3D scenes, it is expected to mature into a fully functional visualization medium.

Future Directions

Some recent activities have broadened visualization research at ORNL into the area of synthetic environments, a term that encompasses both workstation-based visualization and the more totally immersive user interface known as virtual reality. To build this capability, CSMD has acquired a head-mounted display, a head tracking system, and virtual world development software. A powerful new Silicon Graphics computer will provide the foundation for the research planned in this area. This research will examine ways in which humans can interact with complex data sets, using multiple sensory channels (e.g., vision, hearing) and input modalities (e.g., speech, touch, gesture). The effects of synthetic environments on human perception and motor control, and the interaction of the two, will be addressed by a program of experimental research. New application areas for these capabilities will include information visualization for networking and for data mining. Because the goal of developing synthetic environments is to create an interface that is naturally suited to human users, a multidisciplinary team has been assembled to make use of visualization, simulation, and perceptual psychology. We are ready for simulations to provide information as valid as that from theory and experiment. **ornl**

Ray Flanery views a virtual reality model of a crystal through a head-mounted display. *Photograph by Tom Cerniglio.*

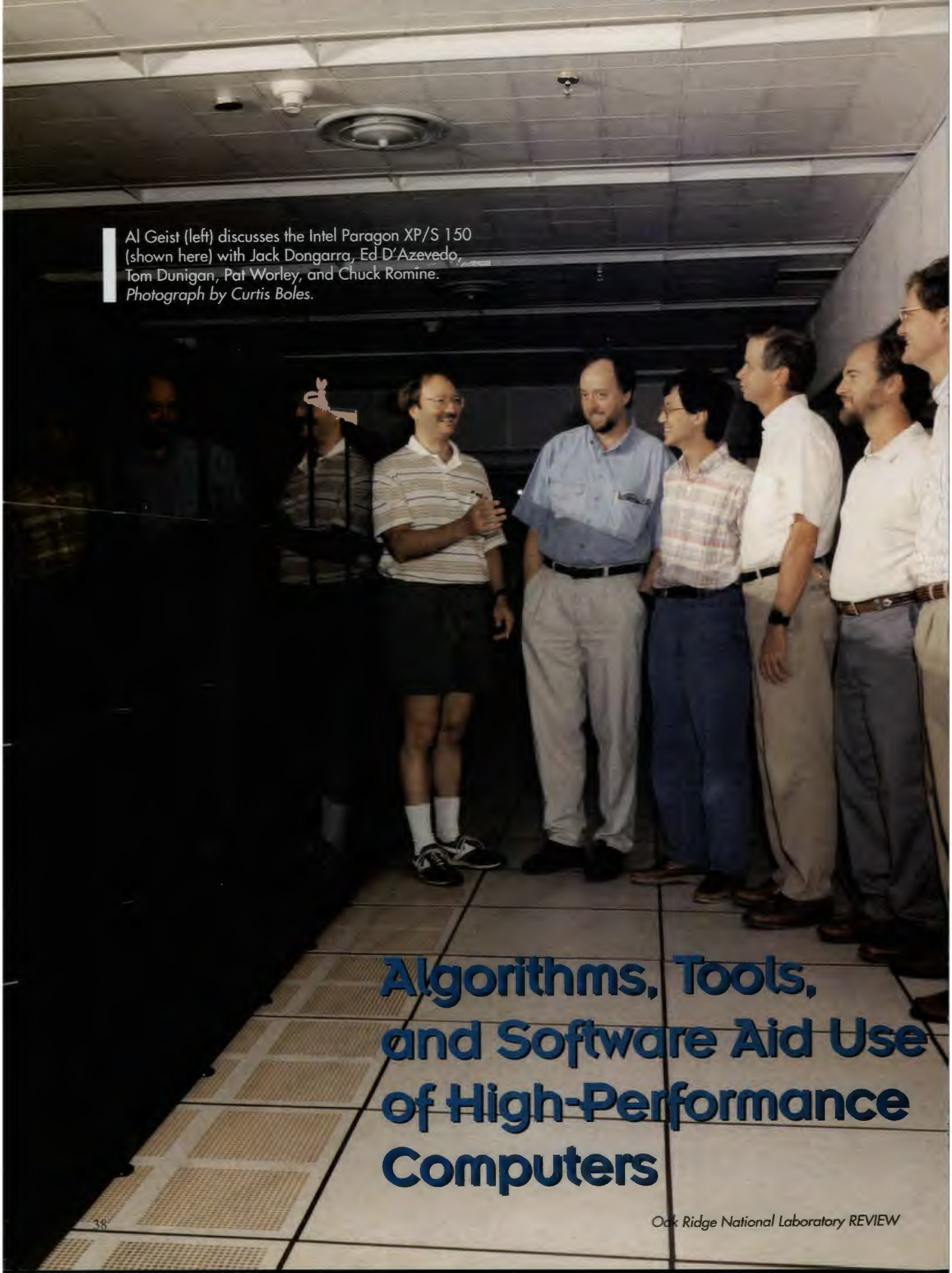
BIOGRAPHICAL SKETCHES

RAYMOND E. FLANERY, JR., is director of ORNL's Advanced Visualization Research Center in the Computer Science and Mathematics Division (CSMD). His research interests include visualization of computational applications, visualization interfaces for data mining, and multimodal interfaces for virtual environments. He received his M.S. degree in mathematics at Youngstown State University in Ohio and came to ORNL in 1987.

NANCY W. GRADY joined ORNL in 1987 as a Wigner Fellow in the Metals and Ceramics Division. She is currently leader of the Visual and Information Sciences Group in CSMD. She holds a B.S. degree in physics and honors mathematics from the University of Tennessee and a Ph.D. degree in mathematical physics from the University of Virginia. Her current research interests include scientific visualization and mathematical techniques for data mining, Web-based collaborative technologies, and information visualization.

JOEL W. REED joined the CSMD research support staff in 1995. He holds B.S. and M.S. degrees in computer science from the University of Tennessee. His interests include using Virtual Reality Modeling Language technology as a solution to Web-based visualization problems.

DANIEL R. TUFANO is leader of CSMD's Human Systems Research Group. He received a B.S. degree in psychology from Georgetown University and M.A. and Ph.D. degrees in psychology from Princeton University. He spent four years performing training effectiveness research at the Army Research Institute. The following ten years he worked at Grumman Aircraft Systems, managing the Advanced Cockpit Technology program. At ORNL his research responsibilities are in three areas: management and display of information to automobile drivers; recognition of computationally reconstructed faces; and locomotion and visual perception of spatial layout in virtual environments. His research is broadly concerned with human perception and performance.



Al Geist (left) discusses the Intel Paragon XP/S 150 (shown here) with Jack Dongarra, Ed D'Azevedo, Tom Dunigan, Pat Worley, and Chuck Romine. *Photograph by Curtis Boles.*

Algorithms, Tools, and Software Aid Use of High-Performance Computers

By Ed D'Azevedo, Jack Dongarra, Tom Dunigan, Al Geist, Chuck Romine, and Pat Worley

ORNL and University of Tennessee at Knoxville (UTK) researchers are at the forefront in developing tools and techniques for using high-performance computers efficiently. Parallel Virtual Machine software enables computers connected around the world to work together to solve complex scientific, industrial, and medical problems. The Distributed Object Library makes it easier to program the Intel Paragon supercomputer, recently enabling the ORNL Paragon to break a computational record in molecular dynamics simulations. The Distributed Object Network I/O Library increases the performance in data input and results output on the Intel Paragon, often by as much as an order of magnitude. ORNL and UTK researchers are also leaders in ongoing efforts to standardize the message-passing parallel programming paradigm and to develop improved techniques for evaluating parallel computers.

In the past decade, the world has experienced one of the most exciting periods in computer development, and ORNL researchers have played key roles in these developments. Computer performance improvements have been dramatic—a trend that promises to continue for the next several years.

One reason for the improved performance is the rapid advance in microprocessor technology. Microprocessors have become smaller, denser, and more powerful. Indeed, if cars had made equal progress, you could buy a car for a few dollars, drive it across the country in a few minutes, and "park" the car in your pocket! The result is that microprocessor-based supercomputing is rapidly becoming the technology of preference for attacking some of the most important problems of science and engineering.

To exploit microprocessor technology, vendors have developed *massively parallel computers*. ORNL has always been at the forefront in acquiring and using the latest of these computers. In 1986, ORNL acquired Serial No. 1 of the Intel iPSC-2, containing 64 Intel 386 processors. More recently, ORNL has installed the Intel Paragon XP/S 150, one of the largest parallel computing systems in the world. It contains 3204 high-speed processors and has a peak performance of 150 gigaflop/s—that is, it can perform 150 billion basic arithmetic operations per second.

Massively parallel systems offer the enormous computational power needed for solving Grand Challenge problems such as simulating the climate. Unfortunately, software development has not kept pace with hardware advances. New programming paradigms, languages, scheduling and partitioning techniques, and algorithms are needed to exploit fully the power of these massively parallel machines.

A major new trend for scientific problem solving is *distributed computing*. In distributed computing, computers connected by a network are used collectively to solve a single large problem. Many scientists are discovering that their computational requirements are best served not by a single, monolithic computer but by a variety of distributed computing resources linked by high-speed networks. This worldwide popularity of distributed computing can be traced back mostly to software developed in ORNL's distributed computing research project.

Combining several parallel supercomputers with distributed computing techniques can produce unprecedented computational power. Recently, researchers at ORNL and Sandia National Laboratories (SNL) combined the 3204-processor computer at ORNL with the 2680-processor computer at SNL to solve a large computational problem in materials science.

In this article, we explore some of the issues involved in the use of high-performance computers. These issues are at the heart of effective use of the fastest supercomputers. In particular, we consider software tools and performance evaluation.

Software Tools

The widespread acceptance of parallel computers as an environment for high-performance scientific computation has been inhibited by the lack of efficient and portable parallel software. Writing parallel software is much more difficult than writing sequential software: parallel programs must express both the sequential computations and the interactions among the sequential computations that define the parallelism.

A number of software tools developed at ORNL, discussed below,

promise to reduce the complexity of parallel programming.

Enabling heterogeneous network computing. Until recently, all computers on a network were considered separate units connected merely to allow users to transfer files and send electronic mail to each other. Today, researchers in high-performance computing are combining computers on the network in such a way that users can exploit their aggregate performance and memory to run a single parallel application.

A collection of computers that differ in their architecture or in their method of representing data are called heterogeneous. Heterogeneous network computing offers several advantages over large-scale parallel computers:

- Cost is reduced by using existing hardware, usually a collection of workstations.
- Performance can be improved by assigning each individual task to the most appropriate architecture.
- Development and debugging use the familiar tools running on the user's personal workstation.
- User-level or program-level fault tolerance (the ability to operate continuously in the event of a failure) can be implemented either in the application or in the underlying operating system.

On the other hand, getting heterogeneous computers to communicate and cooperate with each other is a challenging computer science problem.

To solve this problem, ORNL's distributed computing research project, in collaboration with the University of Tennessee at Knoxville (UTK), produced the Parallel Virtual Machine (PVM) software package. PVM permits a heterogeneous collection of computers linked by a network to be used as a single large parallel computer.

PVM enables users to exploit their existing computer hardware to solve much larger problems at minimal additional cost. The software and documentation are available from the World Wide Web site listed at the end of this article. ORNL researchers are continuing to explore the frontiers of distributed computing, working on security, fault tolerance, high-speed asynchronous transfer mode (ATM) networks, and graphical interfaces to assist users in programming for distributed computing.

Today, hundreds of sites around the world are using PVM to solve important scientific, industrial, and medical problems. Automotive, aerospace, chemical, computer, environmental, medical, pharmaceutical, and oil companies are all using this software as a cost-effective way to design new products. DOE national laboratories, National Science Foundation supercomputer centers, and National Aeronautics and Space Administration research centers, as well as numerous universities around the country, are using PVM both for research and as a teaching tool. With thousands of users, PVM has become the de facto standard for distributed computing worldwide.

Standardizing the message-passing model. The message-passing model is a programming paradigm used widely on parallel computers and on networks of workstations. The basic concept of communicating through messages is well understood, and over the past 10 years, many significant applications have been recast into this paradigm. More recently, several public-domain systems have demonstrated that a message-passing system can be implemented efficiently and portably.

Message passing is used to specify the communication among a set of processes forming a concurrent program. The message-passing paradigm is attractive because it is portable and scalable. Message passing is compatible with distributed-memory multicomputers, shared-memory multiprocessors, networks of workstations, and combinations of these elements. Many diverse message-passing systems were developed, but until 1994, no standard was agreed upon.

In 1992, ORNL and UTK spearheaded an international effort to define a standard interface for message passing. The effort involved more than 80 people from approximately 40 organizations from the United States, Asia, and Europe, including computer vendors and researchers from universities, government laboratories, and industry. This effort recently culminated in the publication of the Message-Passing Interface (MPI) standard.

The MPI standard defines the syntax and semantics of a core of library routines useful to a wide range of users writing portable message-passing programs in Fortran 77 or C. MPI also forms a possible target for compilers of languages such as High-Performance Fortran. Both commercial and public-domain implementations of MPI exist. These run both on tightly coupled, massively parallel processors and on networks of workstations.

Emulating shared memory. The Intel Paragon XP/S 150 at ORNL's Center for Computational Sciences consists of a collection of processors, each with its own local memory, connected by a high-speed communication network. The processors coordinate the computation and exchange of data via message passing. However, efficient coding for these processors requires careful decomposition of data structures and explicit calls to pass data among processors.

Researchers in ORNL's Computer Science and Mathematics Division have developed the Distributed Object Library (DOLIB) to make the Paragon easier to program. DOLIB is a library of Fortran- and C-callable routines that create a shared-memory programming environment for the distributed-memory Paragon.

The original motivation for the creation of DOLIB was in the context of parallel Lagrangian particle tracking on the Paragon, where the message traffic pattern changes dynamically depending on the location of particles at run time. (Lagrangian particle tracking is a numerical technique used in computational fluid dynamics for such applications as the transport of contaminants in groundwater and the advection of moisture in the atmosphere.) Previous efforts to parallelize particle tracking on the Paragon generally involved decomposing the computational grid into subdomains, with padding (or extended "ghost regions") to contain flow-field information from neighboring regions. The time step was then restricted to ensure that no particle could exit the extended region. This approach is relatively simple to program, but creates a serious dilemma. If the extended regions are small (to conserve memory), a severe constraint may be placed on the size of the allowable time step. On the other hand, too large an extended region incurs a heavy cost in memory use and communication traffic. For three-dimensional problems with relatively high-velocity flow, the dilemma may have no acceptable solution.

A more natural approach is to consider the flow field as a globally shared array. Processors "directly" access only the flow-field information they require, using gather and scatter operations. As a result, particles can be allocated dynamically to the processors. DOLIB has been used to parallelize several codes for the Paragon. One such code is a semi-Lagrangian transport (SLT) code, which is used for climate simulations. Using DOLIB, researchers were able to parallelize SLT easily. The performance of the resulting code is competitive with a hand-parallalized code that uses explicit message passing and extended regions. Moreover, on high-resolution refined grids, the amount of memory available for extended regions severely constrains the time step. Thus, the DOLIB version has an advantage.

SOTON-PAR, a molecular dynamics code, has also benefited from DOLIB. ORNL researchers modified SOTON-PAR to use DOLIB's global shared memory. The DOLIB shared memory version allows more efficient use of global aggregate memory, which allows running a billion-particle simulation on the Intel Paragon at ORNL. The DOLIB version shattered the previous world records for simulation size (600 million particles on the 1024-node CM-5 and 400 million particles on ORNL's Paragon). Figure 1 shows that the code has almost ideal scalability with problem size and number of processors.

Speeding the input/output. Getting data in (and results out) of a parallel supercomputer fast enough is a challenge for many high-performance applications. To speed disk input and output on the Intel Paragon, ORNL researchers developed the Distributed Object Network Input/Output (I/O) Library (DONIO). The system uses the aggregate global shared memory provided by DOLIB as a large (gigabyte) disk cache. On most high-performance supercomputers such as the Intel Paragon, the communication network has a much higher bandwidth (bytes per second) than the disk subsystem. By caching data in the memory of remote processors instead of writing to disk, DONIO can achieve

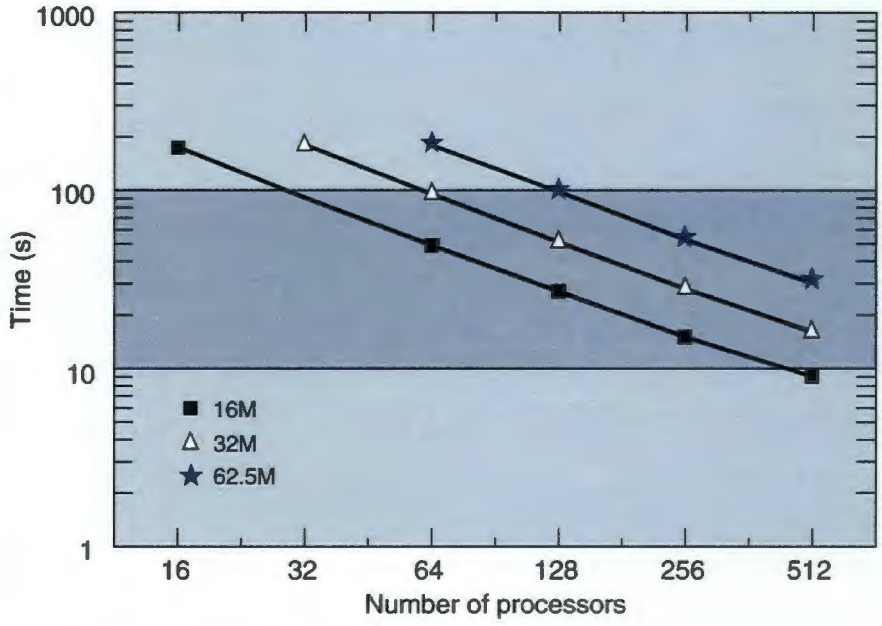


Fig. 1. Using DOLIB, the SOTON-PAR molecular dynamics code shows linear speedup in number of processors and also in the number of atoms.

an order-of-magnitude speedup over native system routines. The library also reads or writes data to multiple disks concurrently to achieve near-peak I/O performance.

The DONIO library has been used in several significant applications. For example, researchers used DONIO in a computational chemistry application to reduce time for checkpointing (saving intermediate results used for resuming computation) from 30 minutes to about 50 seconds. In another application, a code for seismic analysis used DONIO to reduce I/O time from nearly 2.5 hours to only 5 minutes. Researchers at Lawrence Livermore National Laboratory are also interested in adapting DONIO for their PARFLOW saturated groundwater code to run on the Cray T3D.

Performance Evaluation

The software tools described previously are used to provide a programming environment or to improve performance on high-performance computers. Performance evaluation is concerned with measuring performance and determining whether and how performance can be improved. For example, performance studies of I/O on the Paragon were used to optimize the implementation of DONIO on the Intel Paragon.

Several metrics are used in evaluating parallel computer architectures. One of the principal scientific metrics is megaflops, millions of floating-point operations per second that a benchmark or application can achieve on a given computer system. For a parallel computer, we usually measure the mega-flops on a single processor and then calculate the performance when multiple processors are used to execute the benchmarks or applications. Ideally, we hope for *scalability:* that an application will run 10 times faster on 10 processors than it did on one processor, and 1000 times faster on 1000 processors.

Message-Passing Performance

Another indicator of performance involves communication by sending messages. Typically, two separate metrics are involved: *latency*, or the time it takes to send a small message between processors, and *throughput,* or the data rate (in bytes per second) achieved when transferring a large message between processors. Figure 2 illustrates the message-passing performance of several parallel processors using these two metrics. The upper-left region of the plot is the high-performance area, whereas the lower right represents the performance of a typical local area network like Ethernet. Another related metric is the latency and bandwidth of I/O, whether reading/writing to a disk or exchanging messages with some other (slower) external device.

In the following subsections, we discuss benchmarking, in which these and other metrics are measured, and performance evaluation methodology.

Benchmarking. The term *benchmarking* is drawn from its use in surveying, where it represents a mark on a stationary object whose position and elevation have been measured. Once made, the mark is used as a reference point in tidal observations and surveys. Analogously, benchmarking of a computer system is intended to measure new systems relative to a reference point on current systems. In particular, benchmarks are standardized computer programs for which there is a history of measurement data (typically timings) for executions of the programs with specifically defined input and repeatable output.

Benchmarking the performance of a computer is a complicated issue

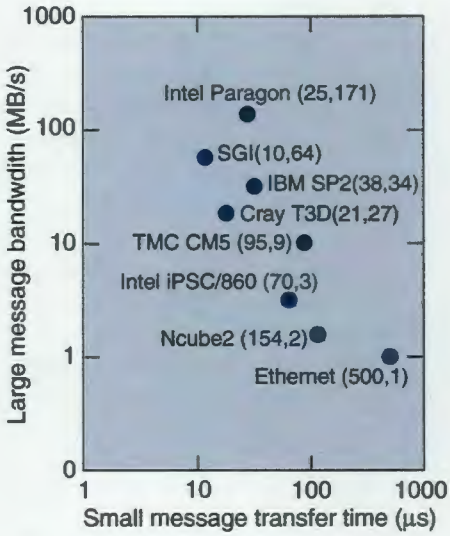


Fig. 2. Message-passing performance.

because it is a function of many interrelated quantities. These quantities include the application, the algorithm, the size of the problem, the choices of high-level language and implementation, the level of human effort used to optimize the problem, and the compiler's ability to optimize, as well as the operating system, architecture, and hardware characteristics of the system under test.

Because of this complexity, benchmarks typically are only one of many criteria used to evaluate computer performance. Nevertheless, such benchmarks are helpful to algorithm designers seeking the optimal coding style for a given system, to system developers seeking to match machine characteristics to the requirements defined by their target workloads and represented to them through the benchmarks, and to individuals and groups seeking to procure the appropriate computing system for a given installation.

Several benchmarks have evolved for both scientific and commercial processors. Among the best known for scientific computing are the Livermore Fortran Kernels, the Los Alamos Benchmarks, the NAS Kernels, and the

LINPACK tests. Recently, motivated by a growing concern in the supercomputing community that existing benchmarks are too simplistic to fully represent scientific computing, researchers have attempted to define new standards. These efforts include the ParkBench activity, initiated by researchers at ORNL and UTK, and the System Performance Evaluation Cooperative (SPEC) project.

Performance evaluation methodology. While benchmarking is primarily concerned with performance measurement, the performance evaluation process also involves deciding which benchmark (and other performance) data to collect and how to use it to answer specific performance-related questions.

For example, the performance evaluation of a computer system may determine whether the system is an appropriate platform for some given task or for a given workload (set of application programs or tasks). This type of evaluation is a crucial part of the procurement process, identifying which computer system to purchase or buy time on. If a particular computer system cannot do the required job in the required time, its cost does not matter.

Performance evaluation can also be used to identify how components of the computer system interact. Such evaluation is important in identifying which components are most limiting to performance and how they might be modified to improve performance. Similarly, evaluation activities are important for providing guidance in the use of the computer, identifying what the computer is good at doing, and which tasks are expensive to perform (and should be avoided or minimized). For example, on distributed-memory machines like the Intel Paragon or IBM SP2, there is a range of costs in accessing data, depending on where those data currently reside: in the local memory of the processor that is scheduled to use the data, in the local memory associated with a different processor but that is accessible via a fast network connection, or in some storage device that is accessible only via a slower network connection. Programming to take advantage of data locality (assigning data to the local memory of processors that are most likely to need the data) is generally a good idea but is not always possible or may require costly restructuring of an existing program. Understanding the relative costs of accessing data from different levels of the memory hierarchy can indicate how important it is to exploit locality (and minimize accesses to nonlocal data).

The evaluation process examines the computer system at a variety of *levels*. In low-level tests, the individual elements of the system are exercised—for example, determining how quickly a processor can compute a result, or determining how quickly a processor can access data from local memory, from nonlocal memory, or from an external storage device. These tests try to determine not only peak performance (the best that can be achieved), but also the performance that is typically achieved, and what factors distinguish between peak and typical performance.

The next level is kernel performance: looking at the ability of the system to solve common algorithmic problems or execute system functions. Here, the focus is on seeing how quickly a single processor can calculate, say, a matrix-matrix multiplication or compute a fast Fourier transform, how quickly a group of processors might accomplish the same or larger versions of these tasks, and how quickly one processor can broadcast data to all of the other processors. The reason behind the performance of a given kernel may not always be clear from these tests, but the kernels are chosen to be important functions whose execution time is of intrinsic interest.

The final level is performance of application programs. Initially, these are programs in the required workload that are just being ported to the new system, or they are already ported and optimized programs that are representative of the programs in the workload. For the first type of program, the performance reflects the minimum that can be achieved, but if these application programs cannot or will not be modified, their performance is the most (or only) relevant measurement in the evaluation process. Usually, however, programs will be adapted to make better use of the computer system over time, and the kernel and low-level performance measurements can be used to indicate how much improvement is possible. The application program tests are also the best evaluation of the compilers, which have been the weakest component in some high-performance computer systems. It is frustrating for an application developer to have access to a fast computer system, only to find that the compilers perform so poorly on application programs that the desired performance is not achieved. For example, Fig. 3 shows megaflops per processor as a function of the number of processors for a climate-related parallel application code run on the Intel Paragon, the IBM SP2, and the Cray Research T3D.

The relative "flatness" of the curves for the Paragon indicates good scalability—that is, per-processor performance is retained when the number of processors increases. One implication of these results is that the interconnection network is fast, and communication costs are manageable. However, the Paragon results also indicate poor performance for the compiled Fortran code when compared to the peak performance of the microprocessors. The results for the SP2 and T3D show better per-processor absolute performance, but are approximately the same fraction of the peak rate for the underlying microprocessor.

A recent addition to the evaluation process is the evaluation of different

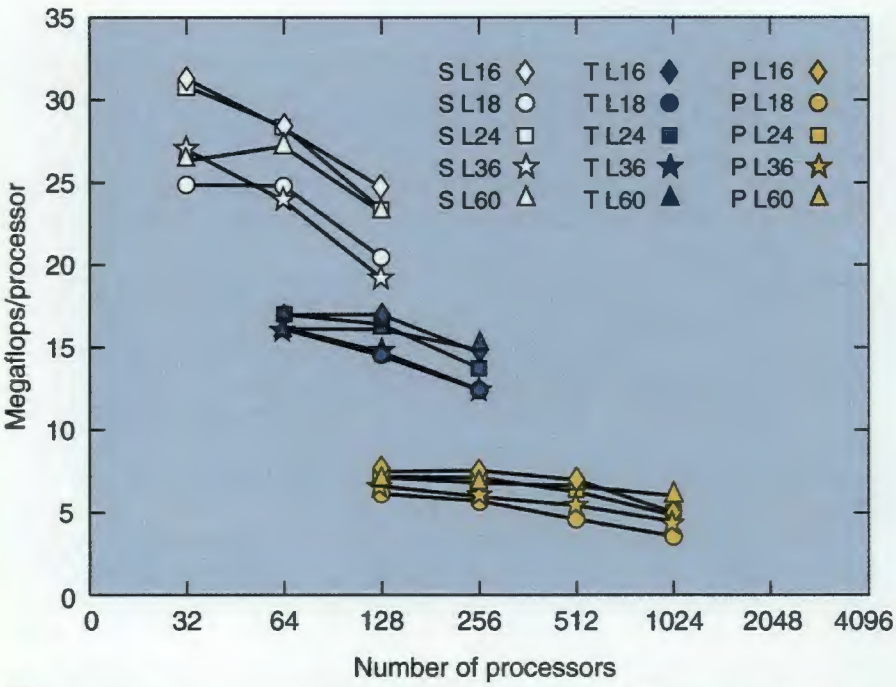


Fig. 3. Per-processor performance for a series of different problem sizes on the Intel Paragon (P), the IBM SP2 (S), and the Cray Research T3D (T).

programming *paradigms,* or models of computation that are used when designing and implementing programs. Examples of this are the *shared* memory programming paradigm, in which data locality is hidden from the programmer, and data movement from remote locations is managed automatically by the system software; the *message-passing* programming paradigm, in which all data movement from nonlocal memory is handled explicitly by the programmer through a special set of system calls; and mixed models like the High-Performance Fortran standard, in which data locality issues can be addressed by specifying what should be local but the data movement required by the program is taken care of automatically. Many of the current high-performance computing systems nominally support two or more of these paradigms, but with vastly different performance characteristics. Moreover, there may be support for more than one type of shared memory or message-passing programming model. For example, most of the current multiprocessor vendors provide both their own proprietary message-passing primitives and one or both of PVM and messaging-passing interface (MPI).

It is important to emphasize that computer systems need to be continually reevaluated. Hardware and software upgrades can change performance dramatically (one hopes) by removing performance bottlenecks in one or more components of the system and by sometimes introducing new performance problems in other components. For this reason, a system administrator or performance specialist should establish a coherent methodology for reevaluating performance at a computer site and for automating the evaluation process as much as possible.

Finally, the evaluation process must take future needs into account. Will the next generation of those programs in the current workload have stricter performance requirements? Is the current computer system scalable; in other words, can increased computational requirements be satisfied by adding more processors or by replacing existing components with faster ones? Answers to these questions typically rely on extrapolation from the characteristics of the current computer system and the current workload. Nevertheless, peak performance measurements can be used reliably to indicate negative results—for example, to show that a larger problem cannot be solved quickly enough or that a computer system is not scalable.

When Is Fast "Fast Enough"?

As parallel computers become ever faster, it is tempting to suppose that they will eventually become "fast enough." In practice, however, the user's appetite for increased computing power is inexhaustible: the extra power is quickly consumed in an attack on problems previously considered intractable.

The continuing evolution of massively parallel computers and distributed computing systems promises unprecedented speed and power. Some effort will always be necessary to achieve the best performance on these systems. However, current research in parallel and distributed computing at ORNL and elsewhere should enable us to more rapidly capitalize on this power. ornl

Further information

- On high-performance computing:
  http://www.ccs.ornl.gov
- On software tools:
  http://www.epm.ornl.gov/cs
  http://www.epm.ornl.gov/pvm
  http://www.netlib.org/mpi/index.html
  http://www.netlib.org/nhse
- On performance evaluation:
  http://www.epm.ornl.gov/ees
  http://www.netlib.org/benchmark
  http://www.netlib.org/parkbench

BIOGRAPHICAL SKETCHES

EDUARDO D'AZEVEDO is a research staff member in ORNL's Computer Science and Mathematics Division (CSMD). He has a Ph.D. degree in computer science from the University of Waterloo, Canada. He first came to the Mathematical Sciences Section at ORNL under an Oak Ridge Associated Universities postdoctoral fellowship in 1990. Since that time, he has been involved in research in numerical linear algebra, triangular mesh generation, and high-performance computing with applications in modeling groundwater flow and contaminant transport.

JACK DONGARRA holds a joint appointment as Distinguished Professor of Computer Science in the Computer Science Department at the University of Tennessee and as Distinguished Scientist in ORNL's Mathematical Sciences Section, CSMD, under the UT/ORNL Science Alliance Program. He specializes in numerical algorithms in linear algebra, parallel computing, use of advanced-computer architectures, programming methodology, and tools for parallel computers. He was involved in the design and implementation of the software packages EISPACK, LINPACK, BLAS, LAPACK, ScaLAPACK, Netlib/XNetlib, PVM/HeNCE, MPI, and the National High-Performance Software Exchange. His current research includes the design of algorithms and techniques for high-performance computer architectures and the development, testing, and documentation of high-quality mathematical software. You can learn more about him through his UT web page: *http://www.netlib.org/utk/people/JackDongarra.html.*

TOM DUNIGAN is a research staff member in CSMD. He has worked at all three Oak Ridge facilities since the mid-1970s. After he joined the Computer Science Research Group in 1982, he established ORNL's first Internet connection. His research interests are in parallel computing and high-speed networking. He has been involved in beta testing and performance analysis of several first-generation parallel computers at ORNL. He has a Ph.D. degree in computer science from the University of North Carolina. He is an adjunct faculty member of the University of Tennessee Computer Science Department.

AL GEIST, who joined ORNL in 1983, is leader of the Computer Science Group in the Mathematical Sciences Section of CSMD. One of the developers of the Parallel Virtual Machine (PVM) software system and one of the designers of MPI, he has published papers in areas such as solar energy, materials science, solid-state physics, parallel computing, scientific computation, distributed computing, and numerical linear algebra. To learn more, see *http://www.epm.ornl.gov/~geist.*

CHUCK ROMINE joined the Mathematical Sciences Section of CSMD in 1986 after receiving his Ph.D. degree in applied mathematics from the University of Virginia. His main areas of research interest include parallel numerical linear algebra and software tools for parallel numerical computation. Most recently, as a member of the Partnership in Computational Science team, he has been developing software tools to support parallel models for groundwater flow and contaminant transport on high-performance supercomputers such as the Intel Paragon at ORNL.

PAT WORLEY is a research staff member in CSMD. He works in numerical analysis, parallel algorithm design, computer performance evaluation, and software tools. He is a principal investigator for the Center for Computational Sciences' Evaluation of Early Systems Project and a member of the ORNL CHAMMP project team, which is part of the Global Change Research Program. He has a Ph.D. degree in computer science from Stanford University. He joined ORNL in 1987 as a researcher in the Mathematical Sciences Section. For more information, see *http://www.epm.ornl.gov/~worley.*

Software Components To Facilitate Application Development

By Jack Dongarra, Noel Nachtigal, Esmond Ng, Barry Peyton, Bill Shelton, and David Walker

ORNL researchers have developed computationally efficient linear algebra packages that are portable across different computer architectures, including workstations and massively parallel processors. These packages include ScaLAPACK, which is a parallel version of the LAPACK library, an iterative methods library known as the quasi-minimal residual package (QMRPACK), and several sparse matrix solvers. These computational tools are used in several important scientific and engineering applications, resulting in state-of-the-art algorithms that perform simulations in a fraction of the time of the original solvers they replaced. These applications range from first-principles electronic structure codes that are being developed as part of the DOE Grand Challenge in materials science to codes used in the automotive and aerospace industries.

Sophisticated mathematical software libraries relieve the scientist of the burden of having to be an expert in parallel programming, numerical methods, and computer science. Grand Challenge application codes make use of these software libraries to solve complex mathematical equations on sequential and parallel computers. Very often these equations can be formulated as linear algebra problems, so most of the software components that we have developed perform linear algebra computations. Numerical linear algebra is the branch of applied mathematics that deals with the computational aspects of matrices—orderly arrays of symbols by rows and columns.

In this article, we discuss the main features and uses of a parallel library for dense linear algebra computations (ScaLAPACK), a package based on the quasi-minimal residual algorithm (QMRPACK), and sparse linear algebra techniques. These software components, which were developed at ORNL, provide a common interface, thus making the codes highly portable between different computer architectures ranging from personal computers and workstations to massively parallel platforms. The algorithms in these software libraries are numerically stable and highly reliable, and they are optimized to achieve the highest possible computational performance.

A good example of the use of these software components is the large system multiple scattering (LSMS) method, whose continuing development is part of a Grand Challenge application in materials science; it is sponsored by DOE's High-Performance Computation and Communications Program (HPCCP). Several of the software libraries have been incorporated into the most computationally intensive sections of the LSMS method, resulting in a highly efficient algorithm. These sections include the calculation of the inverse of a large matrix, solutions of a system of linear equations, and several matrix operations such as dot products, matrix-vector, and matrix-matrix multiplication.

A Parallel Dense Linear Algebra Library

Software libraries are widely used on personal computers, workstations, and conventional supercomputers, so it is natural to want to use the same libraries on parallel supercomputers. The use of software libraries makes it easier to build complex application programs and ensures that these applications are portable between different types of computers. Unfortunately, few high-quality software libraries are available for parallel computers, making applications more difficult to program and often resulting in duplication of effort. The Linear Algebra PACKage (LAPACK) is a popular library of dense linear algebra routines that is used on personal computers, workstations, and conventional supercomputers. The Scalable LAPACK (ScaLAPACK) project is developing a software library for performing dense linear algebra computations on parallel computers. The term *scalable* refers to

The authors in the library of the Computer Science and Mathematics Building: sitting from left are Jack Dongarra, Barry Peyton, and David Walker; standing from left are Bill Shelton, Esmond Ng, and Noel Nachtigal. *Photograph by Tom Cerniglio.*

the ability of the software to make effective use of additional computational resources as the problem size increases; in a highly scalable algorithm, computational efficiency is preserved as the problem size and number of processors increase together. ScaLAPACK and LAPACK both perform dense linear algebra computations. These sorts of computations involve matrices in which most of the entries are nonzero, contrasting with sparse matrices, discussed in the next section, in which a significant fraction of the entries are zero. ScaLAPACK is designed to achieve good performance while being easy to use and simple to port between different computers. Dense linear algebra is important in a number of areas, particularly in the DOE Grand Challenge in materials science, where it has been used to investigate magnetic moment formation and stability in magnet materials. These types of materials are used in magnetic motors, data storage devices, and recording media, representing billions of dollars in annual revenues. In addition, dense linear algebra problems arise in boundary integral methods used in computing water flow past ships and ocean structures (such as oil rigs) and in solving electromagnetic scattering problems. Both LAPACK and ScaLAPACK are being used to help computational scientists solve these and other Grand Challenge problems.

The memory of high-performance computers consists of several hierarchical layers, each with a different access time. Usually layers that have more memory take longer to access. The uppermost levels are the registers that can be accessed most rapidly. The next levels are cached memory and main memory. In addition, on a parallel computer, nonlocal memory residing on a remote processor represents another memory layer.

The performance of an application depends on how data are accessed in these different layers. To get good performance, we want to move as little data as possible between different layers of memory. Where data movement is necessary, we move it in a few big chunks, rather than in many small chunks. These considerations are central to the design of ScaLAPACK and LAPACK, thus leading to the formulation of most library routines as block-partitioned algorithms. In block-partitioned algorithms, most of the work involves operations on two or more matrices, resulting in the efficient use of the memory hierarchy.

A dense linear algebra problem typically involves matrices and vectors. On a parallel computer, these data must be split up and assigned to different processors so that each processor can perform its particular part of the problem. The data distribution must be done carefully to make sure that each processor has the same amount of work to do in each phase of an application. If some processors have more work to do, then other processors may have to wait while they "catch up." This situation, known as load imbalance, results in poorer performance. In ScaLAPACK, matrices and vectors are distributed over processors using a block-cyclic data distribution. In the block-cyclic data distribution of a matrix, the data assigned to a particular process are not contiguous but are scattered in a regular way over the whole matrix. This arrangement ensures that good load balance is maintained in the major parts of an algorithm.

Good performance is not the only goal in designing a software library. It must also be portable and easy to use. One problem in using distributed memory parallel computers is that each processor has its own local memory that is separate from the other processors; therefore, it knows only about its own data—that is, the local portions of the matrices and vectors that have been assigned to it by the data distribution. A processor cannot directly refer to part of a matrix on another processor.

ScaLAPACK is easy to use because matrices and vectors are referenced as global objects. Thus, when referring to a particular matrix entry, we can use global indices, rather than specifying it by giving the processor number and the local indices. This makes programming with ScaLAPACK much easier, and the resulting code looks very similar to the sequential version using LAPACK.

ScaLAPACK addresses the issue of portability by constructing the library routines out of lower-level components. Most computations on a single processor are performed using the basic linear algebra subprograms (BLAS). These routines are widely available, and on many platforms have been optimized to give very high performance. Message passing between processors is done using the basic linear algebra communication subprograms (BLACS). Versions of BLACS have been written based on the parallel virtual machine (PVM) and message-passing interface (MPI), as well as for the native message-passing systems of a number of parallel computers. The parallel BLAS (PBLAS) are parallel versions of most of the operations available in BLAS, and they are based on BLAS and BLACS. PBLAS make it easier for library designers to extend ScaLAPACK to include new algorithms. ScaLAPACK is constructed using BLAS, PBLAS, and BLACS as building blocks; it is therefore portable to essentially any computer that uses PVM or MPI. Since its first release into the public domain in December 1994, more than 1000 copies of the ScaLAPACK software have been distributed. Current work is extending ScaLAPACK to include out-of-core

routines and other types of matrices, such as banded matrices. Further information is available on the World Wide Web at *http://www.netlib. org/scalapack/.*

Sparse Matrices and Structural Dynamics

When an automobile, airplane, space shuttle, or rocket is in motion, it inevitably undergoes stresses and strains induced by a significant amount of vibration. Can a next-generation automobile, airplane, space shuttle, or rocket be designed to be more reliable than today's models under such conditions? This question is extremely important because the cost of building cars must be very low, while the cost of building aircraft and spacecraft will be very high. How do scientists and engineers study this type of problem? One solution is to build prototypes, perform experiments with the prototypes, and construct models to analyze the experimental results. The experimental results will allow scientists to adjust the parameters of the models so that new and improved prototypes can be built. This iterative process eventually converges on prototypes that will survive the experiments. The ultimate products are then constructed on the basis of the prototypes. This is one essential application of structural dynamics.

Structural dynamics modeling is computationally intensive. We have been working with researchers in the Structural Dynamics and Vibration Group at Sandia National Laboratories to help them improve the efficiency of their modeling effort. Our efforts have met with much success.

The heart of many structural dynamics applications is a numerical linear algebra problem, and the Sandia modeling effort is no exception. Ultimately, the overwhelming majority of the total computer time is spent in a small number of linear algebra routines that solve symmetric, positive, definite systems of linear equations, where the coefficient matrices are large and have relatively few nonzero entries; such matrices are said to be sparse. Routines such as these, which are critical to the overall performance of the modeling software, are known as the key kernels within the software.

Efficient solution of sparse linear systems requires careful exploitation and preservation of the zero entries in the coefficient matrices. The way in which we solve such linear systems is to factorize each coefficient matrix into the product of two triangular matrices. The solution to each of the original linear systems can then be obtained by solving two triangular linear systems. An important note about this approach is that extra nonzero entries, or fill entries, are introduced into the triangular factors during the factorization. Thus, a crucial step in the solution process is to arrange the computation so that the number of fill entries is small.

Variable-banded methods, or profile methods, which attempt to limit fill entries around the diagonal of a matrix, are commonly used to solve the linear systems in many structural analysis applications. Such a linear-system solver was originally incorporated into Sandia's structural dynamics modeling code. Unfortunately, these solvers do not make efficient use of either storage or computing time; consequently, the modeling software originally could deal effectively only with models too small to be of practical interest to scientists and engineers.

Fortunately, however, much better technology now exists to solve linear systems of this kind. General sparse solvers, which employ new techniques to limit the number of fill entries introduced and to take advantage of the sparsity pattern, have proven very effective on modern workstations and vector supercomputers, especially after dense matrix operations have been incorporated into the solution method to exploit the memory hierarchies found on modern uniprocessor machines. Over the past few years, we have further improved the algorithms on which this technology is based, and then we developed a sparse linear-system solver based on the new algorithms. As an illustration of advances in sparse matrix technology, a good implementation of one of the profile methods factors a sparse, symmetric, positive definite matrix of order 19,600 in 51.49 s on an IBM RS/6000 workstation; our solver takes only 3.24 s to factor the same matrix on the same machine. The number of matrix elements stored in the profile method is more than 3 million, but our sparse matrix code stores fewer than 1 million matrix elements. More examples are provided in Figs. 1 and 2. Figure 1 compares the numbers of matrix elements stored and manipulated in a profile method (RCM) and in a method (MD) that uses the minimum-degree algorithm to reduce fill. Figure 2 compares the times required to factor the matrices in RCM and MD; the difference between MD and MD/B is that MD does not exploit dense matrix operations while MD/B does. The matrices were derived from finite element discretizations of a square domain; their dimensions range from 10,000 to 40,000.

We have been working with Sandia researchers to incorporate our new fast, sparse linear-system solver in a large-scale structural dynamics modeling effort. Incorporation of our package into the modeling software enabled it to solve large problems of interest to scientists and engineers. This approach increased the problem size that can be dealt with in an effective manner and

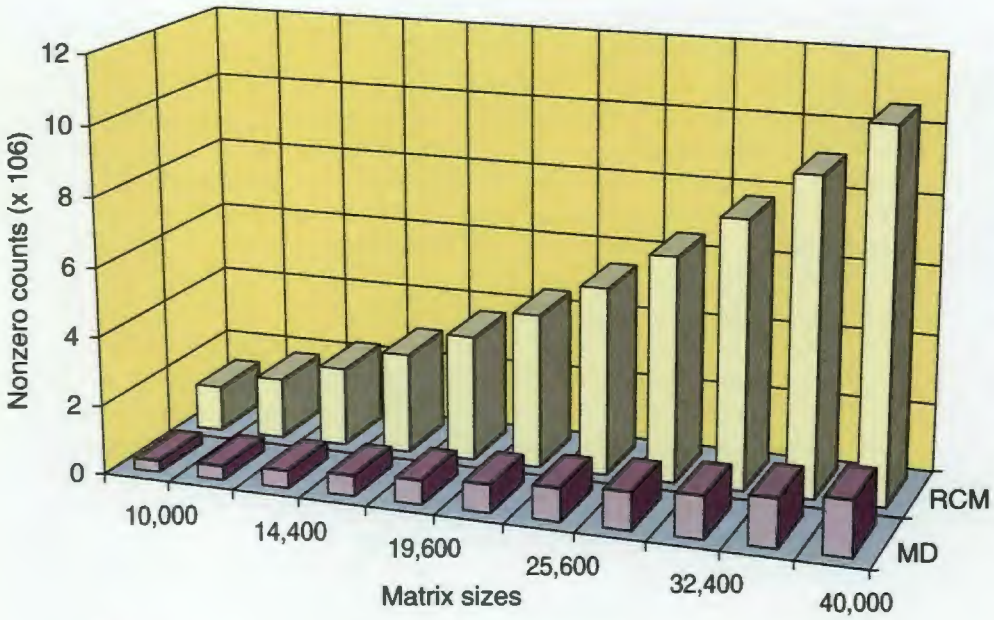


Fig. 1. Nonzero counts in sparse Cholesky factors.

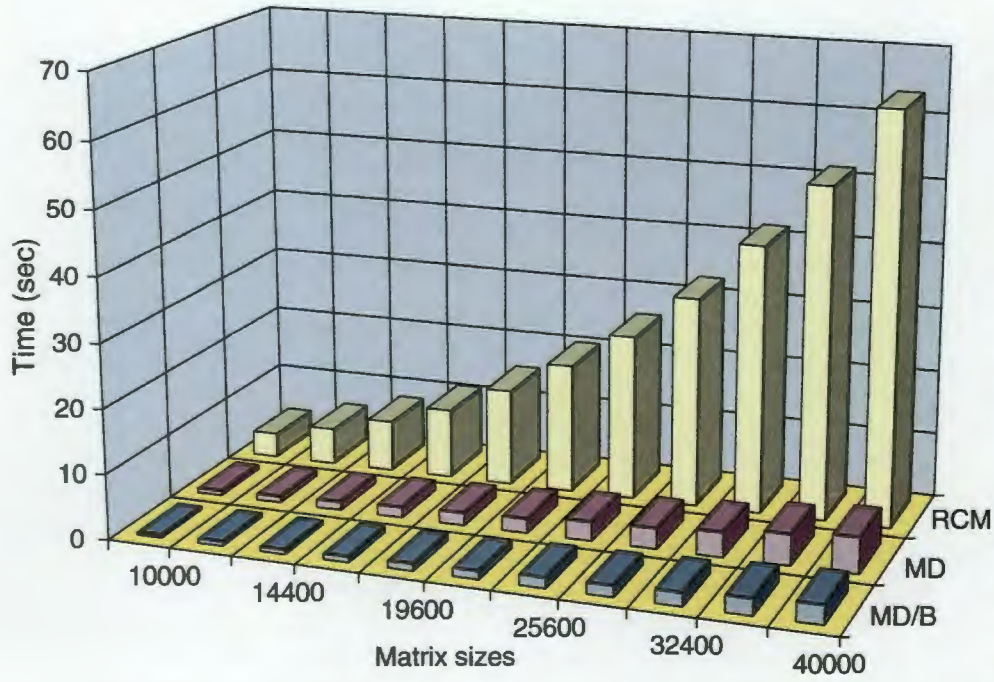


Fig. 2. Performance of sparse Cholesky factorizations.

reduced significantly the time required to solve almost all problems over the approach originally employed in the software. As a result of the collaboration, studies of the response of structures to stresses and strains induced by heavy vibration can now be done much more quickly and with greater accuracy.

The new code enables Sandia and an industrial partner in California to perform state-of-the-art modeling in a fraction of the time required using the solver it replaced. The solver is the most heavily used module within the modeling software, and because of our input, the amount of time required from a product's inception to production could be reduced drastically. Application of Sandia's structural dynamics modeling package could increase the competitiveness of a U.S. automaker, improve the design of missiles developed at Sandia, and help assess the safety of the aging bridges found within the U.S. highway system.

Structural dynamics modeling is not the only application that gives rise to large, sparse, symmetric, positive, definite linear systems. Other examples include numerical solution of self-adjoint elliptic partial differential equations and numerical optimization. In particular, our sparse linear-system solver has been used in interior-point methods for solving linear programming problems.

Applications of an Algorithm

One of the major scientific projects at ORNL involves the computation of material properties starting from first principles. The goal

is to obtain methods that can predict the material properties of an alloy, for example, using as the only inputs the constitutive elements of the alloy; in other words, no experimental data are used. Such methods are called parameter-free methods, and because they require no experimental inputs, relying only on basic principles of physics to describe the interactions among the atoms making up the system, they are also referred to as ab initio methods. If successful, these methods would allow us to predict properties of a material without having to first build samples of that material, thus reducing considerably the time and money spent designing new technologically advanced materials, such as those required by the power-generation or aerospace industries.

One important class of problems in ab initio materials modeling involves the computation of the minimum energy state of a system of electrons interacting in the field of atomic nuclei using an approach called density functional theory. This computation requires the solution of a set of Schroedinger equations, which in turn can be reduced to solving several linear systems of equations whose matrices describe the interactions among the different particles in the system. These matrices are not particularly large—the largest ones treated had only 2000 to 3000 unknowns—but, unfortunately, they are dense and thus have several million nonzero elements. An overwhelming fraction of the total computational effort is spent solving these linear systems, so it is here that we focused our attention.

The previous approach used to solve these linear systems was to factor the matrix into a product of two triangular matrices, and then use these to obtain the solution to the original system. This approach worked well while the matrices were still small. Unfortunately, the amount of time spent factoring each matrix grows rapidly as more and more atoms are included in the atom clusters: the time grows by a factor of 8 every time the number of atoms in the cluster is doubled. As a result, the technique can no longer be used once the cluster of atoms has grown to around 100.

We replaced this factorization technique with a completely different method, an algorithm from the class of iterative methods for the solution of linear systems, the quasi-minimal residual (QMR) algorithm. Like other iterative methods, the QMR algorithm successively computes approximations to the exact solution of the linear system, each time attempting to solve these linear systems to improve upon the last approximate solution. While it can be shown that the algorithm generates a sequence of approximate solutions that does, in fact, eventually converge to the exact solution, the hope is that in practice, it will find very good approximations after only a few iterations, as each iteration is relatively inexpensive.

Whether this is the case depends on the properties of the matrix. In our case, it turns out that the matrices that describe the interactions among atoms in clusters are very well suited for the QMR algorithm and that the algorithm rapidly gives very good approximations to the exact solution. In fact, for the materials tested, QMR solved the system up to 40 times faster when compared to the previous factorization-based method. Even more important, it turned out that when the number of atoms in the cluster is doubled, the time spent using QMR only doubles, instead of growing by a factor of 8; as a result, much larger cluster sizes can be treated. This advance enables better prediction of material properties and pushes the first-principles methods to systems previously envisioned as unattainable.

"Necessary computational tools will be provided to an even larger number of researchers, allowing them to concentrate on their research and not on computer science."

Conclusion

We have developed efficient linear algebra packages for use on high-performance workstations and massively parallel computers. These linear algebra packages have been incorporated in important computational-intensive applications, resulting in significant improvements in performance. Our current work involves increasing the capabilities of linear algebra packages that we have developed. These enhancements will enable these packages to treat a much wider class of matrix problems than is currently possible. As a result, necessary computational tools will be provided to an even larger number of researchers, allowing them to concentrate on their research and not on computer science and numerical linear algebra issues. Recent increases in efficiency are already allowing investigators to push their research into areas once thought intractable. By extending their research into new areas, scientists and engineers will provide important technological information that can be used to develop new efficient products, improving the overall competitiveness of U.S. industries. **ornl**

BIOGRAPHICAL SKETCHES

JACK DONGARRA was profiled in the previous article "Algorithms, Tools, and Software Aid Use of High-Performance Computers."

NOEL NACHTIGAL is a research staff member in the Mathematical Sciences Section of ORNL's Computer Science and Mathematics Division. A native of Romania, Nachtigal obtained his Ph.D. degree in applied mathematics in 1991 from the Massachusetts Institute of Technology. After a 2-year stint as a postdoctoral scientist at the Research Institute for Advanced Computer Science at NASA Ames in Moffett Field, Nachtigal joined the Mathematical Sciences Section as the 1993 Householder Fellow. He is a coauthor of the quasi-minimal residual method for solving non-Hermitian linear systems and of the QMRPACK software package. More recently, he has been involved in research projects in materials science and computational fluid dynamics.

ESMOND G. NG, a native of Kwangtung, China, received his Ph.D. degree in computer science from the University of Waterloo in Waterloo, Ontario, in 1983. He joined ORNL in 1985. He is currently a senior research staff member and a group leader in the Mathematical Sciences Section of the Computer Science and Mathematics Division. Ng is also an adjunct professor in the Department of Computer Science at the University of Tennessee at Knoxville. He serves on the Technical Committee on Computational Linear Algebra of the International Association for Mathematics and Computers in Simulation (IMACS). He is also a member of the IMACS Technical Committee on Parallel- and Supercomputing. His research interests include sparse matrix computations, numerical linear algebra, parallel computing, and mathematical software development and software engineering. He is a co-author of the book *Parallel Algorithms for Matrix Computations*, which was published in 1990 by SIAM Publications.

BARRY W. PEYTON is a research staff member in the Mathematical Sciences Section of the Computer Science and Mathematics Division. A native of Charlotte, North Carolina,

he received his Ph.D. degree in mathematical sciences from Clemson University in 1986. He joined ORNL in 1988. His research interests include sparse matrix computations, numerical linear algebra, parallel computing, and combinatorial algorithms. Peyton was a cowinner of the 1988 Gordon Bell Prize in recognition of the outstanding performance achieved by a parallel version of a sparse matrix code that he codeveloped prior to coming to ORNL. He is a coauthor of the book *Parallel Algorithms for Matrix Computations*, which was published in 1990 by SIAM Publications.

BILL SHELTON has a biographical sketch located with the article "Developing a Grand Challenge Materials Application Code: An Interdisciplinary Approach."

DAVID WALKER is a senior research staff member in the Mathematical Sciences Section of ORNL's Computer Science and Mathematics Division. He holds a B.A. degree in mathematics from Jesus College, Cambridge University, an M.S. degree in astrophysics, and a Ph.D. degree in physics, both from Queen Mary College, University of London. He held postdoctoral appointments at the University of London and at the Jet Propulsion Laboratory. In 1986 he became a staff scientist in the Concurrent Computational Project at the California Institute of Technology, and in 1988 he was appointed to the University of South Carolina mathematics faculty as an associate professor. In 1990 he joined the ORNL staff. His research interests focus on software and algorithms for the scientific use of message-passing computers. He has been closely involved in the development of the ScaLAPACK parallel software library and the MPI message-passing standard. He has also contributed to the design of a parallel version of the Community Climate Model for predicting future climate. Walker has published a number of papers on the parallel implementation of particle-in-cell algorithms for plasma simulations. He has also been involved in the benchmarking of science and engineering applications codes on parallel computers. He has published more than 60 papers on parallel computing and has coauthored three books on the subject. In 1992 he founded a series of conferences on high-performance computing under the auspices of the Gordon Research Conference organization.

High-Performance Computing: Innovative Assistant to Science

By James Arthur Kohl

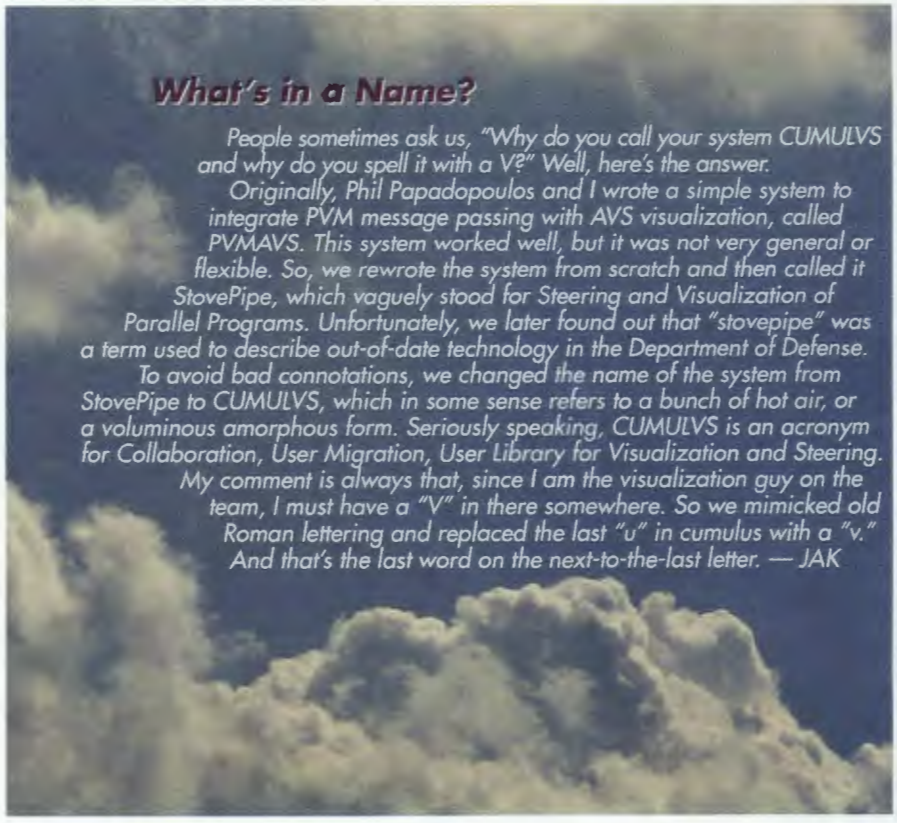
ORNL researchers "push the envelope" to put heavy-duty computer power within scientists' grasp using the CUMULVS system developed at ORNL. It helps scientists simulate experiments and change the parameters in midcourse to influence the results, saving time and money.

Scientists today are frequently turning to high-performance computer simulation as a more cost-effective alternative to physical prototyping or experimentation. The on-line nature of computer simulation encourages more flexible collaboration scenarios for researchers across the country, and the interactivity that is possible can often shorten the design cycle. Yet many issues must be overcome when developing a high-performance computer simulation, especially when many scientists will interact with the simulation over a wide-area network. The scientists must be able to observe the progress of the simulation and coordinate control over it, and the user environment must be capable of withstanding or recovering from system failures. The efficient handling of these issues requires a special expertise in computer science and a level of effort higher than the typical application scientist is willing to expend.

CUMULVS, a new software system developed at ORNL by James Kohl and Philip Papadopoulos, bridges the gap between scientists and their computer simulations. CUMULVS allows a collaborating group of scientists to attach dynamically to an ongoing computer simulation in order to view the progress of the computation and control the simulation interactively. CUMULVS also provides a framework for integrating fault tolerance into the simulation program, for saving user-directed checkpoints, for migrating the simulation program across heterogeneous computer architectures, for automatically restarting failed tasks, and for reconfiguring the simulation while it is running.

With CUMULVS, each of the collaborators can start up an independent "viewer" program that will connect to the running simulation program. This viewer allows scientists to browse through the various data fields being computed and observe the ongoing

Jim Kohl (left) and Phil Papadopoulos enjoy the ambience of Kohl's office, where scientific experiments are simulated and their results are viewed on the computer using CUMULVS. *Photograph by Tom Cerniglio.*



What's in a Name?

People sometimes ask us, "Why do you call your system CUMULVS and why do you spell it with a V?" Well, here's the answer. Originally, Phil Papadopoulos and I wrote a simple system to integrate PVM message passing with AVS visualization, called PVMAVS. This system worked well, but it was not very general or flexible. So, we rewrote the system from scratch and then called it StovePipe, which vaguely stood for Steering and Visualization of Parallel Programs. Unfortunately, we later found out that "stovepipe" was a term used to describe out-of-date technology in the Department of Defense. To avoid bad connotations, we changed the name of the system from StovePipe to CUMULVS, which in some sense refers to a bunch of hot air, or a voluminous amorphous form. Seriously speaking, CUMULVS is an acronym for Collaboration, User Migration, User Library for Visualization and Steering. My comment is always that, since I am the visualization guy on the team, I must have a "V" in there somewhere. So we mimicked old Roman lettering and replaced the last "u" in cumulus with a "v." And that's the last word on the next-to-the-last letter. — JAK

convergence toward a solution. Especially for long-running simulations, it can save countless hours waiting for results that might have gone awry in the first few moments of the run. Once connected, the scientists each view the simulation from their own perspective, receiving a steady sequence of "snapshots" of the program data that is of interest to them. CUMULVS supports a variety of visualization systems for viewing these snapshots, from commercial packages such as AVS, to public domain interfaces such as Tcl/Tk (developed at Sun Microsystems). CUMULVS takes care of the many complicated tasks of collecting information and coordinating communication between the various viewers and the simulation program. The result is a single, simple picture of the computation space, presented as a uniform field of data even if the actual data are distributed across a set of parallel tasks.

Computational Steering

Scientists can use CUMULVS for collaborative "computational steering" in which certain parameters of a physical simulation or of an algorithm can be adjusted while the program is running. In a typical scenario, several scientists would attach to a simulation to view its progress. One of them might discover that something has gone wrong or is heading in the wrong direction. For example, if they were trying to synthesize a new material, they might decide the cooling rate must be changed to make the material stronger. At this point the scientist could adjust, or "steer," certain physical or algorithmic features to try to fix the simulation, or the simulation could simply be restarted with a new set of inputs (such as an altered cooling rate). This type of interaction can save immense amounts of time by shortening the experimentation cycle. The scientist need not wait for the entire simulation to be completed before making the next adjustment. CUMULVS provides mechanisms that allow groups of scientists to cooperatively manipulate a simulation, with automatic locking capabilities that are invoked to prevent conflicting steering requests for any single parameter. Although only one scientist at a time can adjust the value of any single parameter, any number of different parameters can all be adjusted simultaneously.

To interact with a simulation using CUMULVS, the simulation program must be instrumented to describe the primary computational data fields and algorithmic or physical parameters. These special declarations consist of the data type, the size and cardinality of arrays, and any distributed data decompositions. CUMULVS needs declarations only for the data that are to be viewed and the parameters that are to be steered. At the point in the simulation where the data values are deemed "valid," a single library call is made to temporarily pass control to CUMULVS. Here, any pending viewer requests are handled and any steering parameter updates are processed. If no viewers are attached, this library call carries only the overhead to check once for an incoming message, so that there is negligible intrusion to the simulation.

The various communication protocols that CUMULVS uses to coordinate the interactions between the viewers and the simulation are tolerant to computer faults and network failures. In addition, CUMULVS provides a "checkpointing" mechanism for making the simulation program itself fault-tolerant. Using this mechanism, the state of a simulation program can be saved periodically. Then the data stored in the checkpoint can be used to automatically restart the simulation if a computer node should crash or if a network should fail. CUMULVS checkpoints can also be used to migrate parallel simulation tasks across heterogeneous computer architectures on the fly. This capability is typically not possible with traditional checkpointing schemes, but CUMULVS uses a special "user-directed" checkpointing approach. Because the scientist has precisely described the data in the simulation program, CUMULVS has the additional semantic information necessary to automatically migrate a task using a minimal amount of information. CUMULVS can save the state of a simulation task and then restore it, even if the new task's computer is of a different architecture or data format. Beyond that, CUMULVS can actually reconfigure an entire application by reorganizing the checkpoint data to fit a new data decomposition. So, a checkpoint saved on a cluster of workstations can be restarted to continue executing on a large parallel machine with many more nodes, or vice versa.

Simulation Scenario

To better understand the usefulness of these CUMULVS features, consider a sample scenario. Suppose you're an engineer on a big project team that is designing a new high-tech jet airplane. Your job is to make sure that the air flows smoothly over the wings and around the engine intakes. If your design is off by even a small amount, you might bring down a multimillion-dollar aircraft, not to mention making a lifelong enemy out of the poor pilot, assuming he or she survives.

What you need is some way to really test out your ideas, try things out a few different ways, and make sure you've got it right before they start forming those expensive prototype airfoils. So you put your expertise to work, sit down at the computer, and whip up a computational fluid dynamics (CFD) simulation of the air flowing around one of your wings. You sit back and patiently wait for the

results. And you wait. And you wait some more. Whew! Finally, after many hours of waiting for your program to converge on a solution, you get the answer. But something went wrong. Your wing design didn't produce the smooth flow you expected. "What happened?" you ask.

With CUMULVS at your side, the problems with your wing simulation can easily be revealed. You decide to apply CUMULVS to the simulation program to see what's going wrong. In your CFD airflow program you add a few special declarations so that CUMULVS knows what's in your simulation and where. You give your simulation the name "flow" so your viewer can find it. You describe the main computational data fields, "pressure" and "density." You also declare a few of the steerable parameters, like the "Mach number" and the wing's "angle of attack." After recompiling your program, you are ready to go.

This time, you start up your simulation and can immediately attach a CUMULVS viewer to see what's happening. You request the main "pressure" data field—it's huge, but you want to see an overview of the whole array anyway. You tell CUMULVS to view the entire region of computation but at a coarse granularity, showing only every tenth data point. Using this smaller collection of data points for viewing greatly reduces the intrusion to your simulation, and the load on your network, while exploring such an immense dataset. The CUMULVS view of "pressure" appears as requested, and you begin to watch it slowly change as the simulation proceeds. From this high-level view, you can already see that something isn't quite right. It looks like the angle of attack of the wing is off by a mile. But it turns out to be a simple program bug, and you fix it in no time.

Now you're ready to try again, so you start up the simulation and connect up with CUMULVS. Your wing looks much better now, so you disconnect your viewer and let the simulation run while you go out to lunch. When you get back, you connect up again to see how things are going. The simulation is working, getting closer to an answer, but you can see that the performance of the wing will not be as good as was hoped. While watching through your viewer, you tell CUMULVS to adjust one of the wing model parameters to see if you can improve the design. After a moment you see the changes to the wing appear in your viewer, but it takes several more iterations before the effects of the new information begin to be seen in the simulation results.

Parallel Programming

After tediously tweaking your model over the next few hours, you decide that your simulation program is just too darn slow. You need to split your simulation program into smaller, independent pieces that can run simultaneously, or "in parallel," so you can get the job done faster. With several different computers all working together on the problem, your simulation program might run in minutes instead of hours. You use a system like the MPI message-passing standard or PVM (the Parallel Virtual Machine system developed jointly at Emory University, ORNL, and the University of Tennessee by a team led by Al Geist at ORNL and Jack Dongarra at ORNL and the University of Tennessee, both of whom have also been instrumental in the development of MPI). Either of these systems allows you to write a "parallel program." You parallelize the CFD algorithm by breaking the original calculation down into "cells," and then you assign sets of these cells to a collection of parallel "tasks" that will cooperate to solve your problem. After each task finishes its iteration of work, the tasks will talk to each other, sending messages among themselves to share intermediate results on the way to a solution.

You start up a run of your new parallel program on a few workstations, and sure enough, you get the answer back in a fraction of the time. But things are way off again, and it's worse than before. There's a huge region of turbulence off the tip of the wing. Something has gone wrong with the way you reorganized your simulation program. "Now what?!" you exclaim. It's time for CUMULVS again.

Parallel programming is notoriously difficult because it lacks the single thread of control you would have in a conventional serial program. In addition, the data used in your parallel computation are probably spread across a number of distributed computer systems. This is done to capitalize on *locality* by leveraging faster local data accesses against more costly remote data accesses. Often, the data "decompositions" that make your parallel program the fastest are the ones that are the most complicated. CUMULVS helps a great deal with these complex data decompositions because it "un-jumbles" the data and presents them to the scientist in their original form, as if all of the data were present on a single computer.

To help CUMULVS collect the parallel data in your wing simulation, you need to enhance the special declarations that you made for the serial version. This effort involves defining the way each data field has been broken apart and distributed among the parallel tasks. After adding a few extra lines of decomposition declarations for CUMULVS, you are ready to go.

You start up a fresh parallel wing simulation and then attach your CUMULVS viewer to see what is happening. Sure enough, almost immediately you begin to see turbulence form off the wing tip. But it's still not clear to you why it's there. Something must be

wrong with the parallel algorithm. You go back into your simulation code and add some CUMULVS declarations for the "residuals" array. This array doesn't represent the physical model, but instead describes the error associated with your mathematical computation. Viewing the residuals data field with CUMULVS should indicate whether there is an algorithmic problem.

This time when you connect your viewer, you request the residuals data field. "Aha!" you declare. It looks like the residual error in one corner of your computation space is "stuck." One column of the space is not being updated from iteration to iteration, causing a fixed boundary condition that appears as turbulence in the model. You must have figured your array bounds wrong for that pesky parallel data decomposition.

With the bug fixed, you are now up to full speed and back in the task at hand—designing that airplane wing. The parallel simulation runs much faster than the serial version, and you are able to very quickly try a wide range of variations on your design. After a few days of successful experimentation, suddenly everything clicks, and you arrive at a solid arrangement of the wing parameters. You excitedly call up one of your colleagues and ask her to take a look at your design. She hooks up her CUMULVS viewer to the parallel simulation running on your workstation cluster and checks out your new design. "This looks great!" she says. She decides to try some minor enhancements, so she takes the last CUMULVS checkpoint saved for your simulation and reconfigures it to run on her big 512-node multiprocessor system.

She picks up where you left off on your workstation cluster and begins to explore some slight adjustments to your model. She steers one wing parameter, just a little bit, to smooth off a final rough edge, and then calls you up to look at the simulation. You connect another viewer to her simulation and immediately agree that the wing is even better. The two of you contact the rest of the team, and everybody brings up their CUMULVS viewers to take a look at the new wing design. Everyone agrees that it is time to build a physical prototype of the wing. Success at last!

This type of CUMULVS functionality was recently put to the test as part of the High Performance Computing Challenge competition of the Supercomputing '96 conference held in November 1996 in Pittsburgh. CUMULVS won a silver medal for innovation for its contribution to high-performance scientific computing. The ORNL team—consisting of James Kohl, Philip Papadopoulos, Dave Semeraro, and Al Geist—demonstrated a collaborative visualization of three-dimensional airflow over an aircraft wing (much like the hypothetical scenario described above). Figure 1 illustrates a CUMULVS view of the running CFD airflow simulation over a wing. Figure 2 shows a view of the residuals field that helped Dave Semeraro debug the simulation.

In the High Performance Computing Challenge at the Supercomputing '95 conference, CUMULVS won the award for best interface and fault tolerance. In addition to winning awards, it is hoped that CUMULVS will win over many scientists. ornl

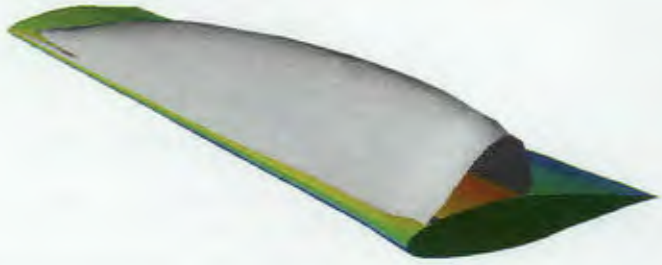


Fig. 1. CUMULVS view for a computational fluid dynamics (CFD) simulation of the airflow over a jet airplane wing. This demonstration won ORNL a silver medal for innovation at the Supercomputing '96 conference.

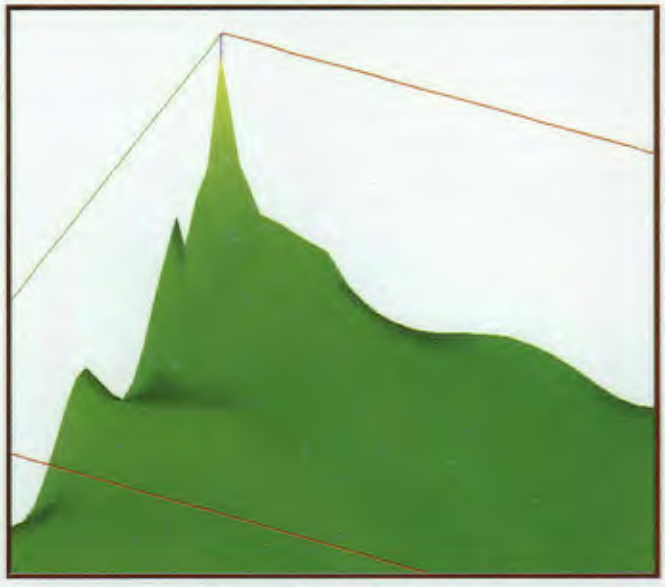
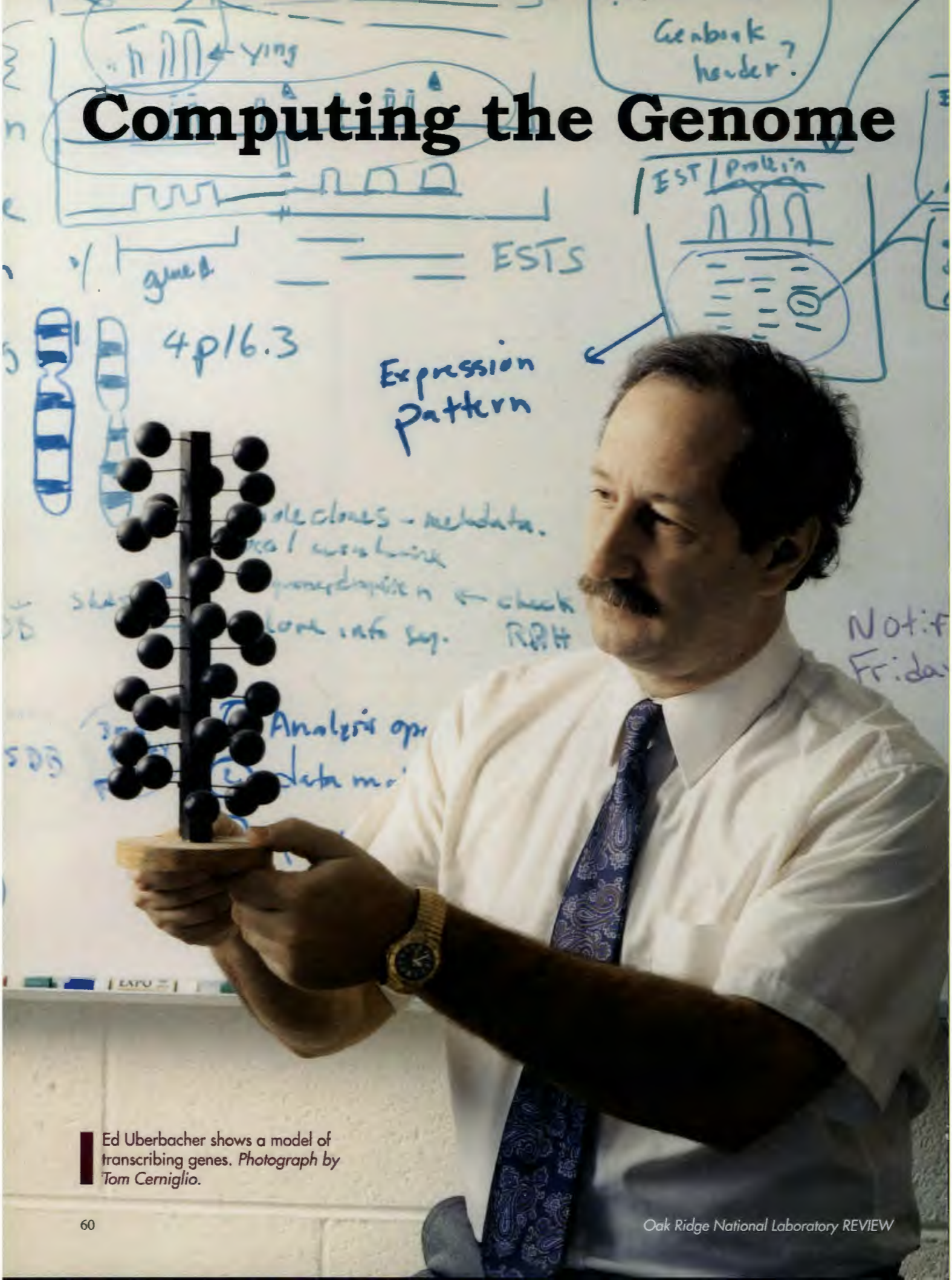


Fig. 2. CUMULVS view of the residuals field for the CFD simulation in Fig. 1. The spike in the corner reveals an omitted computation cell in the parallel decomposition.

BIOGRAPHICAL SKETCH

JAMES ARTHUR KOHL is a staff scientist in the Mathematical Sciences Section of ORNL's Computer Science and Mathematics Division, which he joined in 1993. He received a Ph.D. degree in electrical and computer engineering from the University of Iowa, and he holds B.S. and M.S. degrees in this field from Purdue University. He was involved in visualization projects for parallel programming at the IBM T. J. Watson Research Center in 1992 and at DOE's Argonne National Laboratory, where he worked from 1983 through 1990 on regular short-term appointments. He is currently a member of the Parallel Virtual Machine (PVM) research group at ORNL, where he developed the widely used XPVM visualization interface. In 1996 Kohl received a Division Director's Award from the Computer Science and Mathematics Division for innovative work on user interfaces and reliability in distributed computing environments (the preliminary CUMULVS work). For three consecutive years, he has won recognition on ORNL teams in Heterogeneous and High-Performance Computing Challenges at Supercomputing conferences. He was recently selected as editor for a new weekly e-mail newsletter *PT Digest* for parallel software tools, a joint project by ORNL and the University of Tennessee that has been sponsored by the National HPCC Software Exchange. His research interests include program visualization, user interface design, and parallel computer architecture and software development. Kohl has been a member of the IEEE Computer Society, ACM SIGARCH, SIGSOFT, and SIGCHI. He is a member of the Order of the Engineer, Eta Kappa Nu, Tau Beta Pi, Phi Kappa Phi, Golden Key, Phi Eta Sigma, and Mensa International.

Computing the Genome



Ed Uberbacher shows a model of transcribing genes. *Photograph by Tom Cerniglio.*

By Ed Uberbacher

ORNL is part of a team that is designing and preparing to implement a new computational engine to rapidly analyze large-scale genomic sequences, keeping up with the flood of data from the Human Genome Project.

Just a few short years ago, most of us knew very little about our genes and their impact on our lives. But more recently, it has been virtually impossible to escape the popular media's attention to a number of breathtaking discoveries of human genes, especially those related to diseases such as cystic fibrosis, Huntington's chorea, and breast cancer. What has brought this about is the Human Genome Project, an international effort started in 1988 and sponsored in the United States by the Department of Energy (DOE) and the National Institutes of Health (NIH). The goal of this project is to elucidate the information that makes up the genetic blueprint of human beings.

The Human Genome Project's success in sequencing the chemical bases of DNA is virtually revolutionizing biology and biotechnology. It is creating new knowledge about fundamental biological processes. It has increased our ability to analyze, manipulate, and modify genes and to engineer organisms, providing numerous opportunities for applications. Biotechnology in the United States, virtually nonexistent a few years ago, is expected to become a $50 billion industry before 2000, largely because of the Human Genome Project.

Despite this project's impact, the pace of gene discovery has actually been rather slow. The initial phase of the project, called mapping, has been primarily devoted to fragmenting chromosomes into manageable ordered pieces for later high-throughput sequencing. In this period, it has often taken years to locate and characterize individual genes related to human disease. Thus, biologists began to appreciate the value of computing to mapping and sequencing.

A good illustration of the emerging impact of computing on genomics is the search for the gene for Adrenoleukodystrophy (related to the disease in the movie *Lorenzo's Oil*). A team of researchers in Europe spent about two years searching for the gene using standard experimental methods. Then they managed to sequence the region of the chromosome containing the gene. Finally, they sent information on the sequence to the ORNL server containing the ORNL-developed computer program called Gene Recognition and Analysis Internet Link (GRAIL). Within a couple of minutes, GRAIL returned the location of the gene within the sequence.

Sequencing Applications

The Human Genome Project has entered a new phase. Six NIH genome centers were funded recently to begin high-throughput sequencing, and plans are under way for large-scale sequencing efforts at DOE genome centers at Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory (LANL); these centers have been integrated to form the Joint Genome Institute. As a result, researchers are now focusing on the challenge of processing and understanding much larger domains of the DNA sequence. It has been estimated that, on average from 1997 to 2003, new sequence of approximately 2 million DNA bases will be produced every day. Each day's sequence will represent approximately 70 new genes and their respective proteins. This information will be made available immediately on the Internet and in central genome databases.

Such information is of immeasurable value to medical researchers, biotechnology firms, the pharmaceutical industry, and researchers in a host of fields ranging from microorganism metabolism to structural biology. Because only a small fraction of genes that cause human genetic disease have been identified, each new gene revealed by genome sequence analysis has the potential to significantly affect human health. Within the human genome is an estimated total of 6000 genes that have a direct impact on the diagnosis and treatment of human genetic diseases. The timely development of diagnostic techniques and treatments for these diseases is worth billions of dollars for the U.S. economy, and computational analysis is a key component that can contribute significantly to the knowledge necessary to effect such developments.

In addition to health-related biotechnology, other application areas of great importance to DOE include bioremediation, waste control, energy supplies, and health risk assessment. Correspondingly, in addition to human DNA sequencing, sequencing of microorganisms and other model organisms that are important to biotechnology is also ramping up at a very rapid rate. For example, the recent sequencing of *Methanococcus jannaschii*, a methane-producing microorganism from deep-sea volcanic vents that flourishes without sunlight, oxygen, or surrounding organic material, suggests that life has three branches, not two. Such microorganisms, called archaea, are genetically different from bacteria and from eukaryotes (which includes plants, animals, and people).

The entire genomes for *Haemophilus influenzae* and yeast have also been fully sequenced, although the significance of many genes remains a mystery. The potential for the discovery of new enzymes and chemical processes important for biotechnology (e.g., new types of degradative enzymes), as well as new insights into disease-causing microbes, makes these efforts highly valuable economically and socially.

The rate of several megabase pairs per day at which the Human Genome and microorganism sequencing projects will soon be producing data will exceed current sequence analysis capabilities and infrastructure. Sequences are already arriving at a rate and in forms that make analysis very difficult. For example, a recent posting of a large clone (large DNA sequence fragment) by a major genome center was made in several hundred thousand base fragments, rather than as one long sequence, because the sequence database was unable to input the whole sequence as a single long entry. Anyone who wishes to analyze this sequence to determine which genes are present must manually "reassemble" the sequence from these many small fragments, an absolutely ridiculous task. The sequences of large genomic clones are being routinely posted on the Internet with virtually no comment, analysis, or interpretation; and mechanisms for their entry into public-domain databases are in many cases inadequately defined. Valuable sequences are going unanalyzed because methods and procedures for handling the data are lacking and because current methods for doing analyses are time-consuming and inconvenient. And in real terms, the flood of data is just beginning.

Computational Analysis

Computers can be used very effectively to indicate the location of genes and of regions that control the expression of genes and to discover relationships between each new sequence and other known sequences from many different organisms. This process is referred to as "sequence annotation." Annotation (the elucidation and description of biologically relevant features in the sequence) is the essential prerequisite before the genome sequence data can become useful, and the quality with which annotation is done will directly affect the value of the sequence. In addition to considerable organizational issues, significant computational challenges must be addressed if DNA sequences that are produced can be successfully annotated. It is clear that new computational methods and a workable process must be implemented for effective and timely analysis and management of these data.

In considering computing related to the large-scale sequence analysis and annotation process, it is useful to examine previously developed models. Procedures for high-throughput analysis have been most notably applied to several microorganisms (e.g., *Haemophilus influenzae* and *Mycoplasma genitalium*) using relatively simple methods designed to facilitate basically a single pass through the data (a pipeline that produces a one-time result or report). However, this is too simple a model for analyzing genomes as complex as the human genome. For one thing, the analysis of genomic sequence regions needs to be updated continually through the course of the Genome Project—the analysis is never really done. On any given day, new information relevant to a sequenced gene may show up in any one of many databases, and new links to this information need to be discovered and presented. Additionally, our capabilities for analyzing the sequence will change with time. The analysis of DNA sequences by computer is a relatively immature science, and we in the informatics community will be able to recognize many features (like gene regulatory regions) better in a year than we can now. There will be a significant advantage in reanalyzing sequences and updating our knowledge of them continually as new sequences appear from many organisms, methods improve, and databases with relevant information grow. In this model, sequence annotation is a living thing that will develop richness and improve in quality over the years. The "single pass-through pipeline" is simply not the appropriate model for human genome analysis, because the rate at which new and relevant information appears is staggering.

Computational Engine for Genomic Sequences

Researchers at ORNL, LBNL, Argonne National Laboratory (ANL), and several other genome laboratories are teaming to design and implement a new kind of computational engine for analysis of large-scale genomic sequences. This "sequence analysis engine," which has become a Computational Grand Challenge problem, will integrate a suite of tools on high-performance computing resources and manage the analysis results. In addition to the need for state-of-the-art computers at several supercomputing centers, this analysis system will require dynamic and seamless management of contiguous distributed high-performance computing processes, efficient parallel implementations of a number of new algorithms, complex distributed data mining operations, and the application of new inferencing and visualization methods. A process of analysis that will be started in this engine will not be completed for seven to ten years.

The data flow in this analysis engine is shown in Fig. 1. Updates of sequence data will be retrieved through the use of Internet retrieval agents and stored in a local data warehouse. Most human genome centers will daily post new sequences on publicly available Internet or World Wide Web sites, and they will establish agreed-upon policies for Internet capture of their data. These data will feed the analysis engine that will return results to the warehouse for use in later or long-term analysis processes, visualization by researchers, and distribution to community databases and genome sequencing centers. Unlike the pipeline analysis model, the warehouse maintains the sequence data, analysis results, and data links so that continual update processes can be made to operate on the data over many years.

The analysis engine will combine a number of processes into a coherent system running on distributed high-performance computing hardware at ORNL's Center for Computational Sciences (CCS), LBNL's National Energy Research Scientific Computing Center, and ANL's Center for Computational Science and Technology facilities. A schematic of these processes is shown in Fig. 2. A process manager will conditionally determine the necessary analysis steps and direct the flow of tasks to massively parallel process resources at these several locations. These processes will include multiple statistical and artificial-intelligence-based pattern-recognition algorithms (for locating genes and other features in the sequence), computation for statistical characterization of sequence domains, gene modeling algorithms to describe the extent and structure of genes, and sequence comparison programs to search databases for other sequences that may provide insight into a gene's function. The process manager will also initiate multiple distributed information retrieval and data mining processes to access remote databases for information relevant to the genes (or corresponding proteins) discovered in a particular DNA sequence region. Five significant technical challenges must be addressed to implement such a system. A discussion of those challenges follows.

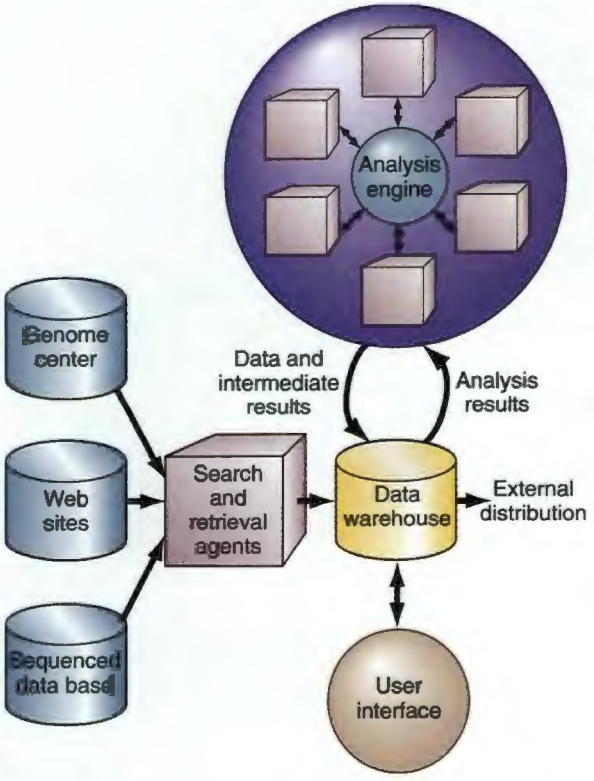


Fig. 1. The sequence analysis engine will input a genomic DNA sequence from many sites using Internet retrieval agents, maintain it in a data warehouse, and facilitate a long-term analysis process using high-performance computing facilities.

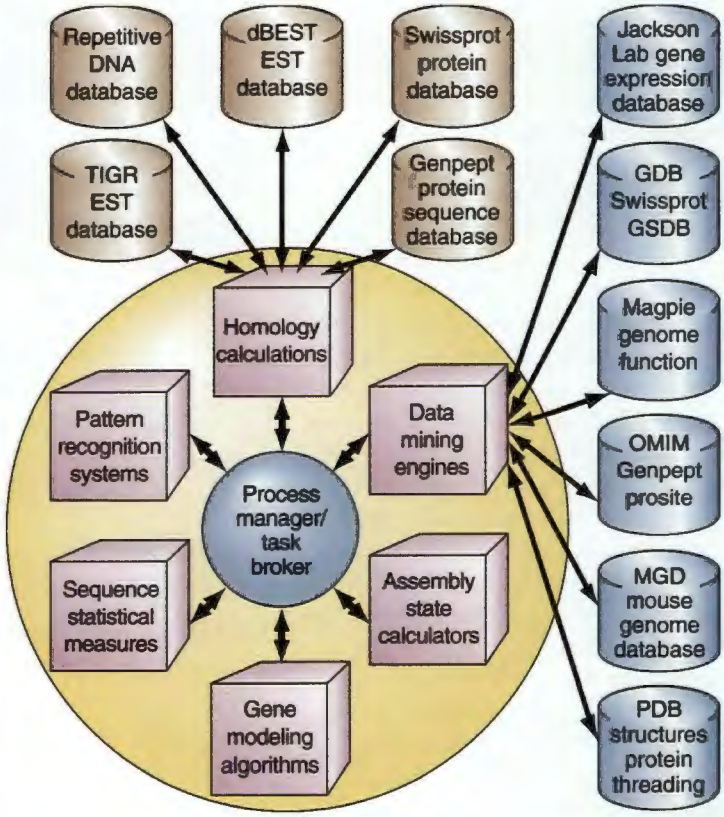


Fig. 2. In the sequence analysis engine, a central task manager coordinates analysis tasks such as pattern recognition and gene modeling and also initiates sequence comparison and data mining using multiple external databases.

Seamless high-performance computing. Megabases of DNA sequence being analyzed each day will strain the capacity of existing supercomputing centers. Interoperability between high-performance computing centers will be needed to provide the aggregate computing power, managed through the use of sophisticated resource management tools. The system must be fault-tolerant to machine and network failures so that no data or results are lost.

Parallel algorithms for sequence analysis. The recognition of important features in a sequence, such as genes, must be highly automated to eliminate the need for time-consuming manual gene model building. Five distinct types of algorithms (pattern recognition, statistical measurement, sequence comparison, gene modeling, and data mining) must be combined into a coordinated toolkit to synthesize the complete analysis.

One of the key types of algorithms needed is pattern recognition. Methods must be designed to detect the subtle statistical patterns characteristic of biologically important sequence features, such as genes or gene regulatory regions. DNA sequences are remarkably difficult to interpret through visual examination. For example, in Fig. 3, it is virtually impossible to tell that part of the sequence is a gene coding region. However, when examined in the computer, DNA sequence has proven to be a rich source of interesting patterns, having periodic, stochastic, and chaotic properties that vary in different functional domains. These properties and methods to measure them form the basis for recognizing the parts of the sequence that contain important biological features.

In genomics and computational biology, pattern recognition systems often employ artificial neural networks or other similar classifiers to distinguish sequence regions containing a particular feature from those regions

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1321 agcagcttct aatttgggtg cgtggttgag agcgctcagc tgtcagccct gcctttgagg
1381 gctgggtccc ttttcccatc actgggtcat taagagcaag tgggggcgag gcgacagccc
1441 tcccgcacgc tgggttgcag ctgcacaggt aggcacgctg cagtccttgc tgcctggcgt
1501 tggggcccag ggaccgctgt gggtttgccc ttcagatggc cctgccagca gctgccctgt
1561 ggggcctggg gctgggcctg ggcctggctg agcagggccc tccttggcag gtggggcagg
1621 agaccctgta ggaggacccc gggccgcagg cccctgagga gcgatgacgg aatataagct
1681 ggtggtggtg ggcgccggcg gtgtgggcaa gagtgcgctg accatccagc tgatccagaa
1741 ccattttgtg gacgaatacg accccactat agaggtgagc ctagcgccgc cgtccaggtg
1801 ccagcagctg ctgcgggcga gcccaggaca cagccaggat agggctggct gcagccccctg
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1921 tctcagcacc ccaggagagg agggggcatg aggggcatga gaggtaccag ggagaggctg
1981 gctgtgtgaa ctccccccac ggaaggtcct gaggggtcc ctgagccctg tcctcctgca
2041 ggattcctac cggaagcagg tggtcattga tggggagacg tgcctgttgg acatcctgga
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Fig. 3. Approximately 800 bases of DNA sequence (equivalent to 1/3,800,000 of the human genome), containing the first gene coding segment of four in the human *Ras* gene. The coding portion of the gene is located between bases 1624 and 1774. The remaining DNA around this does not contain a genetic message and is often referred to as "junk" DNA.

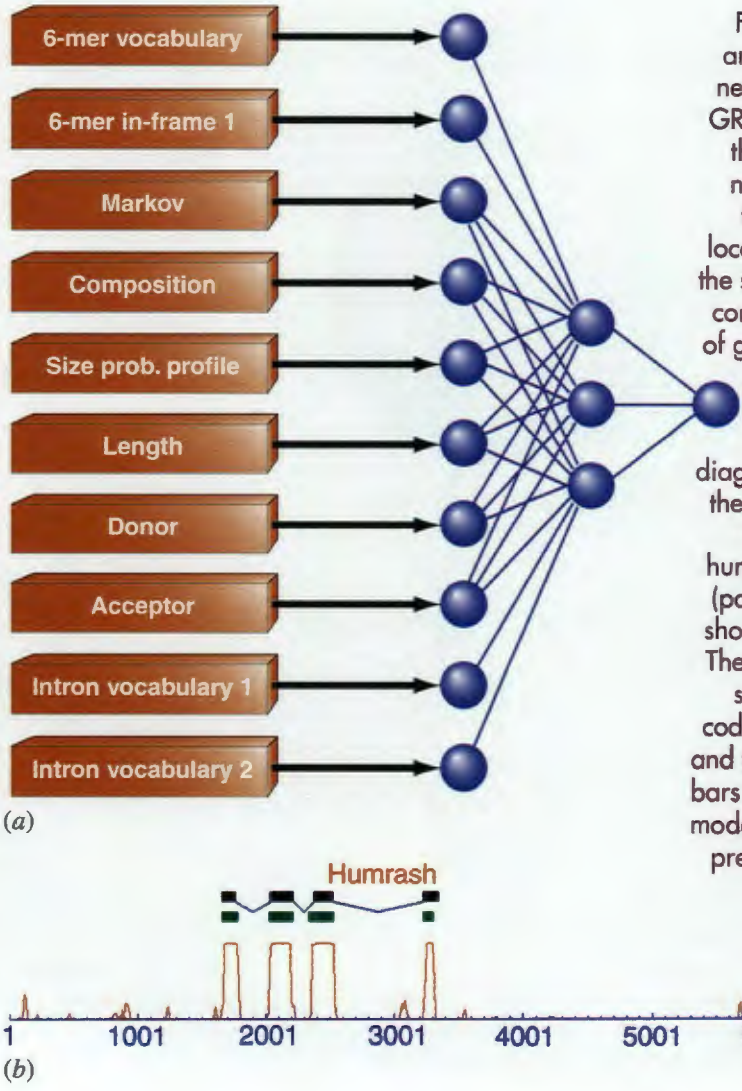


Fig. 4. (*a*) The artificial neural network used in GRAIL combines the results of a number of statistical tests to locate regions in the sequence that contain portions of genes with the genetic code for proteins. (*b*) A diagram showing the prediction of GRAIL on the human *Ras* gene (part of which is shown in Fig. 3). The peaks correspond to gene coding segments, and the connected bars represent the model of the gene predicted by the computer.

that do not. Machine-learning methods allow computer-based systems to learn about patterns from examples in DNA sequence. They have proven to be valuable because our biological understanding of the properties of sequence patterns is very limited. Also, the underlying patterns in the sequence corresponding to genes or other features are often very weak, so several measures must be combined to improve the reliability of the prediction. A well-known example of this is ORNL's GRAIL gene detection system, deployed originally in 1991, which combined seven statistical pattern measures using a simple feed-forward neural network [Fig. 4(*a*)]. GRAIL is able to determine regions of the sequence that contain genes [Fig. 4(*b*)], even genes it has never seen before, based on its training from known gene examples.

High-speed sequence comparison represents another important class of algorithms used to compare one DNA or protein sequence with another in a way that extracts how and where the two sequences are similar. Many organisms share many of the same basic genes and proteins, and information about a gene or protein in one organism provides insight into the function of its "relatives" or "homologs" in other organisms. Experiments in simpler organisms often provide insight into the importance of a gene in humans, so sequence comparison is a very important tool. Often the most accurate and sensitive methods for making this comparison are carried out using massively parallel computational platforms. To get a sense of the scale, examination of the relationship between 2 megabases of sequence (one day's finished sequence) and a single database of known gene sequence fragments (called ESTs) requires the calculation of 10^{15} DNA base comparisons. And there are quite a number of databases to consider.

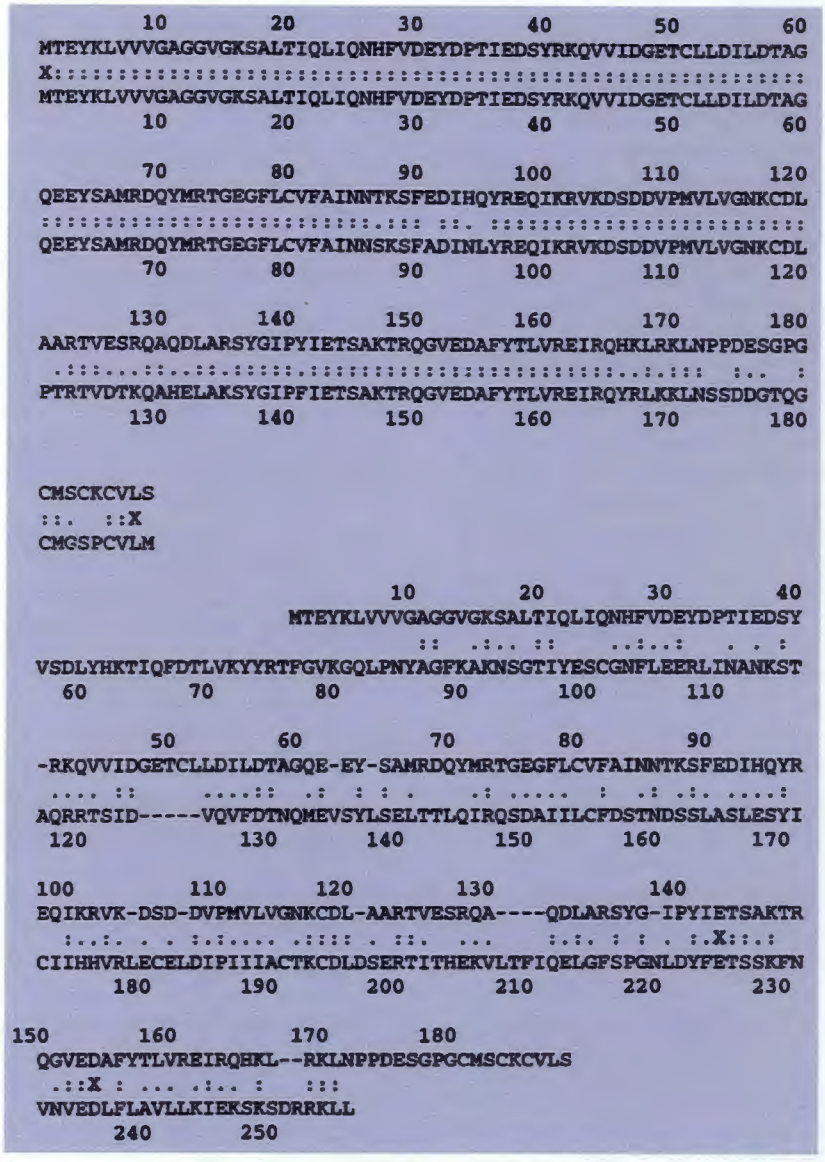


Fig. 5. Alignments of the protein sequences in the *Ras* family. First is the alignment of human *Ras* and mouse *Ras*, followed by human *Ras* with a related protein in yeast. The relationship in the latter case is much more difficult to detect, requiring computationally intensive sequence comparison methods. The letters in the sequence represent a pre-letter code for the 20 amino acids.

Two examples of sequence comparison for members of the same protein family are shown in Fig. 5. One shows a very similar relative to the human protein sequence query and the second a much weaker (and evolutionarily more distant) relationship. The sequence databases (which contain sequences used for such comparisons) are growing at an exponential rate, making it necessary to apply ever-increasing computational power to this problem.

Data mining and information retrieval. Methods are needed to locate and retrieve information relevant to newly discovered genes. If similar genes or proteins are discovered through sequence comparison, often experiments have been performed on one or more homologs that can provide insight into the newly discovered gene or protein. Relevant information is contained in more than 100 databases scattered throughout the world, including DNA and protein sequence databases, genome mapping databases, metabolic pathway databases, gene expression databases, gene function and phenotype databases, and protein structure databases. These data can provide insight into a gene's biochemical or whole organism function, pattern of expression in tissues, protein structure type or class, functional family, metabolic role, and potential relationship to disease phenotypes. Using the Internet, researchers are developing automated methods to retrieve, collate, fuse, and dynamically link such database information to new regions of sequence. This is an important component of ORNL's Functional Genomics Initiative, because it helps to link experimental studies in the mouse to the larger context of the world's genomic information.

The target data resources are very heterogeneous (i.e., structured in a variety of ways), and some are merely text-based and poorly formatted, making the identification of relevant information and its retrieval difficult. Intelligent information retrieval technology is being applied to this domain to improve the reliability of such systems. One challenge here is that information relevant to an important gene or protein may appear in any database at any time. As a result, systems now being developed dynamically update the descriptions of genes and proteins in our data warehouse and continually poll remote data resources for new information.

Data warehousing. The information retrieved by intelligent agents or calculated by the analysis system must be collected and stored in a local repository from which it can be retrieved and used in further analysis processes, seen by researchers, or downloaded into community databases. Numerous data of many types need to be stored and managed in such a way that descriptions of genomic regions and links to external data can be maintained and updated continually. In addition, large volumes of data in the warehouse must be accessible to the analysis systems running at multiple sites at a moment's notice. Our plan involves using the High-Performance Storage System being implemented at ORNL's CCS.

Visualization for data and collaboration. The sheer volume and complexity of the analyzed information and links to data in many remote databases require advanced data visualization methods to allow user access to the data. Users need to interface with the raw sequence data; the analysis process; and the resulting synthesis of gene models, features, patterns, genome map data, anatomical or disease phenotypes; and other relevant data. In addition, collaborations among multiple sites are required for most large genome analysis problems, so collaboration tools, such as video conferencing and electronic notebooks, are very useful. A display of several genes and other features from our GRAIL Internet server is shown in Fig. 6. Even more complex and hierarchical displays are being developed that will be able to zoom in from each chromosome to see the

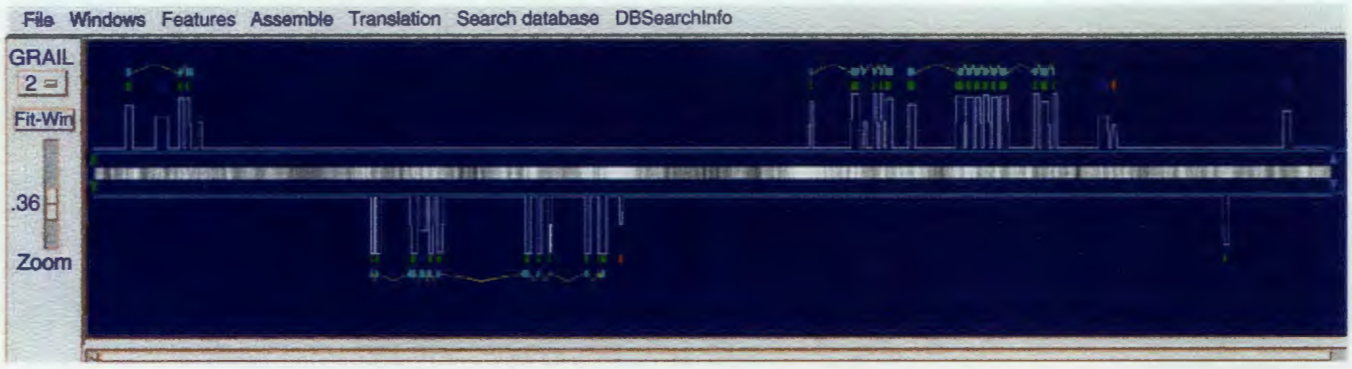


Fig. 6. Diagram showing a region of 60 kilobases of sequence (horizontal axis) with several genes predicted by GRAIL (the up and down peaks represent gene coding segments of the forward and reverse strand of the double-stranded DNA helix). Visualization tools like the GRAIL interface provide researchers with an overview of large genomic regions and often have hyperlinks to underlying detailed information.

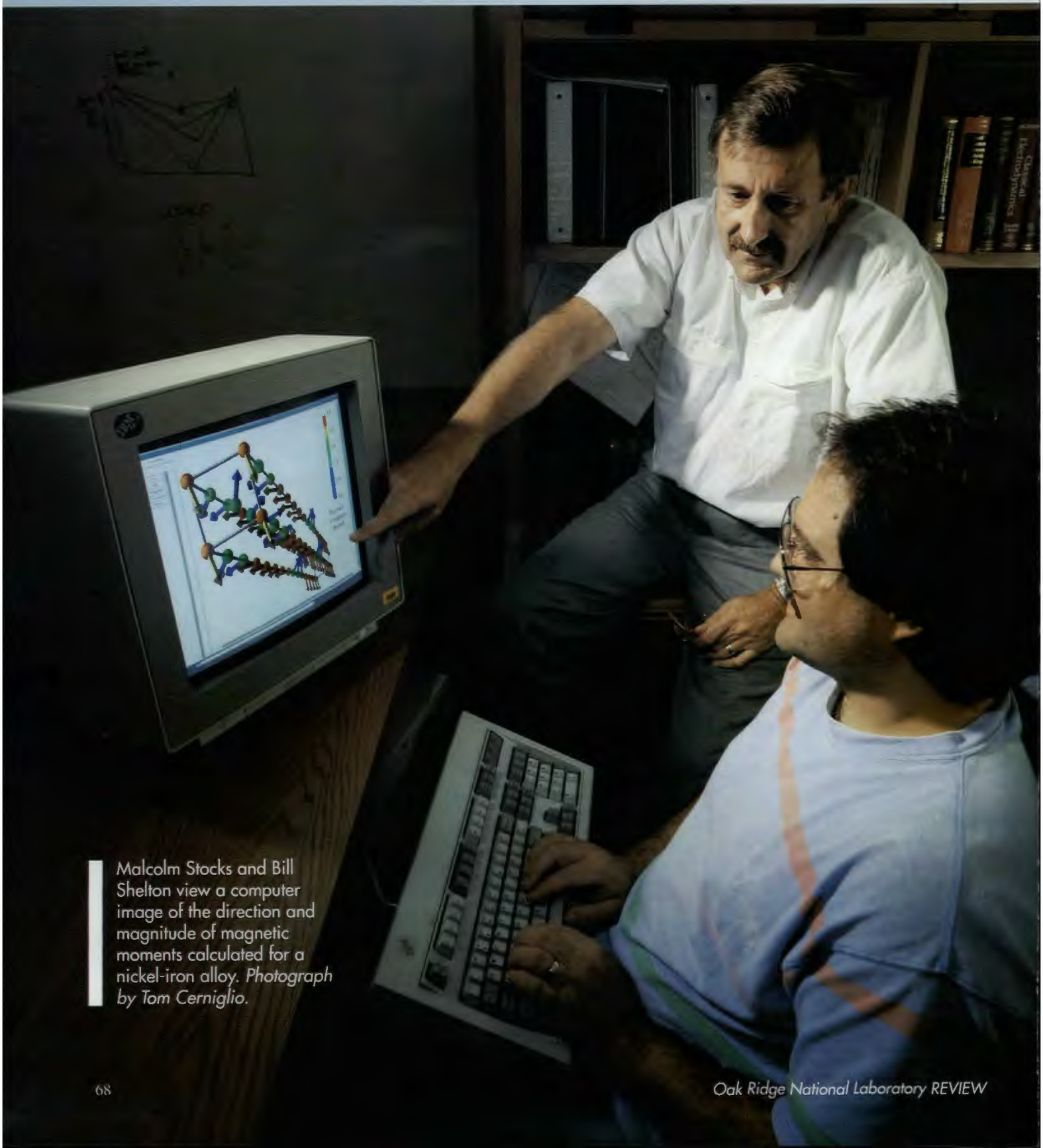
chromosome fragments (or clones) that have been sequenced and then display the genes and other functional features at the sequence level. Linked (or hyperlinked) to each feature will be detailed information about its properties, the computational or experimental methods used for its characterization, and further links to many remote databases that contain additional information. Analysis processes and intelligent retrieval agents will provide the feature details available in the interface and dynamically construct links to remote data.

The development of the sequence analysis engine represents part of the rapid changes in the biological sciences paradigm to one that makes much greater use of computation, networking, simulation and modeling, and sophisticated data management systems. Unlike any other existing system in the genomics arena, the sequence analysis engine will link components for data input, analysis, storage, update, and submission in a single distributed high-performance framework that is designed to carry out a dynamic and continual discovery process over a 10-year period. The approach outlined is flexible enough to use a variety of hardware and data resources; configure analysis steps, triggers, conditions, and updates; and provide the means to maintain and update the description of each genomic region. Users (individuals and large-scale producers) can specify recurrent analysis and data mining operations that continue for years. The combined computational process will provide new knowledge about the genome on a scale that is impossible for individual researchers using current methods. Such a process is absolutely necessary to keep up with the flood of data that will be gathered over the remainder of the Human Genome Project. **ornl**

BIOGRAPHICAL SKETCH

EDWARD C. UBERBACHER is head of the Computational Biosciences Section in ORNL's Life Sciences Division. He received his Ph.D. degree in chemistry from the University of Pennsylvania. In 1980, he conducted postdoctoral studies at the University of Pennsylvania Department of Biophysics and ORNL's Biology Division through the University of Tennessee–ORNL Graduate School of Biomedical Sciences. In this work, he investigated the structure and function of genetic materials using crystallography and tomographic image reconstruction in the electron microscope. In 1985 he became a consultant at ORNL's Center for Small-Angle Scattering Research, pursuing structural and dynamic studies of macromolecules in solution through use of neutron and X-ray scattering techniques. In 1987, he also became a research assistant professor at the Graduate School of Biomedical Sciences and an investigator in the Biology Division, where he focused on X-ray and neutron crystallography, scattering, and other biophysical methods. In 1988 he became a consultant in ORNL's Engineering Physics and Mathematics (EP&M) Division, where he developed artificial intelligence and high-performance computing methods for genomic DNA sequence analysis. In 1991 he joined the staff of the EP&M Division as the Informatics Group leader and received an R&D 100 award for the development of the Gene Recognition and Analysis Internet Link (GRAIL) system for analyzing DNA sequences. In 1997 he assumed his current position at ORNL. He is also an adjunct associate professor in the Graduate School of Biomedical Sciences at the University of Tennessee at Knoxville.

Developing a Grand Challenge Materials Application Code: An Interdisciplinary Approach



Malcolm Stocks and Bill Shelton view a computer image of the direction and magnitude of magnetic moments calculated for a nickel-iron alloy. *Photograph by Tom Cerniglio.*

By William A. Shelton and G. Malcolm Stocks

The combination of massively parallel processors and newly developed computation methods at ORNL is enabling scientists to simulate magnetic and other properties of metallic alloys based on the electronic structure of thousands of atoms. Such computer simulations are less costly and time-consuming than laboratory experiments and could help U.S. aerospace, biotechnology, electronics, and power generation industries become more competitive in products based on advanced materials.

Fig. 1. Advanced materials are showing up in everyday products: (a) A variety of materials make automobiles tougher and lighter. (b) Newer materials enhance the performance of catalytic converters. (c) Quasi-crystals are used in the electronics industry. (d) Carbon-fiber-reinforced composites provide strength for car bumpers and tires. (e) Bioskin is used for burn victims. (f) Turbine blades are used in the aerospace and power generation industries.

Throughout history, materials science has played an extremely important role in society. Today's significant developments in materials science include lightweight, corrosion-resistant, ductile alloys used to make turbine blades for the aerospace and power generation industries and artificial skin used in medicine (see Fig. 1).

Clearly, materials science has a profound effect on our economy. For example, in the early 1970s, the birth and growth of the microelectronics industry sparked a surge in the Japanese economy and a large shift in the global marketplace. Therefore, to improve its competitiveness in the global economy, the United States must be at the forefront of materials research to better position itself for development, commercialization, and use of the next new technology.

A key factor for any industry is the research and development (R&D) costs associated with bringing a product to market. Unfortunately, at the present time the laboratory development of new, technologically advanced materials is largely performed using phenomenological parameters (based on human experience). This type of approach, while successful, is an expensive and time-consuming process.

For successful competition in the global marketplace, R&D resources must be used efficiently to enable timely release of a product at the lowest possible price. Reducing R&D costs and the time needed to bring a product to market requires strong collaborations among materials theorists, experimentalists, and computational scientists. Computational scientists are essential because the cost of performing computer simulations, or computer experiments, is far lower than the cost of conducting laboratory experiments. In addition, results can often be obtained faster from simulations than from laboratory experiments.

A key difficulty in simulating the properties of materials such as metallic alloys is that physical mechanisms responsible for particular properties exist on varying length scales ranging from the microscopic to the continuum. While theoretical models do exist across these length scales, these models often are based on phenomenology, requiring some form of experimental input that diminishes their usefulness. On the other hand, on the microscopic scale there are so-called first principles, or ab initio, methods that incorporate the underlying physics and therefore do not require any adjustable parameters. These methods calculate the physical properties of crystalline materials at the microscopic level, where the crystal is made up of atoms in a periodic arrangement (see Fig. 2). In each atom, electrons orbit a nucleus composed of protons and neutrons. The outermost electrons, or valence electrons, hold the crystal together (cohesion). They are also responsible for most of a material' s properties, ranging from its phase stability to its ability to conduct heat and electricity.

These atomistic methods calculate the energetics of a system of electrons in the field of atomic nuclei using quantum mechanics. In addition, it is possible to use the output from calculations using ab initio methods to determine parameters used as the input for models that operate at much larger

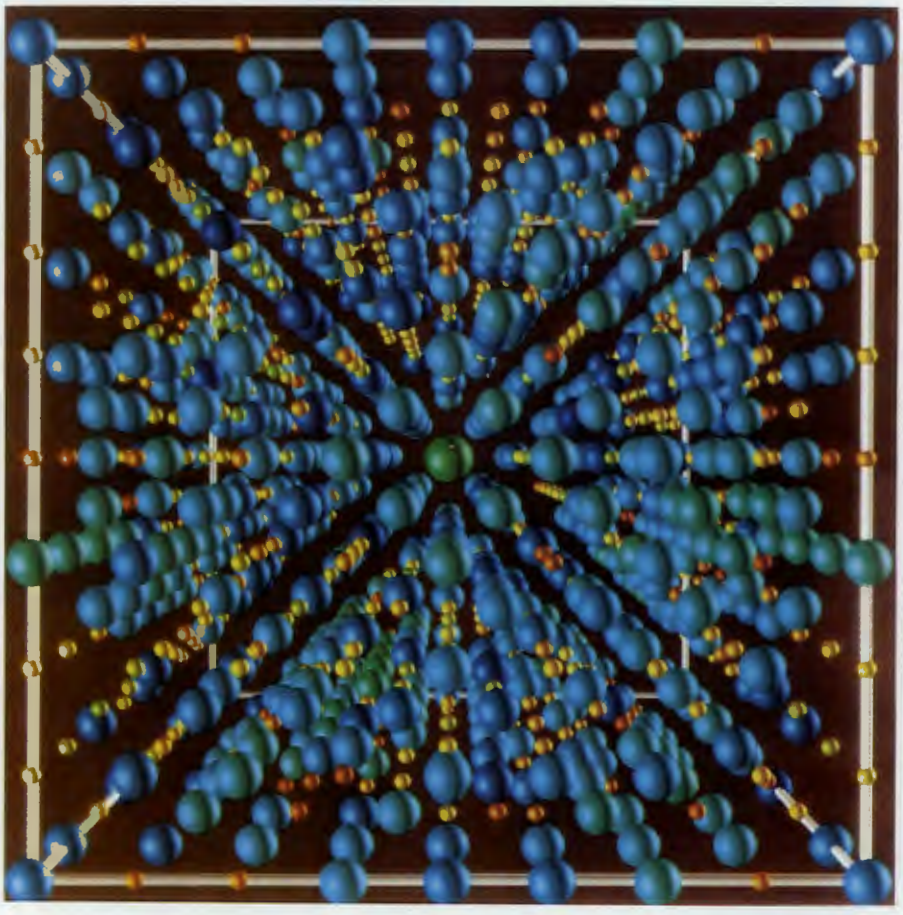


Fig. 2. Crystalline materials are made up of atoms in a periodic arrangement.

length scales. This type of approach connects the different modeling efforts on various length scales, enabling calculations of materials properties without performing a laboratory experiment. This approach can aid in the design of technologically advanced materials at a fraction of current development costs.

Unfortunately, contributions arising from theoretical investigations have been limited. A major hurdle in implementing the above strategy is overcoming poor $\vartheta(N^3)$ scaling (where N is the number of atoms making up the system) inherent in traditional ab initio methods. $\vartheta(N^3)$ scaling arises because of either the necessity of solving an eigenvalue-eigenvector problem or the need to calculate the inverse of a matrix. This limitation reduces both the types of properties that can be realistically simulated and the types of parameters that can be reliably extracted for use in other large-scale simulations. Solving this problem requires the development of new ab initio methods that offer significantly improved scaling.

New Tools for Materials Theorists

The introduction of massively parallel processors (MPPs) in the 1980s has provided materials theorists with the tools to begin development of new ab initio methods for uncovering the physical mechanisms responsible for a material's intrinsic properties. As part of DOE's High Performance Communication Computation Program (DOE-HPCCP) in materials science, we have developed the first fully parallel, local-density-approximation (LDA)-based ab initio electronic structure method that scales linearly [$\vartheta(N)$] as the number of atoms is increased. This new method, referred to as the locally self-consistent multiple scattering (LSMS) method, is a real-space multiple scattering, Green-function-based method. For the first time, this new technique using ab initio methods makes possible an accurate simulation of the properties of materials whose behavior depends on the electronic structure of systems comprising hundreds to thousands of atoms.

The development of such a large-scale application requires interdisciplinary work involving quantum physics, materials science, applied mathematics, and computer science. This type of approach—formulated by materials theorists at ORNL—has been extremely successful, resulting in a highly efficient algorithm that can be used for investigations of materials properties of systems that were originally considered untenable because of the number of particles necessary to accurately perform the simulations.

At the heart of multiple scattering theory is the calculation of the single-site Green function. Determining the single-site Green function requires calculation of the scattering path operator. The scattering path operator describes the scattering of an electron beginning at site i and ending at site j and includes all possible scattering paths. The total scattering path of an electron consists of both a "single scattering path," by which an electron scatters from a single site, as well as a "multiple scattering path," by which an electron scatters from multiple sites and returns to a site multiple times after being rescattered (see Fig. 3). For condensed systems, multiple scattering theory can be viewed as a succession of scattering events with the added advantage of expressing the scattering properties of the entire system in terms of the scattering properties of the individual atoms. Using this type of method along with standard approaches employed in traditional electronic structure methods leads to a $\vartheta(N^3)$ algorithm. Calculation of the scattering path operator requires the inverse of a matrix whose size is proportional to the number of atoms, N, making up the system and hence $\vartheta(N^3)$ scaling.

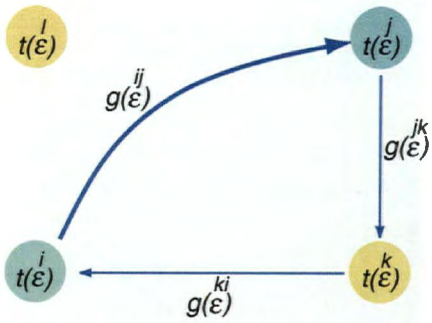


Fig. 3. An example of one scattering path an electron can take within a four-atom cluster.

On the other hand, by making use of MPP machines and formulating this approach in real space with an approximation to the calculation of the scattering path operator leads to a $\vartheta(N)$ method. In this new real-space approach, every atom must calculate its own scattering path operator and single-site Green function. Formally, to calculate the scattering path operator for site i requires inclusion of all scattering events with all the other sites, leading to the inversion of a matrix whose size is proportional to N. However, truncating the number of atoms in the calculation of the scattering path operator to m reduces the size of the matrix to be inverted. Because each atom must perform this inversion, which scales as $\vartheta(m^3)$, the total scaling for the entire N atom system is $\vartheta(m^3N)$. Now the $\vartheta(N)$ scaling can be realized by noting that once m is determined, adding more atoms outside of the m atom cluster does not affect the calculation of the scattering path operator. In other words, once m is fixed, the algorithm naturally scales linearly as N is increased because every atom must perform the matrix inversion, whose size is the same. Therefore, each atom requires the same amount of time to perform this operation (see Fig. 4).

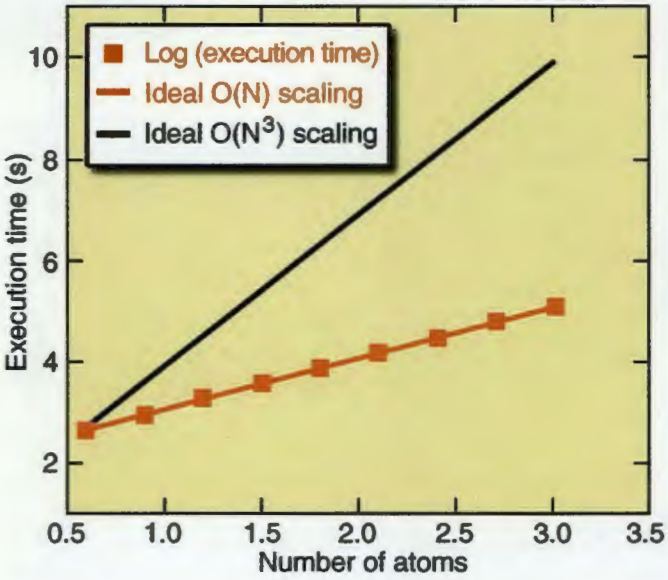


Fig.4. This plot is the log of the execution time vs the log of the number of atoms making up the crystal. The plot demonstrates the linear scaling of the LSMS method.

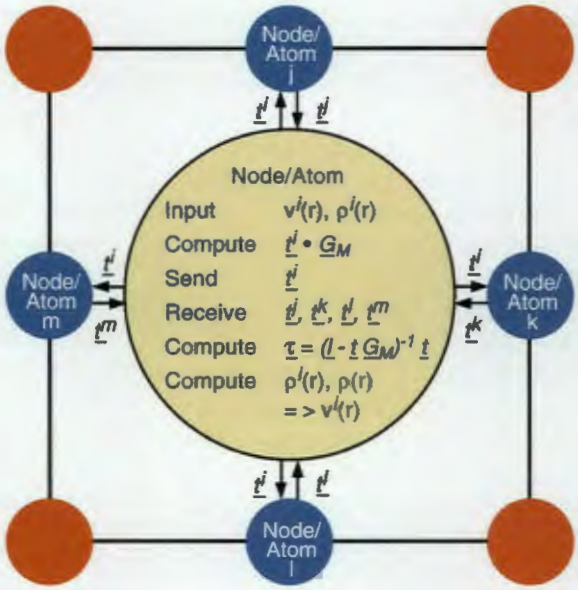


Fig. 5. A schematic of the LSMS algorithm highlighting the information that is exchanged within a nearest-neighbor LIZ.

A key component of this approach is the decomposition of the atoms making up the crystal onto computer nodes on a large-scale MPP machine. To simplify this discussion, we will use a strategy in which we assign an atom to a computer node (generally one can assign multiple atoms to a computer node). This type of decomposition requires communication between an atom and the other atoms within its *m* atom cluster. The information that is sent is the single-site transfer matrix that contains information about the sending atom's scattering properties. The single-site transfer matrix is used to construct the scattering path operator and single-site Green function for the receiving atom's site.

ORNL Contributions

A key contribution made by ORNL computer scientists (including the authors) was the design and development of a computationally efficient message-passing algorithm to handle communication between atoms. On a distributed message-passing machine, two pieces of information are crucial to ensuring that a particular atom receives the correct message: the node number of the computer node on which an atom resides and the message tag. The node number is used in a way similar to a postal address; like anyone who gets mail, an atom can receive messages from more than one source. The message tag is used to separate these messages so that the atom can pick up the messages in a specific order.

Our algorithm is similar to a molecular dynamics algorithm in which two integer lists are constructed for each atom. One list contains the node numbers of the atoms that are to receive information from this atom. The second list contains the message tags. These tags are numbered using the row block index of the matrix. A row block consists of several rows of a matrix. This numbering scheme is necessary because each row block of an atom's scattering path operator describes a part of the total scattering process associated with the atom sending the message (see Fig. 5). The algorithm is computationally fast and memory-efficient, requiring the storage of only two single-site transfer matrices at a time, one for the local atom's matrix and the other for the sending atom's matrix. Once it has been used in the construction of a row block of the atom's scattering path operator, its memory location is reused for the next incoming message.

As previously mentioned, the most time-consuming part of this method is taking the inverse of a matrix. Even though this is a linear method, the time goes up drastically for increasing cluster size, *m*, because the method involves inverting a matrix whose size is proportional to *m*. The scattering path operator is a double-precision, dense, complex, nonsymmetric matrix. Because the matrix is nonsymmetric, there is no symmetry that can be exploited to speed up the calculation of the inverse.

A major contribution made by ORNL's applied mathematicians was to develop a hybrid method for solving for the inverse of the scattering path

operator. A key feature of this method is that only a small portion of the inverse is needed. Using direct methods such as lower upper (LU) triangular-based methods to obtain this part of the inverse still results in a $\vartheta(m^3)$. So instead, an iterative method known as the quasi-minimal residual method (QMR) was employed. This method can be used for both symmetric and nonsymmetric problems, and equally important, it is extremely efficient in its use of computer memory. Iterative methods typically work well for sparse matrices (matrices containing lots of zeros) but not so well on dense matrices (matrices containing very few zeros). Normally, this is true because the full inverse is usually being calculated. However, because we are interested only in a small portion of the inverse, an iterative approach might just work, and indeed it works extremely well. There are certain situations where it is known not to work as well as a direct method. Therefore, the final algorithm is a hybrid one that switches between the QMR and a direct method, providing maximum computational efficiency.

Recently, materials theorists at ORNL have formulated a new version of the LSMS method. This new approach results in a sparse scattering path matrix. Again, the applied mathematicians are working with the application scientists on providing a direct sparse solver. This solver takes advantage of the sparsity pattern to develop a computationally fast algorithm that uses significantly less computer memory than the previous version of the LSMS computer code.

Simulating Materials Properties by New Computer Methods

Accurately simulating particular materials properties such as magnetic interactions may require more computational resources than can be provided by a single large MPP machine, requiring instead several large machines that are networked together. These machines can consist of several different architectures and can reside on different networks. This type of computing is referred to as heterogeneous computing. Efficient use of these resources requires fault tolerance. Fault tolerance provides the user with the ability to restart an application after a machine failure, provided either that the remaining computational resources can supply the necessary capabilities or that additional computational resources become available to run the application.

Currently, the ORNL team is involved in a networking project with DOE's Sandia National Laboratories (SNL) to link together the two largest computers in the world to solve an important scientific problem. The two machines that are networked together are the 1024-node Intel Paragon XP/S 150 at ORNL's Center for Computational Sciences and the 1800-node Intel Paragon at SNL. The LSMS computer code is being used for this project to study the magnetic structure of technologically important magnetic alloys. This project requires a strong collaboration with computer scientists. A key objective is to demonstrate the effectiveness of linking together large-scale MPP machines to solve important scientific and technological problems. The major obstacle to overcome is the time it takes to communicate information between machines.

The parallel virtual machine (PVM) software library developed in ORNL's Computer Science and Mathematics Division is used to handle the communication between the machines. PVM supports heterogeneous computing and dynamic configuration, permitting a user to add or delete computational resources dynamically during a PVM session. Also, PVM takes advantage of high-performance network interfaces such as the asynchronous transmission mode (ATM), which currently provides the lowest latency and highest bandwidths and, thereby, the maximum message-passing performance.

ORNL computer scientists, led by Al Geist, are also developing a parallel application development system called CUMULVS (see Kohl's article "High-Performance Computing: Innovative Assistant to Science" starting on p. 54). CUMULVS supports fault tolerance, interactive visualization, and computational steering so that parameters of a simulation can be viewed and changed by participants during the simulation to "steer" it toward a desired outcome. Because it is based on PVM, it is heterogeneous and supports the use of high-speed network interfaces. CUMULVS supports fault tolerance through user-directed checkpointing (saving) of data and heterogeneous task migration. That is, the user can specify the essential data that must be saved to restart the application. CUMULVS writes these data out on each machine so that all machines have a coherent view of the data. CUMULVS can restart the application either on the remaining computational resources or by dynamically adding new computational resources via PVM and using the checkpointed data as the input. The interactive visualization feature supports multiple viewers connected to a running application. In this way, scientists collaborating on the same problem can view the data at the same time on their own machines at their own respective institutions.

We are currently incorporating CUMULVS into the LSMS code because performing some of our scientific investigations requires a large number of computer resources obtainable only by linking together

multiple platforms. The possibility of a machine failure increases with the number of machines networked together. Fault tolerance assures us that a failure within the environment is recoverable, allowing our simulation to continue. In addition, the ability to view a simulation provides us with a powerful tool to monitor it; if something goes wrong, we can stop the job, minimizing the loss of computer cycles.

Modeling Importance to Magnetic Alloys

To demonstrate the wide applicability of the LSMS method, we have applied it to the investigation of two magnetism problems affecting materials that contain both chemical and magnetic disorder. Chemical disorder is substitutional disorder in which an atomic site in the crystal is randomly occupied by atoms making up the system. Because we are assuming complete random disorder, the probability of occupation of an atomic site by an atom of a particular element is equal to that element's concentration in the alloy. Consider a copper-nickel alloy, for example. For collinear magnetic disorder (where the moments point either parallel or antiparallel to the spin axis of quantization) the size (magnitude) of the moments are randomly distributed on the magnetic atomic sites (i.e., nickel sites are magnetic whereas copper sites are not). For noncollinear magnetism, both the size (magnitude) and the directions are randomly distributed on the magnetic atomic sites. A major advantage in using the LSMS method is that it naturally accounts for any local fluctuations. Specifically, LSMS naturally incorporates the effects of short-range order on the energetics as a result of either chemical or magnetic disorder. An example of short-range correlation is short-range order of a particular

ORNL and Others Recognized for "Metacomputing" Approach

At the Supercomputing '96 conference held in November 1996 in Pittsburgh, Pennsylvania, a team of researchers from ORNL, Sandia National Laboratories, and the Pittsburgh Supercomputing Center (PSC) received a gold medal for performing a complex pacesetting calculation on a high-performance, multisite, multicomputer system linked by high-speed networks. Their "metacomputing" approach connected ORNL's Paragon supercomputers with Sandia's Paragon and Pittsburgh's Cray T3D supercomputers using high-speed networks provided by ESnet and vBNS.

The first code being implemented is a first-principles materials science electronic structure method developed at ORNL. In this project the code is being used to model the magnetic properties of metallic alloys. The algorithm decomposes the atoms of the material of interest across the nodes of a massively parallel computer by assigning each atom in the structure to an individual processor of the parallel machine. In this way, very complex models consisting of large numbers of atams can be simulated.

The purpose of this simulation was to investigate the underlying magnetic interactions that give rise to the complex magnetic structure observed in neutron-scattering experiments performed on disordered copper-nickel alloys. These neutron-scattering data, obtained by ORNL scientists at the High Flux Isotope Reactor, have existed for over two decades without a satisfactory intepretation. Previous simulations performed on the ORNL XP/S-150 Paragon that have involved a few hundred atoms had accurately described the structure in the neutron-scattering experiments, attributing it to relatively short-range interactions between magnetic atoms.

The purpose of the computer "experiment" demonstrated at Pittsburgh was to use the power of the metacomputer to simulate the thousands of atoms required to study the nature of the long-range interactions, thereby providing a more complete understanding of the neutron-scattering data. The three-lab team used the high-speed network for a 1000+ processor (atom) run between Paragons at Oak Ridge and Sandia. The code was also used to test the connection between ORNL's machines and PSC's Cray. The results demonstrate that tying geographically distributed heterogeneous supercomputers together for a single application is a viable way to produce otherwise unobtainable scientific results. This distributed approach is expected to be immensely beneficial to the national research community.

The three laboratories' metacomputing approach—which will ultimately use all of ORNL's Paragons, most of Sandia's Paragon, and all of PSC's Cray, for a total of nearly 3000 processors—received the gold medal award in the concurrency category of the High-Performance Computing Challenge competition at the Supercomputing '96 conference. The award, which was the only gold medal given in this competition, recognized the recipients for demonstrating excellence in large-scale heterogeneous supercomputing. ORNL researchers from the Center for Computational Sciences and the Metals and Ceramics, Computer Science and Mathematics, and Computing, Information, and Networking divisions participated in the effort.

atomic site with its surrounding neighbors. If a random disordered alloy is truly random, then there is no correlation between a site and its neighbors; in the case of the nickel-copper alloy, the nickel site is not affected by whether its neighboring atoms are nickel or copper. In many alloys, short-range order is extremely important and must be accounted for in the model if one hopes to calculate a material's properties accurately. LSMS incorporates short-range order in the construction of the system by using short-range order parameters, for example, to construct a crystal lattice with atomic sites occupied by atoms with appropriate neighboring atoms. Traditional band structure methods either cannot or can only approximately treat these types of effects.

Magnetic materials represent a multibillion-dollar industry. A fundamental understanding of magnetism in alloys has the potential to influence the design of magnetic materials for applications ranging from power generation to data storage. Magnetism has a profound effect on many alloy properties such as phase stability, thermal expansion, and electrical conductivity.

Magnetism is a consequence of electron spin. In metals the same electrons that give rise to cohesion (the energy that holds the crystal together) can, if they are reasonably well localized about atomic sites (e.g., d-electrons in cobalt, nickel, and iron), also give rise to magnetism. Magnetism occurs when it is energetically favorable on the atomic sites to have an excess of electrons of one spin; this spin imbalance gives rise to magnetic moments associated with individual atoms. In a ferromagnet the local magnetic moments point in the same direction (collinear parallel), resulting in a macroscopic magnetic moment (there are more electrons with spins that point parallel to the spin axis of quantization than electrons whose spins point antiparallel); in an antiferromagnet, an equal number of moments point up and down (collinear antiparallel) in an ordered arrangement, resulting in no net macroscopic magnetic moment.

In our first investigation, we have been studying the nature and effect of magnetic inhomogeneities in nickel-copper (Ni-Cu) alloys. This investigation uses the standard approach of assuming that the electron spin points either parallel or antiparallel to the spin axis of quantization (we assume that the z-axis is the spin axis of quantization in spin space). The second investigation involves the use of a new theory concerning noncollinear magnetism. In noncollinear magnetism the electron spin in the global frame of reference (the laboratory frame) is not restricted to any direction, but in its local frame of reference (on the atom), it points along the traditional spin axis of quantization (z-axis). As will be seen, this extra degree of freedom allows for a very rich magnetic structure that has not previously been simulated using an ab initio approach.

Our second investigation is applied to the disordered nickel-iron (Fe) Invar alloy, Ni.35Fe.65. Invar alloys are interesting for both scientific and technological reasons. In 1920 the Nobel Prize in physics was awarded to the Swiss-born French scientist Charles E. Guillaume for discovering this unique magnetic alloy. Invar alloys exhibit a negligible coefficient of thermal expansion (hence INVAR-iable), called the Invar effect. These alloys are used in many industries that need a material that does not expand in a particular temperature range. Such a material is needed for shadow masks for televisions and computer monitors, the surrounding tubing for fiberoptic cables, and high-precision laboratory equipment.

The purpose of our investigation of the Ni.80Cu.20 alloy is to uncover the nature of the magnetic correlations found in neutron-scattering experiments performed more than two decades ago by Joe Cable and colleagues at ORNL's High Flux Isotope Reactor. The onset of magnetism and the nature of the ferromagnetic state when nickel is alloyed with nonmagnetic copper to form a weakly ferromagnetic disordered Ni-Cu alloy have been matters of scientific interest. The results of the LSMS calculation for a ferromagnetic disordered Ni.80Cu.20 alloy show that the local magnetic moments associated with individual sites are inhomogeneously distributed.

In the LSMS calculation the random alloy is modeled by randomly occupying the sites of the 256-atom unit cell by atoms of nickel and copper (shown as large blue spheres and small red spheres, respectively, in Fig. 6). In the illustration, the arrows emanating from the nickel sites represent the magnitudes of the calculated local magnetic moments. (The magnetic moments associated with copper sites, which are antiparallel to the nickel moments, are too small to be seen.) The magnitudes of the nickel moments are encoded both in the length and in the color of the arrows. The local nickel-site magnetic moment varies from a minimum of approximately 0.29 Bohr magnetons (blue arrows) to a maximum of approximately 0.6 Bohr magnetons (red arrows). Interestingly, the magnetic moment on a nickel site correlates with the total magnetic moment on the nearest-neighbor shell of atoms surrounding it: large red arrows tend to be surrounded by other reddish arrows, while small blue arrows are surrounded by either copper sites having no moment or other blue arrows. So far, our calculations show excellent agreement with the measured neutron-scattering cross sections and also provide an atom-by-atom picture of magnetism (see Fig. 7). From this it

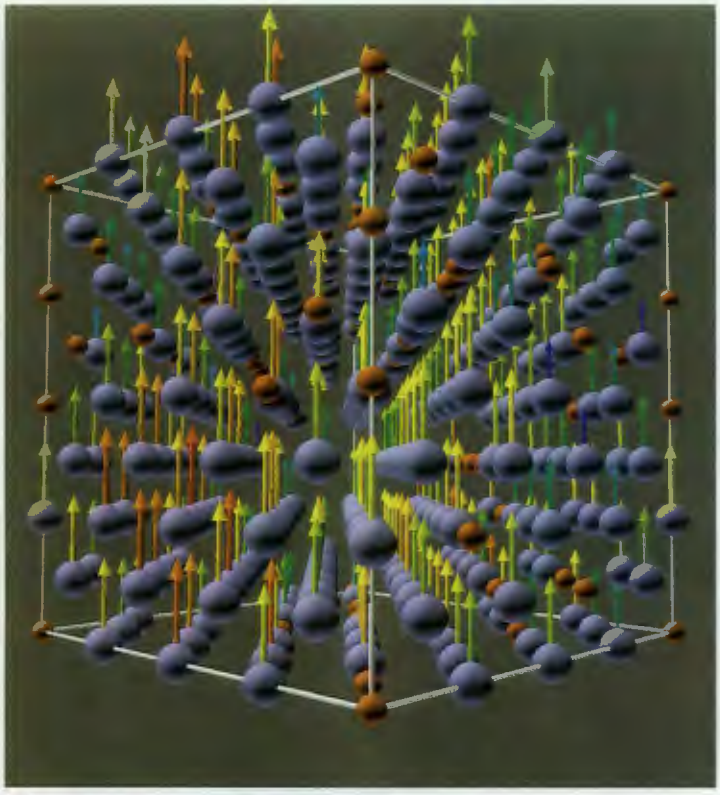


Fig. 6. A schematic of the 256-atom Ni-Cu unit cell.

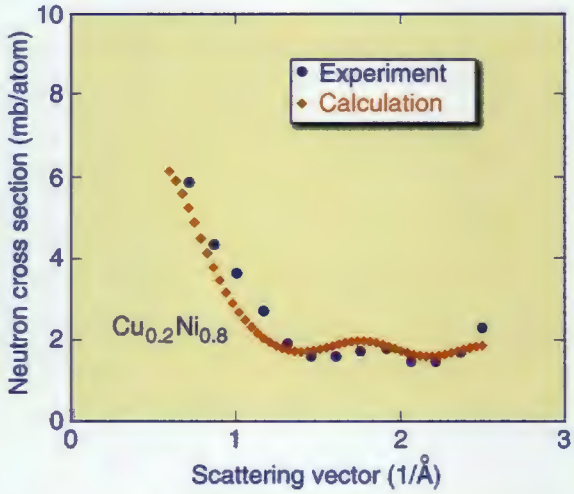


Fig. 7. Comparison of the experimental neutron-scattering cross sections with those obtained from the LSMS method.

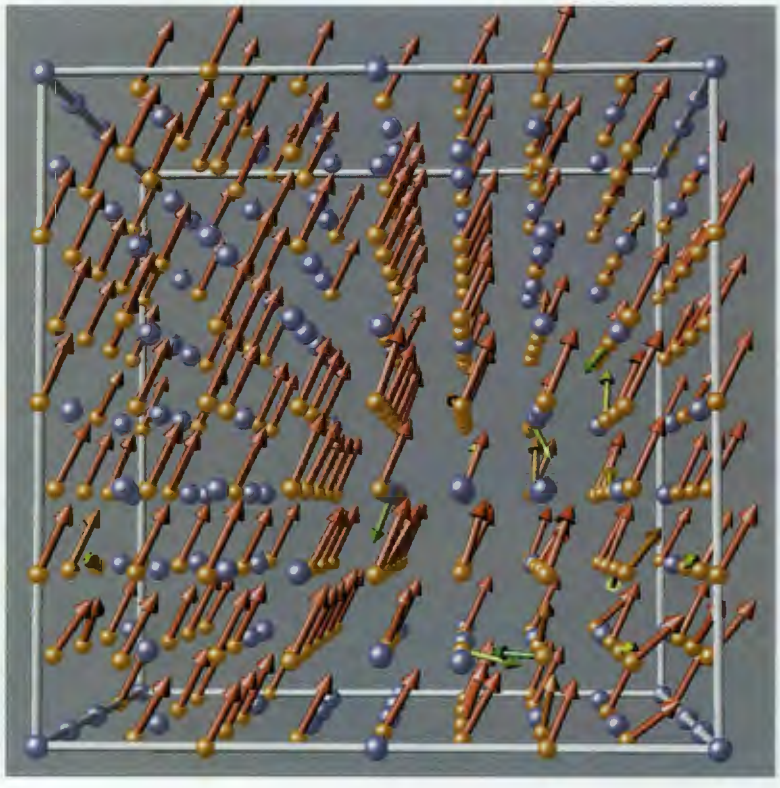


Fig. 8. A schematic of the 256-atom Ni-Fe spin canting unit cell.

can be seen that the magnetic moments are higher for nickel sites whose neighbors are nickel atoms having strong magnetic moments than for nickel sites surrounded by either nickel atoms having weak magnetic moments or by virtually nonmagnetic copper atoms. The results of these simulations are being used to reinterpret results of neutron-scattering measurements of magnetic correlations in these alloys.

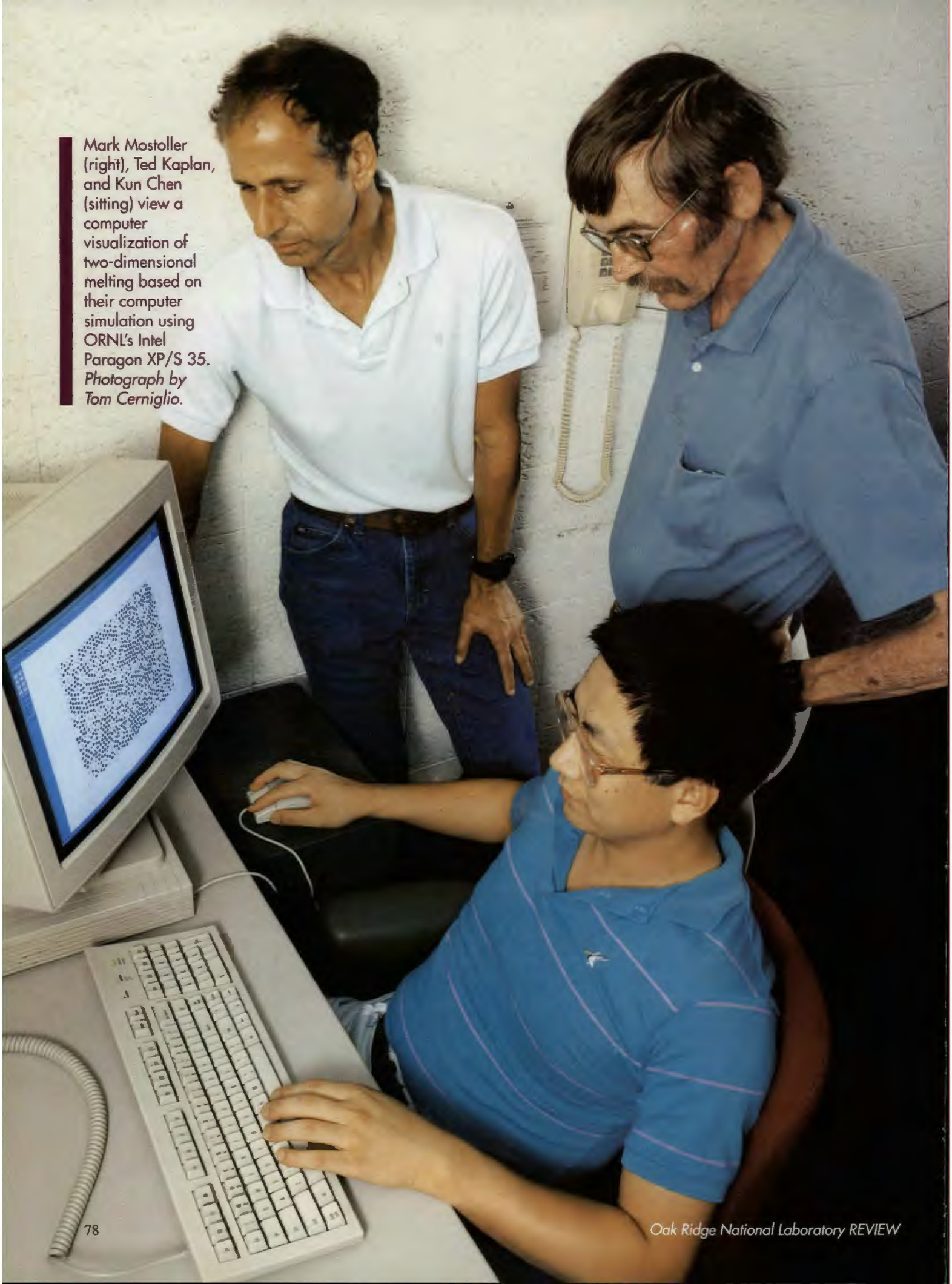
This past year, 1996, marked the hundredth anniversary of Guillaume's discovery of Invar. Despite the venerability of the subject, the mechanisms responsible for the Invar effect, though thought to be related to Invar's complex magnetic behavior, are still deeply mysterious. Our preliminary investigations of the ground state (T = 0 K) magnetic structure of large-cell (256-atom) models of disordered Ni.35Fe.65 alloys (the classic Invar system) are pointing to unusual magnetic behavior involving noncollinear arrangements of the local magnetic moments associated with iron-rich clusters within the otherwise disordered alloy (see Fig. 8). In particular, there is a nickel atom whose nearest neighbors are all nickel atoms and whose local moment, peculiarly enough, is exactly antiparallel to its surrounding nickel moments (the local magnetic structure is antiferromagnetic). If these magnetic structures remain stable, they will have important implications for our understanding of magnetism in this material, implications that could be investigated experimentally using neutron diffraction.

Our interdisciplinary team made several other important contributions to computational modeling of materials, in addition to the major ones covered here. The strong interaction among various ORNL scientists is a key to the success of this large-scale scientific project which can play an important role in sustaining our economic competitiveness. **ornl**

BIOGRAPHICAL SKETCHES

BILL SHELTON is a research staff member in the Mathematical Sciences Section of ORNL's Computer Science and Mathematics Division. He holds a Ph.D. degree in theoretical condensed matter physics from the University of Cincinnati. He also held a National Research Council (NRC) fellowship at the Naval Research Laboratory, working with Dr. Warren Pickett. In 1992 he joined the ORNL staff. His research interests include high-performance heterogeneous scientific computing, the development of scalable first-principles electronic structure algorithms, and the development of applied mathematical techniques and numerical algorithms to scientific problems, software tools, and parallel algorithms. He has published over 60 papers in materials science, high-performance computing, and parallel processing. He has also won several high-performance computing awards, including the Gordon Bell Prize, the Cray Research Award, and several High-Performance Computing Challenge Awards.

MALCOLM STOCKS is a Lockheed Martin Corporate Fellow in the Theory Group of ORNL's Metals and Ceramics Division. He holds a Ph.D. degree in condensed matter physics from Sheffield University. Prior to joining ORNL in 1976, he was a lecturer at the University of Bristol, U.K., from 1972 to 1976. His research interests include materials science, high-performance heterogeneous scientific computing, and the development of scalable first-principles electronic structure algorithms and parallel algorithms. He has published over 200 papers in materials science, high-performance computing, and parallel processing. He has also won several high-performance computing awards, including the Gordon Bell Prize, the Cray Research Award, and a High-Performance Computing Challenge Award.



Mark Mostoller (right), Ted Kaplan, and Kun Chen (sitting) view a computer visualization of two-dimensional melting based on their computer simulation using ORNL's Intel Paragon XP/S 35. *Photograph by Tom Cerniglio.*

How Solids Melt:
ORNL Simulations Support Theory

By Mark Mostoller, Ted Kaplan, and Kun Chen

Chocolate melts in our mouths, but how it turns from solid to liquid isn't clear in our minds. Recently, three ORNL researchers have used the Intel Paragon XP/S 35 to help confirm a theory developed in the 1970s about how substances melt in two dimensions. They simulated two-dimensional systems containing 576, 4,096, 16,384, 36,864, and 102,400 atoms with an interatomic force model often used for rare-gas solids. Results for the two largest systems show the existence of a new "hexatic" phase between the solid and liquid phases, as predicted by the theory. This two-dimensional simulation helps explain the melting process.

Every solid melts if taken to a high enough temperature. For example, hydrogen melts at about 14 Kelvin (or K, the number of degrees above absolute zero); ice at 273 K, iron at 1810 K, and tungsten at nearly 3700 K, making it very useful as the filament material in light bulbs. Melting in three dimensions (3D), or the conversion from solid to liquid, is a first-order phase transition in which a latent heat must be provided. Thus, ice keeps a drink cold by taking in its latent heat, which causes the ice gradually to melt.

Melting is a fundamental phenomenon that all of us have witnessed and think we understand, but, paradoxically, there is no generally accepted picture of how solids melt at an atomistic level. Instead, there are empirical rules such as the Lindemann criterion, named after the man who presented it 85 years ago. The atoms in a crystal vibrate around fixed positions, just like a guitar string when plucked. The size, or amplitude, of the vibrations increases with increasing temperature. According to the Lindemann criterion, a crystal will melt when the vibrational amplitudes of its constituent atoms reach some critical magnitude, say 10 to 15% of the interatomic spacing.

Physics is a search for the elegance and simplicity that underlie nature's often apparently chaotic and complex behavior. The Lindemann picture of melting is simple, but it certainly is not elegant. It proposes that the disorganized vibrations of the atoms in a solid somehow cause the solid to melt *at a very precise temperature*. Other phase transitions do not occur in such a disorganized fashion. Superconductivity, for example, occurs because electrons with opposite spins form pairs that can move through the lattice without resistance. A number of famous physicists, including Richard Feynman, have proposed theories for melting in 3D that involved more efficient mechanisms to mediate the process, but none of these theories has proven true.

In two dimensions (2D), the situation is different. In the 1970s, an elegant theory for melting was developed by John Kosterlitz, David Thouless, Burt Halperin, David Nelson, and Peter Young (the KTHNY theory, after the initials of its authors' last names). Many experiments and computer simulations have since been done to prove or disprove the theory, with ambivalent results. The experiments have often been quite imaginative. They have used layers of rare gas on graphite, charged polystyrene spheres in solution, and monolayers of metal spheres (metal shot to hunters) shaken between confining plates. Experimental results generally have been supportive of the KTHNY theory. In contrast, simulations, in which complications such as interactions of rare gas atoms with the graphite substrate can be avoided by studying ideal 2D systems, have given predominantly negative results. A number of people, including Burt Halperin and David Nelson, thought the reason for these results could lie in the system sizes and time scales employed in the simulations.

Enter ORNL

Here our part of the story begins. In 1992, the Intel Paragon XP/S 150 became a promise that would soon be funded. Mark Mostoller and Ted Kaplan began an effort in numerical simulations, hoping to harness the power the new machine would provide. They persuaded a close friend of long standing, Mark Rasolt, to join them in this new venture. Rasolt was a very creative and productive theorist who periodically spent time at Harvard University, where Halperin and Nelson are professors. Rasolt saw the development of our new capabilities in simulations and the arrival of the Paragon as an opportunity to test the KTHNY theory at the required system sizes and time scales

for the first time. He also thought that if the mechanism for 2D melting could be confirmed, the studies could be extended to melting in 3D.

Together we prepared a proposal to the Laboratory Directed Research and Development Program which Rasolt presented in September 1992. Everyone acknowledged that the proposal carried a high risk of failure because it would use a then nonexistent machine to examine a fundamental problem that great physicists had been unable to solve. In November 1992, shortly after learning that the project had been funded, Rasolt died of a massive heart attack at Los Angeles International Airport while returning from a conference in Australia. He was 49 years old.

It was hard to continue the work then, and it is hard to tell the story now. Kaplan took over leadership of the project. In August 1993, Kun Chen joined us as a postdoctoral researcher. The Intel Paragon XP/S 35 came on line in April 1994, and the XP/S 150 began operation in January 1995. Our tools had arrived, and we set to work.

Theoretically Speaking

A principal feature of the KTHNY theory of melting is its prediction of a new phase between solid and liquid. A crystalline solid has two kinds of order, translational and orientational. Translational order means that, if you start at a particular atom and take steps along well-defined paths over long distances, you will arrive in close proximity to another atom. Orientational order means that, if you look at two atoms separated by large distances, their neighbors will be oriented relative to some fixed axis in the same way. A liquid has no long-range order of either kind, but it has short-range order: any atom will have some average number of nearest neighbors clustered around an average neighbor distance with no preferred orientation. KTHNY's new phase, called the *hexatic phase*, has no translational order but retains orientational order. In short, you can't predict where the atoms are, but you can predict their neighbor environment.

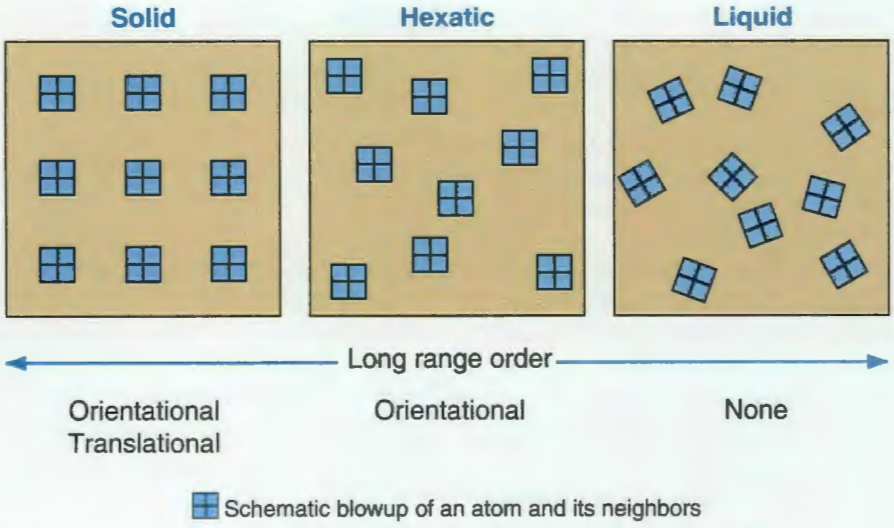


Fig. 1. A cartoon picture of the order present in the solid, hexatic, and liquid phases in two dimensions.

Figure 1 shows a cartoon representation of the three phases. The theory predicts that under certain conditions, the system will transform from solid to hexatic to liquid in two continuous phase transitions that do not involve a latent heat. All of these predictions rest on a picture that invokes specific defects (dislocations and disclinations) rather than the action of all atoms vibrating willy-nilly.

Perfected Method for the Paragon

What have we done that is new? Here's the list.

1. We chose to do our simulations with a recently perfected method for treating a constant pressure (P) and temperature (T) statistical ensemble. A constant volume and temperature ensemble allows mixed solid and liquid phases that can mimic the hexatic and confuse analysis. The constraint of constant volume can also cause a problem when equilibrating the system because vacancies cannot be introduced freely.
2. We chose a longer interaction range for the interatomic potentials than previous simulations. For present purposes, this is a detail, but an important one.
3. Our use of the Paragon supercomputer was the real key to our success. Chen has simulated systems of 576, 4096, 16,384, 36,864, and 102,400 atoms at very long time scales, making him one of the largest users of the new massively parallel processing machines. To give an idea of the computer usage involved, a run of 5 million time steps for the 36,864-atom system at a given P and T takes about 10.5 days running continuously, using 128 nodes on the XP/S 35.

These were our innovations and computational advantages. Our results provide the strongest evidence yet that the KTHNY theory of 2D melting is valid. In small samples like those treated in previous work, we found ambiguous evidence for a first-order transition buried in fluctuations larger than the transition itself. It was not until the system size reached 36,864 atoms that a metastable hexatic phase emerged. This phase lasted for about a million time steps before relaxing down into a liquid. The metastable hexatic phase persists for longer times (3 million time steps) in the larger 102,400-atom system.

Conclusions

We concluded that previous simulations were performed on systems that are too small and that they were carried out over time scales that are too short. The Paragon and our own insights have made it possible to find confirmation of a theory for 2D melting.

Our research was supported by ORNL's Laboratory Directed Research and Development Program and reported in "Melting in Two-Dimensional Lennard-Jones Systems: Observation of a Metastable Hexatic Phase," *Physical Review Letters* **74**, 4019 (1995). For this paper, we received a Lockheed Martin Awards Night publication award.

What's left to do? Create a visualization of the 2D melting process at the atomic level and add a dimension so we can understand 3D melting.

What's the problem? Getting enough Paragon time.

What's the lesson? National laboratories that have managers who will take risks can continue to solve fundamental problems. **ornl**

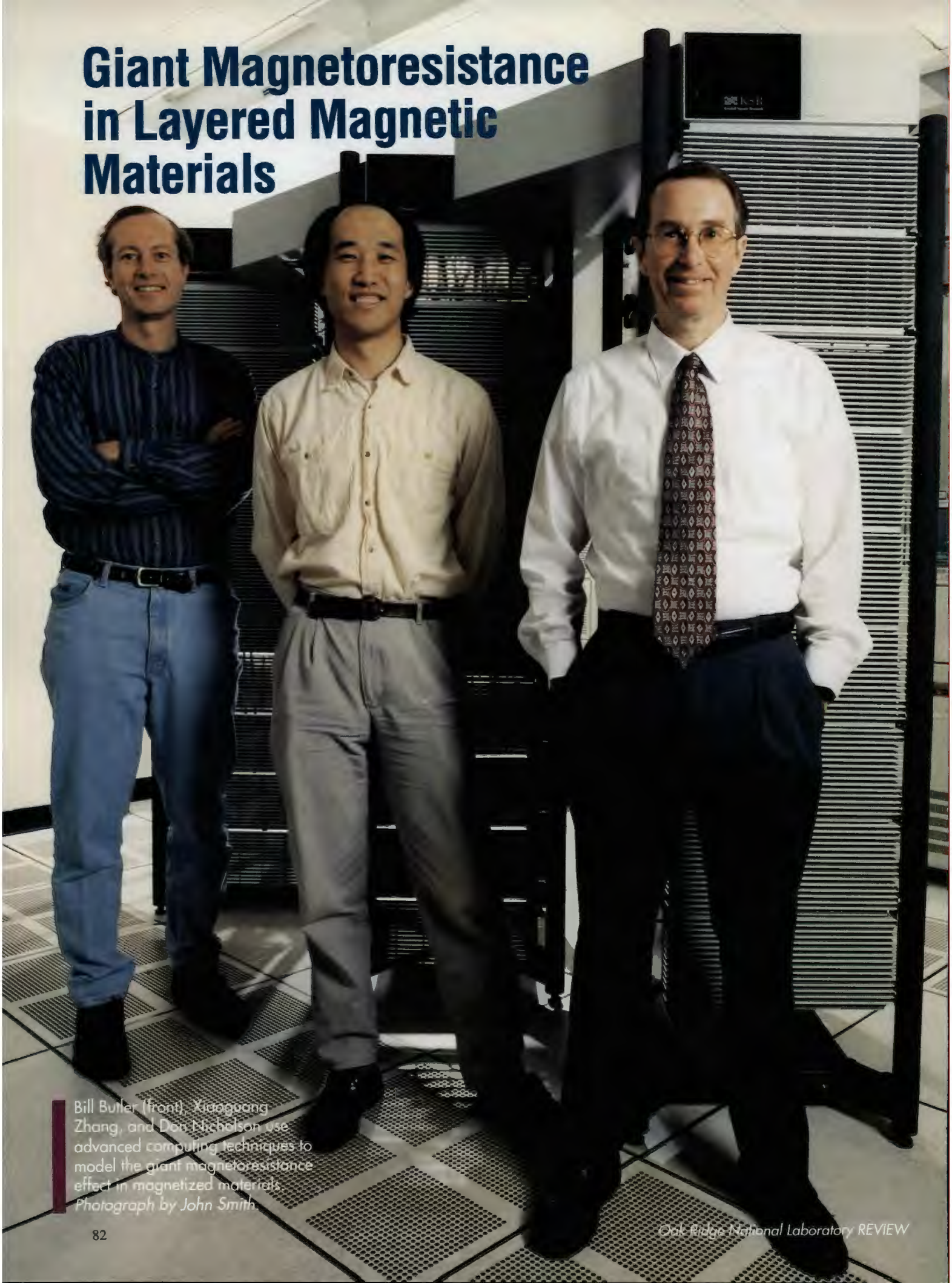
BIOGRAPHICAL SKETCHES

MARK MOSTOLLER was born in Somerset, Pennsylvania, and grew up in Pittsburgh. He received his Ph.D. degree in applied physics from Harvard University. He was a staff member in ORNL's Solid State Division from 1969 until spring 1997. He has worked on lattice vibrations, random alloys, electronic and vibrational properties at surfaces and interfaces, and numerical simulations of the structure and properties of materials. He received Martin Marietta technical achievement awards in 1990 and 1992 and a Lockheed Martin publication award in 1995.

TED KAPLAN is a theoretical physicist in ORNL's Computer Science and Mathematics Division. Born in New York City, he received both his undergraduate and Ph.D. degrees from the Massachusetts Institute of Technology. He has been at ORNL since 1972, when he joined the Solid State Division. His research has included the theory of random alloys, fractal interfaces, chaos, rapid solidification, and thin film growth. Most recently, he has worked on large-scale numerical simulations of the properties of materials. He received a Lockheed Martin publication award in 1995.

KUN CHEN, a native of Xiamen, China, was a postdoctoral researcher in the Solid State Division at ORNL from August 1993 to August 1996. He received his B.S. degree from Beijing University and his M.S. degree from Xiamen University. After teaching at Xiamen for 2 years, he came to the United States in 1988 and received his Ph.D. degree from the University of Georgia in 1993. He received a Lockheed Martin publication award in 1995.

Giant Magnetoresistance in Layered Magnetic Materials



Bill Butler (front), Xiaoguang Zhang, and Don Nicholson use advanced computing techniques to model the giant magnetoresistance effect in magnetized materials. *Photograph by John Smith*

By Bill Butler, Xiaoguang Zhang, and Don Nicholson

By working at the atomic level, performing first-principle calculations of variations of electrical resistivity in layered magnetic alloys, ORNL researchers hope to improve magnetic storage systems. This research in the Metals and Ceramics and Computational Physics and Engineering divisions uses advanced computing techniques to model the giant magnetoresistance (GMR) effect in materials that have structures "layered" at the atomic scale. The GMR effect is a large decrease in electrical resistivity that occurs when the magnetization of two layered samples is aligned by an external magnetic field. A better understanding of GMR could lead to the development of increased data storage density on magnetic disk drives and nonvolatile thin-film magnetic storage devices for computer operating memory whose data would not be destroyed by ionizing radiation or power outages. The goal of this research is to help ORNL's industrial partners develop new products that meet the needs of the Department of Energy and are competitive in the international marketplace.

Most of us are familiar with electrons, the tiny negatively charged particles that carry current in a metal wire when it is connected to a battery. The negative charge of the electron is a familiar property, as is its small mass, which enables it to move easily through a metal. However, in addition to charge and mass, electrons have a third property called spin that is often overlooked. It has become possible to take advantage of the spin of electrons to control the way they move through thin metallic conductors. Exciting new technologies may emerge from this newly acquired ability to control electrons, such as computer memory systems that hold more data and are immune to ionizing radiation and power interruptions.

In a rough sense, you can think of an electron as a tiny negatively charged particle that spins about an axis like a child's top. A spinning charged object creates a magnetic field. However, in most materials, for every electron that spins in one direction there is an electron that spins in the opposite direction so that their magnetic fields cancel exactly. Therefore, most materials are not magnetic. In a few metals—iron, cobalt, and nickel are the most common—electrons gain energy if most of them spin in the same direction. As a result, a net magnetic field is generated in that direction, making the material magnetic.

In the presence of a magnetic field, the laws of quantum mechanics dictate that an electron can spin in one of two directions: Either its own magnetic field, as a result of its spin, aligns with the external field, which physicists call the "up" direction; or its own field aligns opposite to the external field, which is the "down" direction. In a magnetic material most electrons are aligned in the direction of the net magnetic field—that is, there are more up electrons than down electrons. This distinction between up and down electrons is carried over to nonmagnetic materials, although the choice of direction is then arbitrary.

In a nonmagnetic material, the up- and down-spin electrons are expected to respond in exactly the same way to an applied electric field. However, in magnetic metals it was expected that the up- and down-spin electrons might respond quite differently. Unfortunately, there was no way to measure the electrical current carried independently by two kinds of electrons; only the sum of the two currents could be measured.

The discovery of "giant" magnetoresistance (GMR) in 1988 gave scientists the ability to detect and understand the two different kinds of electrons in a metal, opening the possibility of exciting new technological applications (see sidebar on p. 89). Magnetoresistance is a change in the electrical resistivity of a material that is caused by application of a magnetic field. Because magnetoresistance typically is quite small, it was surprising and quite exciting when a group of scientists led by Professor Albert Fert of the University of Paris reported that if a thin metallic film is made of alternating layers of iron and chromium, and if the chromium layers are the right thickness (about 6 atomic layers), the electrical resistivity of this film can be cut in half by placing it in a magnetic field. This GMR was associated with a change in the relative alignment of the net spins on two iron layers. When the net electron spins (or magnetization) on the adjacent iron layers were in opposite directions, the resistance

Building Better Memory Devices

Computer users may no longer need to fear the loss of valuable data every time they hear thunder or see the lights flicker if a project under a new cooperative research and development agreement between ORNL, Honeywell Solid State Electronics Center, and Nonvolatile Electronics, Inc., is successful. Researchers at ORNL are working with their industrial partners to refine a new type of memory based on the giant magnetoresistance (GMR) effect that can survive power interruptions (see article and sidebar on applications of GMR). The new memory system also can endure ionizing radiation, making it especially attractive for military and space applications.

The key to making the new type of memory work efficiently is to be able to deposit high-quality magnetic films. The entire film may be only 50 atoms thick, and some of the layers may be only the thickness of a few atoms. Honeywell and Nonvolatile have called on some of the unique capabilities at ORNL to determine how well these ultrathin films are being deposited so they can learn how to deposit them better. Four different types of experimental techniques are being used to "see" what these films are like at the atomic level.

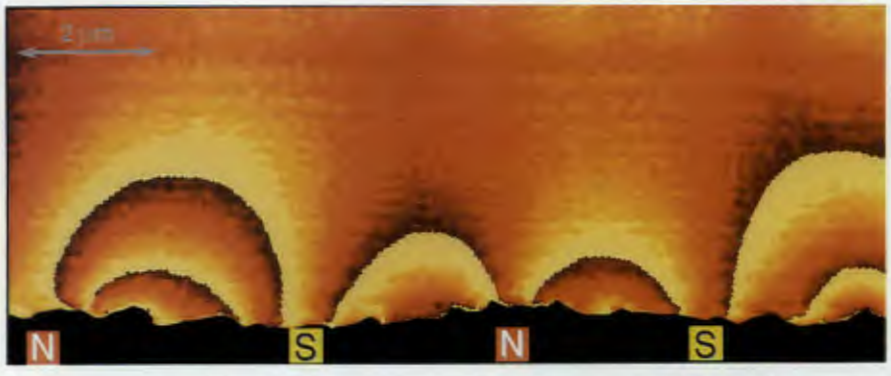
Gene Ice and Eliot Specht, both scientists in the X-Ray Research Group in ORNL's Metals and Ceramics Division, are using X-ray diffraction and reflection to get an overall view of the thickness of the films and the perfection of their crystallinity. So far, their work on the films has been performed in their laboratory at ORNL; later, some of the films will be investigated at the ORNL beamline at the Advanced Photon Source at Argonne National Laboratory.

Mike Miller, a scientist in the Microscopy Microanalytical Sciences Group of ORNL's Metals and Ceramics Division, is using an atom probe field ion microscope to analyze the films atom by atom. Miller's atom probe removes atoms from a sample one by one and determines their elemental identity and their atomic position. With this information he hopes to develop an atomic-scale picture of the structure of the GMR films.

Steve Pennycook and Yanfa Yan, both scientists with ORNL's Solid State Division, are using a scanning transmission electron microscope to shoot a tightly focused beam of electrons through the films. The beam is focused down to a size that is as small as or smaller than an atom. By analyzing the intensity of the transmitted electrons, they can see columns of atoms, and by analyzing the energy of the transmitted electrons, they can perform a chemical analysis of these columns.

Edgar Voelkl and Bernard Frost, both scientists at the High Temperature Materials Laboratory, are looking at a different aspect of these ultrathin films. They are able to image the magnetic fields of the microscopic memory cells. This information is important to understanding how reliably and quickly information can be stored in the cells. The information about the structure of the films obtained by these experimental groups will be used to make more realistic models of the GMR effect.

The work at ORNL is supported by DOE's Office of Energy Research, Laboratory Technology Research Program. The outcome of the work will be the development of better magnetic memory devices.



This image, obtained from an electron hologram, shows the magnetic fields outside magnetic memory cells in a prototype magnetic random access memory device that uses the giant magnetoresistance effect. The electron hologram was obtained by Bernhard Frost and Edgar Voelkl.

was high; when they were in the same direction, the resistance was low.

Understanding GMR

To understand what might be causing this effect, we calculated how electrons behave in a layered iron-chromium system similar to the one investigated by Professor Fert's group. We also looked at other systems that show GMR, such as layers of cobalt and copper. These calculations took advantage of a computational approach developed by Professor James MacLaren of Tulane University, called the "Layer Korringa Kohn Rostoker technique." Korringa, Kohn, and Rostoker were scientists who, during the 1940s and 1950s, devised an elegant technique for calculating how electrons move through a periodic lattice—that is, a system in which all atoms are lined up in precise rows and columns like soldiers in formation. Professor MacLaren extended this technique so that it works very efficiently for layered systems. (Imagine that soldiers in some of the rows are wearing different uniforms). In the article beginning on page 68, Bill Shelton and Malcolm Stocks describe another technique based on the Korringa Kohn Rostoker approach, which is even more general.

Figures 1 and 2 show the number of up- and down-spin electrons that we calculated for each atomic layer of a system consisting of eight chromium layers embedded in iron and for a system consisting of ten copper layers embedded in cobalt. Both

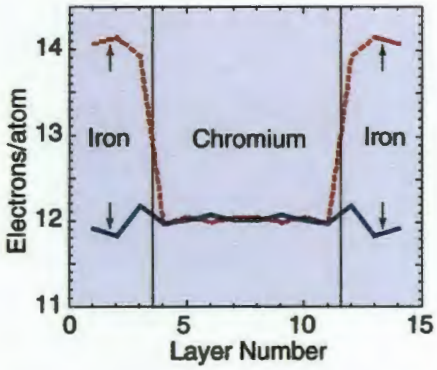


Fig. 1. The number of down-spin electrons per atom hardly changes between the iron and chromium layers, but the number of up-spin electrons is higher for iron than for chromium.

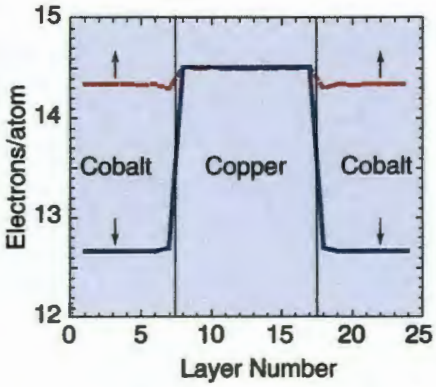


Fig. 2. The number of up-spin electrons per atom hardly changes between the cobalt and copper layers, but the number of down-spin electrons is much lower for cobalt than for copper.

of these systems show a large GMR. These figures give an important clue as to what is happening. For the iron-chromium layers, note that the number of down-spin electrons is about the same in the iron and chromium, but the number of up-spin electrons is very different. Conversely, the number of up-spin electrons is very similar on each layer of the copper-cobalt system, but the number of down-spin electrons changes abruptly at the interfaces.

Figures 1 and 2 provide a qualitative understanding of how the GMR effect might arise. The electrical resistance of a metal arises from irregularities and discontinuities in the atomic lattice potential, called defects, as seen by the electrons. Electrons carrying a current are like balls rolling down a hill. If the slope is smooth, then the balls go very fast. But if it has a lot of bumps, the balls will be slowed down. Defects in the atomic lattice are like those bumps. When electrons hit these defects—a process physicists call scattering—the electrons are slowed down. Therefore, scattering can generate electrical resistance.

Consider the case in which the ferromagnetic layers are cobalt and the nonmagnetic layer is copper. The up-spin electrons hardly notice any difference in the number of electrons per atom as they travel from the ferromagnetic layer to the nonmagnetic layer (see Fig. 1). To them the lattice potential is smooth and almost defect free. On the other hand, the down-spin electrons see a large difference in electron numbers between atoms of copper and cobalt. They see many bumps at the interface (because copper and cobalt atoms often mix with each other there), so they are very likely to scatter there. When excess spins in the two ferromagnetic layers have the same direction (illustrated by the left-hand side of Fig. 3 for cobalt and copper), up-spin electrons can travel freely from one ferromagnetic (cobalt) layer across the interface to the other ferromagnetic layer, and down-spin electrons will scatter strongly at both interfaces. When the excess spins in the two ferromagnetic layers have opposite directions (illustrated on right-hand side of Fig. 3), both the up- and down-spin electrons will scatter at one of the interfaces. The electrical resistivity for the aligned case should be lower because up-spin electrons in this case experience very little resistance and act like a short circuit. Think of the limiting case in which up spin electrons for the aligned case have no resistance, and down-spin electrons have resistance 2R, with R being the contribution from each interface. Because the up spin provides a short-circuit channel, the resistance of the whole system is zero. For the case in which excess spins on two cobalt layers are aligned in opposite directions, both up and down spins have resistance R because both scatter off one interface.

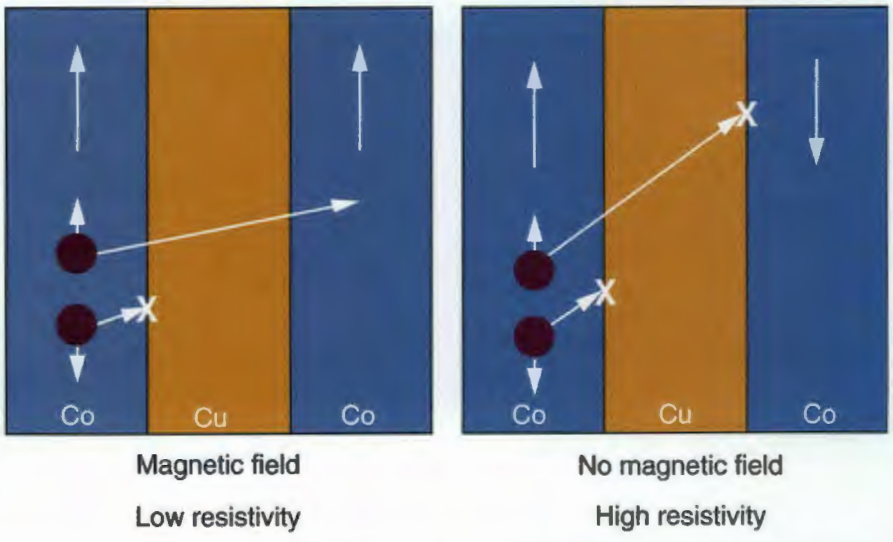


Fig. 3. When excess spins in both cobalt layers are aligned, up-spin electrons pass from layer to layer without scattering.

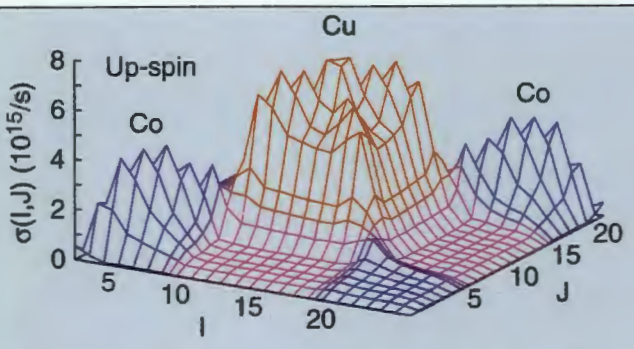


Fig. 4. Nonlocal up-spin conductivity for the case in which the excess spins are aligned on the cobalt layers.

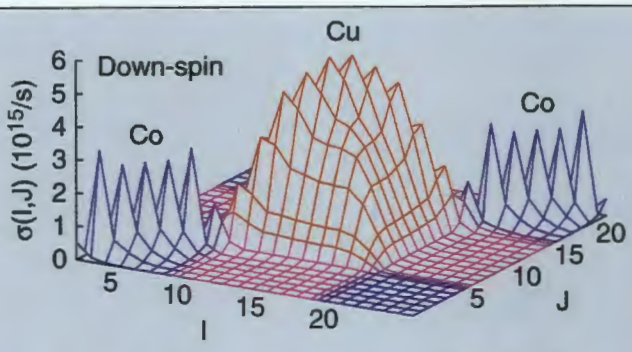


Fig. 5. Nonlocal layer-dependent conductivity for the down-spin electrons for the case in which excess electrons on the cobalt layers are aligned.

In this case the total resistance is R/2, which is certainly greater than the value zero for the aligned case.

From this oversimplified argument, it is evident that resistance will be lower when excess spins in the magnetic layers are in the same direction. Thus, if excess spins are pointing in different directions in different magnetic layers when no magnetic field is applied, applying an external magnetic field can turn them so that they point in the same direction, resulting in a drop in resistivity.

Calculating Electrical Conductivity

The understanding that came from our initial calculations helped us formulate qualitative ideas to explain possible causes of the GMR effect. However, we needed a more detailed understanding of GMR, so we decided to calculate the electrical conductivity of these materials. Calculation of electrical conductivity, which is the inverse of electrical resistivity, is difficult. In these materials it was particularly tough because the layers must be extremely thin to show a large GMR effect. No one knew how to calculate the electrical conductivity of materials that are inhomogeneous on such a fine scale. In the past, physicists had only attempted to calculate the resistivity of such systems using the simplest of "toy" models. We knew it was important to include information about how electrons interact with and scatter from atoms in the layers. We were able to perform these calculations and develop a realistic description of the resistivity of these layered materials partly because of the availability of parallel supercomputers at ORNL.

The other necessary ingredient was an interlaboratory team that had the experience and capabilities to attempt such a formidable task (and perhaps were sufficiently naive to believe it could be done). In addition to the authors, the other team members are Thomas Schulthess of Lawrence Livermore National Laboratory, Richard Fye of Sandia National Laboratories, and Virgil Speriosu and Bruce Gurney, both of the IBM Almaden Research Center. IBM is interested in the GMR effect as a means of increasing the density of data stored on magnetic disks (see sidebar on p. 89). Speriosu and Gurney provided the experimental measurements that we compared with our calculations. The work was funded by DOE's Office of Defense Programs with additional support from DOE's Office of Basic Energy Sciences. Many of the computations were performed on the parallel supercomputers at ORNL's Center for Computational Sciences.

Figure 4 shows some of the results of our calculations of the conductivity of layered cobalt-copper systems. To understand the conductivity of a layered conductor, it is important to realize that the conductivity is nonlocal. We usually think of the conductivity, σ, in terms of the formula $J = \sigma E$, which states that the current at any point, J, is proportional to the applied electric field at that point, E. But in a material made of very thin layers, an electron may be accelerated by a field at one point and then travel a distance, l, before it scatters off an impurity or other irregularity. Because the properties and the fields may change over distances smaller than l, we must consider *nonlocal* conductivity, which relates the current in a particular atomic layer to the field applied in all of the other atomic layers, $J(I) = \Sigma_J \sigma(I,J) E(J)$. Figures 4 through 7 show $\sigma(I,J)$, the current induced in layer I by a field applied in layer J. Figure 4 shows this calculated nonlocal conductivity for the up-spin electrons.

The results are color-coded. Blue represents electrons accelerated by an electric field applied in a cobalt layer which contribute to the conductivity in a cobalt layer. Red represents electrons accelerated in a copper layer that contribute to the current in a copper layer. Purple represents electrons accelerated by a field in a copper layer which contribute to the current in a cobalt layer, or vice versa. Note that the blue region in the near corner represents

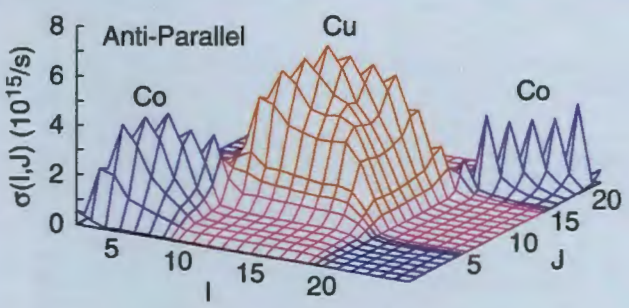


Fig. 6. Conductivity for the case in which excess spins on the cobalt layers are aligned in opposite directions.

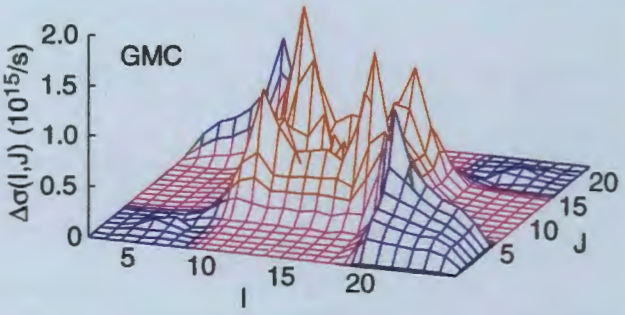


Fig. 7. Giant magnetoconductance (GMC) is the inverse of giant magnetoresistance.

conductivity from electrons accelerated in one of the cobalt layers which contributes to the conductivity in the other.

Figure 5 shows a similar plot for the down-spin electrons. The conductivity for the down-spin electrons is localized within the layers. If an electron is accelerated by a field in one layer, it contributes only to the current in that layer.

Figure 6 shows the nonlocal conductivity for the case in which the excess spins on the cobalt layers are aligned in opposite directions. In this case the conductivities on the left-hand side of the figure are similar to those of the up-spin electrons of Fig. 4, and those on the right-hand side are similar to the conductivities of the down-spin electrons of Fig. 5.

Figure 7 shows giant magnetoconductance. (Conductance is the inverse of resistance.) Thus, giant magnetoconductance is the difference between total conductivity for the case in which excess spins are parallel (i.e., the sum of the conductivities in Figs. 4 and 5), and the total conductivity for the case in which excess spins are antiparallel (i.e., Fig. 6 and its mirror image).

Giant magnetoconductance comes from two effects. The blue region in the near corner of Fig. 7 represents electrons accelerated in one cobalt layer which travel through the copper and contribute to the conductivity in the other cobalt layer. This type of contribution to the GMR is not too surprising. It corresponds to the simple picture of GMR illustrated in Fig. 3.

Waveguide Effect for Electrons

The largest contributions to GMR come from electrons accelerated by a field in the copper layer that help produce a current in that layer. This type of contribution was very surprising to us until we traced its origin to an effect well known to physicists and engineers—the waveguide effect.

This phenomenon is becoming more familiar, thanks to advertisements by phone companies that encourage you to use their services because they promise that your conversations will travel along optical fibers. What they are referring to are optical waveguides. Light waves can travel for miles within a thin glass fiber, even around bends and corners if they are not too sharp. An optical waveguide is a glass fiber that has a glass core surrounded by more glass with a lower index of refraction than the core. Light waves within the core traveling approximately parallel to the length of the fiber will be reflected back into the core. Thus, they can travel for several miles if no impurities are present to scatter or absorb them.

Our calculations predict that a similar phenomenon affects up-spin electrons in a copper layer with cobalt on either side. Like light, electrons propagate as waves. Because the effective index of refraction for electrons in copper is higher than for up-spin electrons in cobalt, some up-spin electrons can be confined to the copper because of their wavelength and, because of copper's low resistivity, they can travel further without scattering. The down-spin electrons for the aligned case will enter the high-resistivity cobalt at both interfaces, and both types of electrons will enter the cobalt at one or the other of the interfaces for the nonaligned case.

The net result is that the waveguide effect can make a big contribution to the GMR for some systems. The size of the channeling effect depends on how nearly perfect the interfaces are between the cobalt and copper layers. We are currently comparing our theoretical calculations with measurements of GMR for cobalt-copper films performed at the IBM Almaden Research Center in California under a cooperative research and development agreement. It may turn out that interfaces in films currently being deposited are not smooth enough to give a strong channeling effect. If so, there will be a strong impetus to increase the effect by finding ways to deposit films with smoother interfaces. An increase in the GMR of the type we predict would have a profound impact on many technologies. **ornl**

Applications of Giant Magnetoresistance

Giant magnetoresistance already has magnetic appeal: It allows more data to be packed on computer disks. If improvements are made in the interfaces between magnetic layers in thin-film structures, the number of new applications could prove irresistible.

For example, it would be possible to make computer operating memories [random access memory (RAM)] that are immune to power disruptions and ionizing radiation. GMR motion sensors could be developed to increase the efficiency and safety of home appliances, automobiles, and factories. Magnetoelectronic devices may someday complement or even replace semiconductor electronic devices.

GMR recently moved out of the laboratory and into our computers with the development of "read sensors" for magnetic disk drives. Because the capacity of disk drives continues to grow rapidly as they shrink in size, GMR read sensors become increasingly important.

Disk drive manufacturers write more and more data into smaller amounts of space. The data are written as tiny regions of magnetization on a disk covered with a thin film of magnetic material. The information (bits of 1 or 0) is stored as the direction of the magnetization of these regions. The information is read by sensing the magnetic fields just above these magnetized regions on the disk. As the density gets higher, these regions get smaller, so the fields that must be sensed to read the data become weaker. Read sensors that employ the GMR effect provide the best technology currently available for detecting the fields from these tiny regions of magnetization. These tiny sensors can be made in such a way that a very small magnetic field causes a detectable change in their resistivity; such changes in the resistivity produce electrical signals corresponding to the data on the disk which are sent to the computer. It is expected that the GMR effect will allow disk drive manufacturers to continue increasing density at least until disk capacity reaches 10 gigabits per square inch. At this density, 120 billion bits could be stored on a typical 3.5-inch disk drive, or the equivalent of about a thousand 30-volume encyclopedias.

GMR also may spur the replacement of RAM in computers with magnetic RAM (MRAM). RAM holds the data that your computer must get to quickly in order to operate. Today's technology uses semiconductor RAM because it is fast, dense, and relatively inexpensive. In semiconductor RAM, data are stored as small regions that have an excess or deficit of electrons. This use of electrical charges to represent data has two serious drawbacks. First, because these charges leak away, the data must be refreshed several times a second by an electrical circuit. Thus, if the power goes off before the data can be written back to the hard disk for permanent storage, they will be lost. Second, because ionizing radiation temporarily destroys a semiconductor chip's semiconducting properties, it can destroy data. Using GMR, it may be possible to make thin-film MRAM that would be just as fast, dense, and inexpensive. It would have the additional advantages of being nonvolatile and radiation-resistant. Data would not be lost if the power failed unexpectedly, and the device would continue to function in the presence of ionizing radiation, making it useful for space and defense applications.

One exciting aspect of GMR devices is their extremely small size. Currently, computer and electronics manufacturers are struggling to shrink their devices and keep them working at feature sizes of about 0.5 μm. Operating GMR-based devices are already 50 times smaller than that, and they tend to work better at smaller sizes. It has already been shown that GMR can be used to make a transistor.

The application of GMR in motion sensors is also likely to be important in our homes, automobiles, and factories. It provides a convenient way of sensing the relative motion and position of objects without physical contact. Just attach a magnet to one object and a GMR sensor to another. Alternatively, if one of the objects contains a magnetic material such as iron or steel, the object in motion will alter any magnetic field that is present. These small changes in the magnetic field could be detected by a GMR sensor.

Applications of this effect could become widespread in the industrial, commercial, and military worlds. Here's a possible list: sensitive detectors for wheel-shaft speed such as those employed in machine-speed controllers, automotive antilock brakes, and auto-traction systems; motion and position sensors for electrical safety devices; current transformers or sensors for measuring direct and alternating current, power, and phase; metal detectors and other security devices; magnetic switches in appliance controls, intrusion alarms, and proximity detectors; motor-flux monitors; level controllers; magnetic-stripe, ink, and tag readers; magnetic accelerometers and vibration probes; automotive engine control systems; highway traffic monitors; industrial counters; equipment interlocks; and dozens of other applications requiring small, low-power, fast sensors of magnetic fields and flux changes. Furthermore, suitable film-deposition processes could also permit fabrication of GMR devices on electronic-circuit chips to produce highly integrated GMR sensors at low cost and high volumes for mass industrial markets. With its promise for tomorrow's technologies, GMR is bound to attract lots of attention.—*Bill Butler and Steve Smith*

BIOGRAPHICAL SKETCHES

WILLIAM H. BUTLER has been leader of the Theory Group in ORNL's Metals and Ceramics Division since 1985 and was manager of computer planning at ORNL in 1984–85. He holds a Ph.D. degree in solid-state physics from the University of California at San Diego. Before coming to ORNL in 1972, he was assistant professor of physics at Auburn University. He received the DOE–Basic Energy Sciences Division of Materials Sciences Award for Outstanding Sustained Research in Metallurgy and Ceramics in 1983 and the DOE–Basic Energy Sciences Division of Materials Sciences Award for Outstanding Scientific Achievement in Metallurgy and Ceramics for 1995 for outstanding computational research on GMR.

XIAOGUANG ZHANG is a member of the research staff in ORNL's Computational Physics and Engineering Division. He has a Ph.D. degree in physics from Northwestern University. Before joining the ORNL staff in 1995, he worked as a postdoctoral fellow at DOE's Lawrence Berkeley National Laboratory, as a postdoctoral scholar at the University of Kentucky, and as a postdoctoral research associate in ORNL's Metals and Ceramics Division. He received the DOE–Basic Energy Sciences Division of Materials Sciences Award for Outstanding Scientific Achievement in Metallurgy and Ceramics for 1995 for outstanding computational research on GMR.

DONALD M. NICHOLSON is a senior research scientist in ORNL's Computational Physics and Engineering Division. He has a Ph.D. degree in solid-state physics from Brandeis University. He joined the ORNL staff in 1986 as a member of the Metals and Ceramics Division. He received the DOE–Basic Energy Sciences Division of Materials Sciences Award for Outstanding Scientific Achievement in Metallurgy and Ceramics for 1995 for outstanding computational research on GMR.

EDGE DISLOCATIONS IN SILICON

Mark Mostoller (left), Matt Chisholm, and Ted Kaplan show their models of a "dreidl," which has a closed symmetric structure of five-fold and seven-fold rings that resembles a child's dreidl, or Hanukkah top. Silicon and germanium can have dreidl structures. *Photograph by Tom Cerniglio.*

By Mark Mostoller, Ted Kaplan, and Matt Chisholm

In the past half century, the world has been transformed by an electronic revolution that is based largely on silicon technology. Semiconductor devices using this technology have become smaller and smaller, yet far more powerful, over time. Defects have a profound effect on device performance. The controlled introduction of substitutional impurities (dopants) like boron and phosphorous in silicon, for example, is what makes transistors work. In this country, only a few incongruously important groups like the air traffic controllers at O'Hare airport in Chicago have lagged this revolution and still use electronic equipment with vacuum tubes.

Dislocations are line defects that are generally thought to be bad actors because among other things, they tend to suck in the dopants that make devices perform. The same negative view is held of planar defects like grain boundaries, which can be viewed as arrays of dislocations. In the worst case, if all the dopants so carefully introduced were to segregate to dislocations, the device would fail to work at all. Any electrical activity associated with dislocations was thought to be due to such impurity segregation or to the presence of so-called dangling bonds.To explain the latter requires a short refresher course on the crystal structure of silicon.

Silicon crystallizes in the diamond cubic structure (shown in Fig. 1), which is responsible for the hardness of the diamond form of carbon. Notice two things about the structure. First, each atom has four neighbors at the corners of a tetrahedron around it. Second, if you pick, say, a blue atom and follow nearest-neighbor bonds until you return to the same atom, the atoms are members of six-fold rings. If, in some defect structure, a silicon atom has fewer than four neighbors, it is said to have dangling bonds.

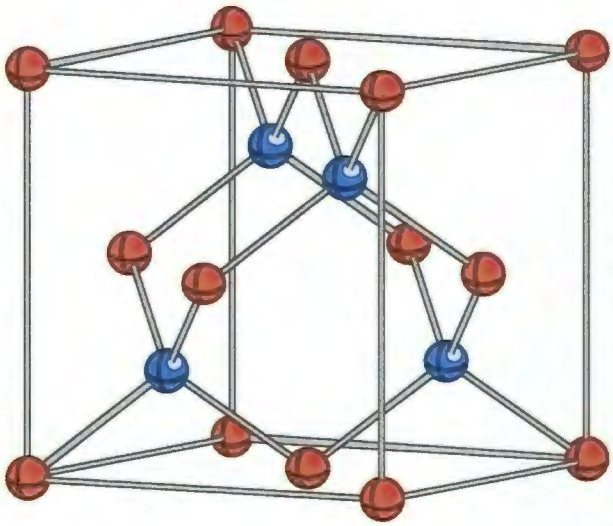


Fig. 1. The diamond-cubic crystal of silicon, with atoms on the cube corners and faces in red, and those inside in blue; each blue atom has four neighbors, and each lies in six-fold rings.

It is important to determine the atomic and electronic structure of dislocations in semiconductors because they can have such profound effects on electrical and mechanical properties. Our work began with a microscope in ORNL's Solid State Division. By using a technique called Z-contrast imaging, we can now look at materials with atomic-scale resolution. Matt Chisholm had been using this technique to investigate bicrystals of germanium on silicon [Ge/Si(001)]. He observed a 4% lattice mismatch between germanium and silicon; for this system, a regular square grid of edge dislocations formed at the interface, 100 Å apart. The microscope images showed that the cores of the dislocations had the structure shown in Fig. 2, in which five-fold and seven-fold rings are stacked together. We confirmed this observation by doing large-scale simulations in systems of roughly 20,000 atoms, using classical interatomic forces that give a good description of pure silicon and germanium. At the intersections on the grid, we found a closed symmetric structure (also shown in Fig. 2), which we called

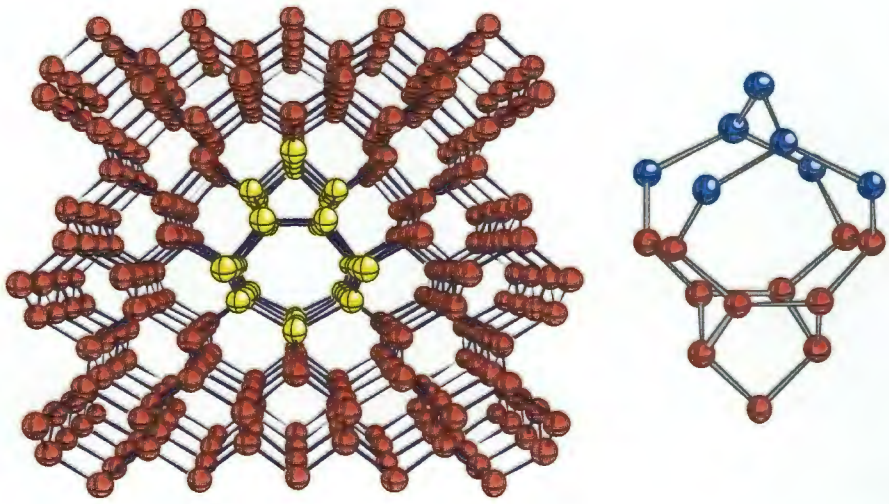


Fig. 2. Looking down the core of an (a/2) <110> edge dislocation in Si (left), with atoms in the core marked in yellow, and the dreidl (right) that forms at the intersections of the dislocation grid in Ge/Si(001) bicrystals.

the "dreidl" after the child's Hanukkah top that it resembles. Again, we see a structure that consists of linked five-fold and seven-fold rings. This discovery was reported with the headline "Atomic Dreidls" in the February 10, 1994, issue of the weekly *AIP Physics News Update* of the American Institute of Physics. The simulations showed that in both the individual dislocations and their intersections, all atoms retain their tetrahedral coordination, albeit with changes in bond lengths and angles. There are no dangling bonds.

In 1993, we were joined by postdoctoral scientists Feng Liu and Victor Milman, who both had experience in first principles calculations of material structure and properties. (Liu is now at the University of Wisconsin at Madison, and Milman is with Molecular Simulations in Cambridge, U.K.) Milman was among the first to get his code working on the new Intel Paragon machines, which occasioned a certain amount of muttering and lamentation on his part. We were interested in the electronic properties that these defects in Ge/Si(001) might have; but systems of 20,000 atoms are too large, even with a Paragon, to perform electronic structure calculations. Instead, we chose a simpler system of dislocation dipoles in silicon, in which all of the dislocations run along the same direction, but whose cores alternate between five-fold on top of seven-fold rings and seven-fold on top of five-fold rings.

Using a combination of first-principles, classical, and tight-binding calculations running on the XPS/35, workstations, and a Cray YMP, respectively, we treated supercells of from 64 to 576 atoms. The 576-atom sample is among the largest systems for which such first-principles calculations have been done, and this turned out to have important results. As the system size grows and the separation of the dipoles increases, the strain becomes more concentrated in the dislocation cores. So despite the absence of dangling bonds, electronic states localized at the cores rise about 0.2 eV into the band gap, as shown in Fig. 3. (Semiconductors and insulators have an energy band gap between the highest occupied electronic states and the lowest unoccupied levels, whereas metals have no gap.) This finding suggests that dislocations themselves, with no dangling bonds and without segregated impurities, may be electrically or optically active. Previous work by others on similar systems was done for smaller samples. They had found no such deep gap states for dislocations in pure silicon. Now we know why. ornl

"This finding suggests that dislocations themselves, with no dangling bonds and without segregated impurities, may be electrically or optically active."

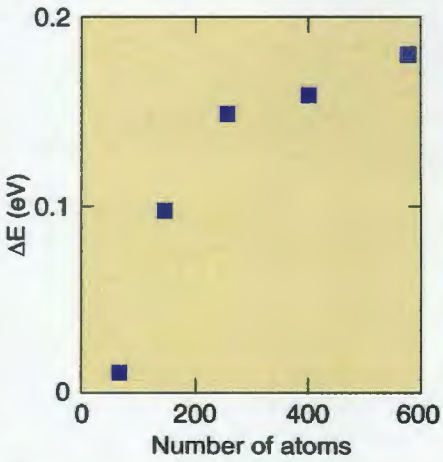


Fig. 3. Shift in energy of the highest occupied electronic state into the bulk band gap for edge dislocation dipoles in Si as a function of system size.

Further information

- Mark Mostoller, M. F. Chisholm, and Theodore Kaplan, "New Extended Point Defect Structure in Diamond Cubic Crystals," *Phys. Rev. Lett.* **72**, 1494 (1994).
- Feng Liu, Mark Mostoller, V. Milman, M. F. Chisholm, and Theodore Kaplan, "Electronic and Elastic Properties of Edge Dislocations in Si," *Phys. Rev. B* **51**, 17192 (1995).

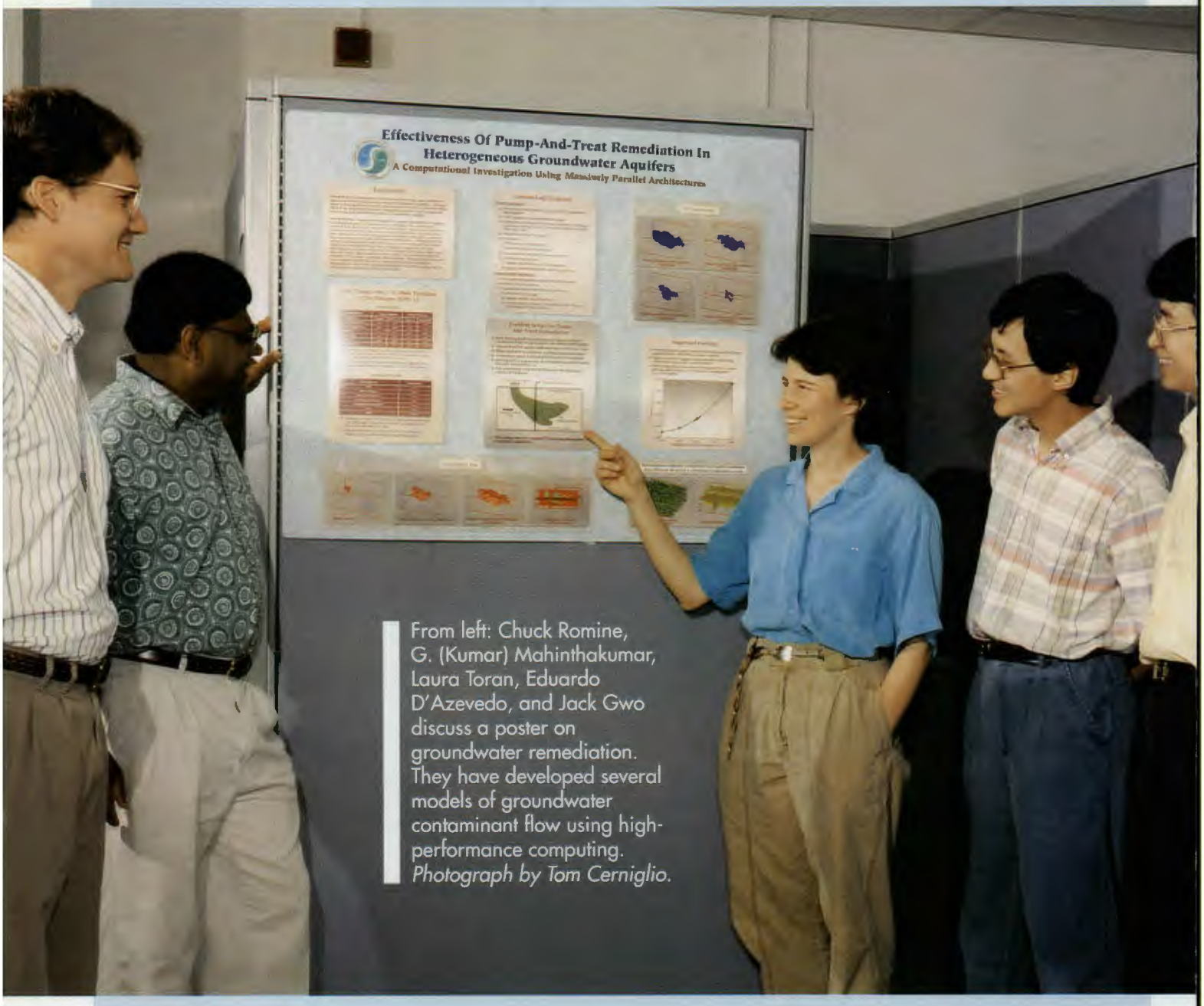
BIOGRAPHICAL SKETCHES

MARK MOSTOLLER was born in Somerset, Pennsylvania, and grew up in Pittsburgh. He received his Ph.D. degree in applied physics from Harvard University. He was a staff member in ORNL's Solid State Division from 1969 to spring 1997. He has worked on lattice vibrations, random alloys, electronic and vibrational properties at surfaces and interfaces, and numerical simulations of the structure and properties of materials. He received Lockheed Martin technical achievement awards in 1990, 1992, and 1996.

TED KAPLAN is a theoretical physicist in ORNL's Computer Science and Mathematics Division. Born in New York City, he received both his undergraduate and Ph.D. degrees from the Massachusetts Institute of Technology. He has been at ORNL since 1972, when he joined the Solid State Division. His research has included the theory of random alloys, fractal interfaces, chaos, rapid solidification, and thin film growth. Most recently, he has worked on large-scale numerical simulations of the properties of materials. He received a Lockheed Martin publication award in 1996.

MATT CHISHOLM is a materials scientist in the Solid State Division. Born in Sayre, Pennsylvania, he received his B.S. degree from Northwestern University. After 4 years at Reynolds Metals Company, where he worked on aluminum alloys for cans, cars, and aircraft, he obtained his Ph.D. degree from Carnegie-Mellon University. Subsequently, he worked for IBM before joining the ORNL staff in 1988. His primary research interest is the determination of the structures of defects in crystalline materials. His primary research tools are the unique direct imaging electron microscopes in the Solid State Division.

High-Performance Computing in Groundwater Modeling



From left: Chuck Romine, G. (Kumar) Mahinthakumar, Laura Toran, Eduardo D'Azevedo, and Jack Gwo discuss a poster on groundwater remediation. They have developed several models of groundwater contaminant flow using high-performance computing. *Photograph by Tom Cerniglio.*

High-performance computing is opening up new opportunities for modeling and understanding complex groundwater systems. Computationally intense models that describe concentrations and movements of specific contaminants in groundwater may be more effective than simple groundwater models in evaluating remediation options.

By Laura Toran, Jack Gwo, G. (Kumar) Mahinthakumar, Eduardo D'Azevedo, and Chuck Romine

Fig. 1. Burial grounds for low-level radioactive waste on the Oak Ridge Reservation. Leaching of this waste is partly responsible for the area's contaminated groundwater.

Consider the plight of a hazardous waste site manager supervising cleanup and containment operations for an area having contaminated groundwater (see Fig. 1). She faces a variety of scientific, engineering, and political challenges. Typically, the waste source is unknown, the complex geology of the site creates uncertainty about the transport of groundwater contaminants, and the funding to find answers is severely limited. In the past, available modeling tools were narrowly focused predictive models, fraught with uncertainty. Today, however, new computationally intense groundwater models that account for uncertainty may provide new insight.

High-performance computing can improve groundwater modeling by providing the ability to (1) use larger and more detailed computational grids, (2) run more simulations under different conditions to evaluate remediation options and determine uncertainty, and (3) develop more complete computational models of physical processes. High-performance computing uses high-speed, large-memory-capacity computers such as the parallel computers at ORNL's Center for Computational Sciences (CCS). These parallel computers link processors or individual workstations together to increase computational power.

Not all modeling problems would benefit from high-performance computing, but one of the key benefits of research in this area is that the lessons learned can provide lessons in other areas. We give several examples of practical groundwater contaminant transport problems that have been solved with high-performance computing at ORNL. These serve to illustrate both the advantages and the difficulties in using high-performance computing for environmental problems.

Subsurface Heterogeneity and Groundwater Remediation

Geologic heterogeneity is one of the most important factors affecting groundwater remediation. Two of the common remediation techniques are pump-and-treat remediation and bioremediation (see Fig. 2). In pump-and-treat remediation—which involves pumping the contaminated groundwater out, cleaning it up, and (sometimes) reinjecting it into the ground—extraction of dissolved contaminants from regions of low permeability is difficult. Bioremediation—the use of bacteria and other microbes to break down pollutants—is hampered because regions of low permeability can affect delivery of nutrients or cause microbial clogging. On the other hand, regions of high permeability can shorten residence times for bacteria, preventing them from effectively degrading the contaminants.

Although it is very difficult to obtain fine-scale heterogeneity information directly by field measurements, geostatistical techniques may be used to generate this information synthetically (with a degree of uncertainty) from sparse field data. Once we generate such data, attempting to resolve fine-scale

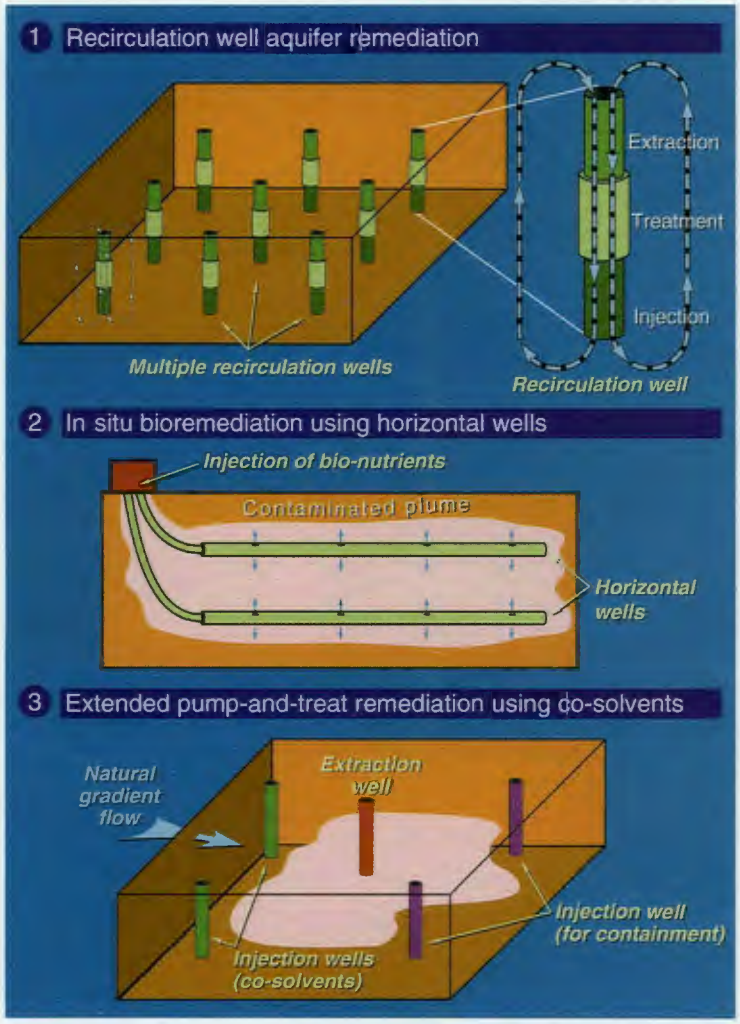


Fig 2. Various remediation strategies being analyzed by ORNL researchers using high-performance computing.

heterogeneity effects on large three-dimensional field-scale systems can result in very large problems requiring hundreds of millions of grid points. A combination of powerful algorithms and current-generation high-performance computers provides means of solving these systems very efficiently.

ORNL researchers have developed parallel-solution algorithms based on multigrid and Krylov subspace methods that can solve groundwater flow and transport problems requiring tens of millions of finite elements in less than a minute on the 1024-processor, massively parallel Intel Paragon supercomputer. These groundwater codes are now being used to study the impact of soil heterogeneity on various remediation strategies.

Figure 3 shows the results from a hypothetical simulation that was performed to determine the viability of pump-and-treat remediation under heterogeneous conditions. The simulations used about 3.2 million finite elements requiring 128 parallel processors of the Intel Paragon XP/S 150 at ORNL. The heterogeneous permeability field was generated with a geostatistical simulator using sparse field data obtained from a sandy aquifer in New England. Contamination occurs over approximately 24 years of landfill leaching while remediation takes approximately 5 years to remove 95% of the contaminants. The extraction well was placed at the vertically averaged concentration weighted centroid of the plume.

Cost-Benefit Analysis

One of the most effective ways of reducing remediation costs is to improve decision making in the presence of uncertainty. The complexity of underground environments and the paucity of geologic data, the various efficiencies of remediation techniques under differing conditions, the ever-changing federal and state regulations, even the fluctuation of interest rates—all contribute to uncertainties. Designing a decision rule for even a moderately complex site such as ORNL has proven to be overwhelming. Moreover, the situation may get worse because of dwindling federal funds for site characterization and remediation. Today's waste management professionals are expected to do a better job than their predecessors with fewer resources at their disposal. One improvement in their arsenal is the emergence of highly efficient computational algorithms on high-performance computers that form the basis for new decision-making tools.

Researchers at ORNL have developed an economic decision framework for improving aquifer remediation designs. Our approach seeks to adopt field and laboratory data into groundwater contaminant transport models running on ORNL high-performance parallel computers. The framework accounts for variations in aquifer properties, remediation designs, and compliance limits by running hundreds of computer simulations on the Intel Paragon and Kendall Square (KSR1) computers at CCS.

Results from these simulations are used to determine the effect of regulatory change on the choice of remediation designs (Fig. 4), the size of the exploration budget, and the most sensitive aquifer parameters that may warrant further explorations. A change in the compliance limit (e.g., the maximum allowable radioactivity of groundwater discharge) can alter a previous decision and result in modification of the remediation strategy. Our study suggests that at or near the most strict compliance limit, the best remediation alternative is to contain the waste

plume. However, at less strict compliance limits, the best remediation alternative is to monitor only, accepting the risk of failure to meet the regulatory requirement. Results shown in Fig. 4 can be translated into maximum exploration budgets based on the opportunity cost of choosing one remediation alternative against another and can therefore be used to guide site characterization efforts.

This economic framework is only an initial effort to guide site remediation decision-making, yet the computational needs have already become immense. For future large-scale, long-term decision-making analyses, studies of this nature may well exceed the capacity of today's largest computational facility. Future high-performance computational algorithms and supercomputers will become increasingly important tools for our complicated environmental restoration problems.

Uranium Concentration Study

One promising way to advance our understanding of contaminant transport is to use high-performance computing to conduct more realistic simulations of transport processes. Geochemical transport modeling offers a good example of this potential. With limited computing power, transport models typically must lump the complex geochemistry into a single term (i.e., the retardation factor), a rather crude approximation. Accurate geochemical transport modeling requires that interactions between chemicals that can change the mobility of the contaminant (for example, alteration of the acidity level, or pH) be treated explicitly at each node, a computationally intensive task. High-performance machines such as the Intel Paragon at ORNL's CCS enable the development of such models.

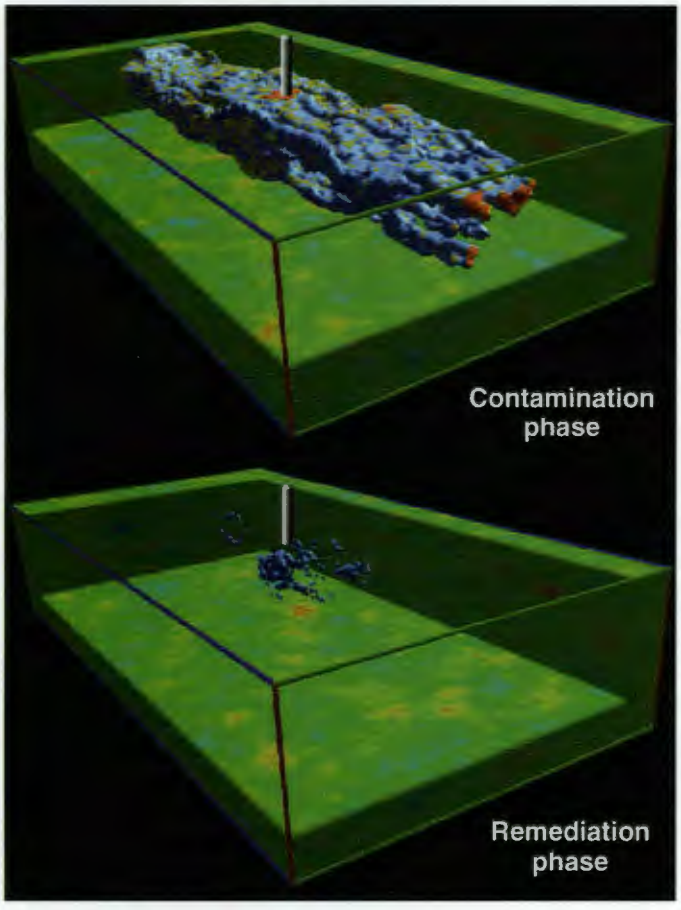


Fig 3. Simulations on the Intel Paragon analyze the impact of heterogeneity on pump-and-treat remediation.

We used a parallel code developed by researchers at the University of Texas and Pennsylvania State University—the Parallel Aquifer and Reservoir Simulator linked to the Kinetic Equilibrium Model or PARSim-KEMOD—to evaluate whether fissile uranium in a low-level waste (LLW) facility can be concentrated by hydrogeochemical processes to levels that might lead to nuclear criticality—the point at which a nuclear reaction is self-sustaining and potentially hazardous. Increases in concentration could not be predicted by simple transport models alone. Our analysis using the code was completed in less than an hour on four processors of an Intel Paragon.

This investigation represents the first attempt to jointly study the potential for nuclear criticality at LLW facilities using both quantitative hydrogeochemical modeling and nuclear criticality safety calculations. We postulated that uranium concentration results from sequential processes of mobilization of uranium by formation of soluble complexes, followed by immobilization of the soluble species by processes of adsorption or precipitation. The goal of our preliminary study was to conduct a sensitivity analysis of factors that could influence the mobilization and immobilization of uranium. Our results indicate that very few model runs could produce both mobilization and immobilization conditions. Adsorption typically does not concentrate uranium sufficiently to create levels of concern for criticality. Precipitation of uranium under reducing conditions is possible, but the stability of reducing zones in LLW facilities has not yet been evaluated. A further limiting factor is that the mass density of uranium required to reach criticality safety concerns is greater than the source term in many cases. This modeling can be used to suggest ways to limit mobilization and immobilization of uranium and to guide the development of design regulations to improve the safety of LLW facilities.

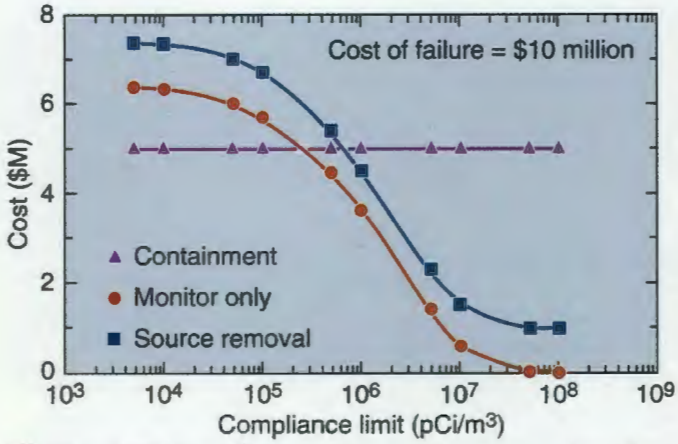


Fig. 4. High-performance computing can analyze the costs and benefits of remediation alternatives in light of changing regulations. An accurate cost-benefit analysis can reduce remediation costs.

Grand Challenges: Groundwater Transport and Remediation

Computational scientists from ORNL have been part of a multidisciplinary team that has developed a suite of codes for a sophisticated parallel supercomputer that can simulate groundwater flow and contaminant transport. The codes incorporate many important complex geochemical and biological processes and solve these problems efficiently on a variety of parallel architectures. The code is designed to solve Grand Challenge problems in groundwater contaminant transport and remediation—highly difficult problems that cannot be solved any other way.

A user-friendly graphical interface will allow the user to "steer" the simulation by changing input parameters and, at the same time, view the simulation output. Such interactive modeling is particularly difficult to support in a parallel environment. The innovative interface and communication libraries that have emerged from this project are adaptable to other projects as well. For example, the DOLIB library (for shared-memory emulation on the Intel distributed-memory Paragon supercomputer) and the EDONIO library (for highly efficient disk input/output, or I/O) that ORNL researchers developed for this project are being used to benefit several other projects.

The Future

Although we have available enormous computational power, improvements in algorithms and solvers are still needed to tackle finest-resolution (submeter-scale) simulations. State-of-the-art numerical techniques such as adaptive meshing, multigrid, and particle methods are needed in the next generation of high-performance groundwater codes. Advances in modeling complex remediation strategies such as in situ bacterial bioremediation, chemical treatment, or soil venting requires a better fundamental understanding of biological and geochemical processes. We envision closer multidisciplinary collaboration between environmental scientists and mathematicians in the future. Model formulation and field experiments will go hand-in-hand, and high-performance computing will be a valuable tool for understanding reaction pathways or estimating variables that are difficult to measure experimentally.

A new research emphasis is on building an integrated problem-solving environment (PSE) that makes high-performance computing readily accessible for scientists. The PSE may offer services that simplify submission and monitoring of multiple simulations and provide services for fault-tolerance and task migration, real-time visualization, and computational steering to explore remediation questions such as "What happens if we place a well here?" The PSE may be a combination of extended versions of an existing graphical preprocessor such as the Groundwater Modeling System (GMS) and a visualization tool such as G3D.

Perhaps the most challenging problem to overcome is lack of application software. Writing efficient parallel programs to take full advantage of a high-performance multiprocessor like the Intel Paragon requires a new way of thinking (programming methodology) and effective software tools to deal with the inherent complexities. While automatic parallelization tools such as Forge or High-Performance Fortran (HPF) are now commercially available, these tools are in their infancy. They still require substantial programmer intervention either in adding compiler directives or restructuring code. Without this intervention, the resulting compiled code usually performs poorly.

Massively parallel multiprocessors such as the Intel Paragon XP/S 150 machine at CCS currently represent the pinnacle of high-performance computing. However, shared-memory symmetric multiprocessors with only a handful of processors (e.g., the SGI Power Challenge) or network clusters of fast workstations (e.g., the IBM SP2) bring high-performance parallel computing to the masses. At the low end, a two-processor Intel 266-megahertz Pentium PC costing a few thousand dollars offers the equivalent performance of several Paragon nodes.

High-performance computing is an emerging new technology that opens up new opportunities for modeling and understanding complex groundwater systems. **ornl**

BIOGRAPHICAL SKETCHES

LAURA TORAN is a hydrogeologist formerly in ORNL's Environmental Sciences Division. She came to the Laboratory in 1986 as a Wigner Fellow after receiving a Ph.D. degree in geology from the University of Wisconsin. Her research interests include coupled geochemistry and transport modeling, application of supercomputers to groundwater problems, fracture flow and transport, and groundwater microbiology. She recently joined the Geology Department of Temple University in Philadelphia.

JIN-PING GWO is a computational hydrogeologist and staff researcher at ORNL's Center for Computational Sciences (CCS). He has a Ph.D. degree in civil engineering from Pennsylvania State University. He specializes in multiple-domain fracture flow and solute transport, development of supercomputer models, and the application of these models to risk-based cost-benefit analysis. His research interests also include hydrogeochemistry, interactions of surface and subsurface waters, reservoir simulations and multiphase mass transfer, optimization of hydrological systems, and global climate modeling.

G. MAHINTHAKUMAR is a research staff member in ORNL's CCS. In 1994 he received a Ph.D. degree in civil engineering from the University of Illinois at Urbana–Champaign (1994). His research specialty is high-performance computing applications in groundwater remediation.

EDUARDO D'AZEVEDO is a research staff member in ORNL's Computer Science and Mathematics Division. He has a Ph.D. degree in computer science from the University of Waterloo in Canada. In 1990 he came to the division's Mathematical Sciences Section under an Oak Ridge Associated Universities postdoctoral fellowship. Since that time he has been involved in research in numerical linear algebra, triangular mesh generation, and high-performance computing with applications in modeling groundwater flow and contaminant transport.

CHUCK ROMINE joined the Mathematical Sciences Section in 1986 after receiving his Ph.D. degree in applied mathematics from the University of Virginia. His main areas of research interest include parallel numerical linear algebra and software tools for parallel numerical computation. Most recently, as a member of the Partnership in Computational Science (PICS) team, he has been developing software tools to support parallel models for groundwater flow and contaminant transport on high-performance supercomputers such as the Intel Paragon at ORNL.

Analysis of Material Performance in Automotive Applications

Srdan Simunovic (left), Gustavo Aramayo, and Thomas Zacharia view a computer simulation of a collision between two cars. *Photograph by Tom Cerniglio.*

By Srdan Simunovic, Gustavo Aramayo, and Thomas Zacharia

Cars and trucks will use fuel more efficiently if they are built of materials lighter than steels used today. But will these materials absorb energy as well as or better than steel to protect passengers during a vehicle collision? Crash testing of prototypes can provide answers. However, computer modeling of materials and vehicles yields solutions in less time and at a lower cost. ORNL researchers have shown that complex models can be developed and modified to run rapidly on massively parallel computers.

Intense competition in the mass-production vehicle market is driving down the time cycle for new vehicle development. The cycle currently takes between 2 and 4 years, and it consists of conceptual design, mechanical design and analysis, materials and process selection, tooling and equipment development and setup, product manufacturing and assembly validation, and finally, production operations. Very little time is allowed for development of new materials and processes because changes in these areas might have major impacts on all stages of operation and could cause significant delay or negative consequences. For the design team to accept a new material or process, it must have no risk associated with manufacturing and use at the time the commitment is made. In-depth understanding of the science of materials synthesis, processing, and performance is a fundamental need of the automobile industry.

Accurate materials models are essential for the development of realistic vehicle deformation simulations. They are derived from a collection of experimental data and accumulated experience with the material. The knowledge about material behavior for conventional automotive structural materials such as mild steel is considered reasonably complete. However, further improvements in vehicle efficiency mandate the introduction of stronger and lighter materials—such as higher-strength steels, aluminum and magnesium alloys, and composite materials—into the load-bearing systems. The behavior of these materials is not yet sufficiently well understood for the variety of conditions that vehicles experience during service to be used confidently for mass automotive production.

One project currently under way aims to accelerate the introduction of lightweight materials to automotive applications through advanced computational simulations for assessing design and performance. The project includes (1) development of improved computer codes for deformation analysis, (2) development of improved vehicle models with experimental validation of the models, (3) improved understanding of design methodologies and vehicle assembly procedures, and (4) development of a lightweight materials database. The combination of computational simulations on supercomputers and rigorous experimental validation will enable assessment of the performance of low-weight materials in automobiles more economically and in a much shorter time than the trial-and-error approach would require.

Development of Vehicle Computational Model

The structure of mass production automobiles has been changing rapidly during the past two decades. Most new cars no longer are made of separate frame and body structures; instead each has an integral system known as a unitized body (unibody). The unibody, which consists of a large number of welded stamped metal parts, is the main energy-absorbing structure of the vehicle. Front and rear subframes are attached to the unibody very late in the assembly process. The front subframe usually carries the transversely positioned engine, transmission, front suspension, and wheel assembly; the rear subframe carries the rear suspension and rear axle. The complexity of the unibody-subframe structure does not allow for obvious simplifications in simulation models as in cases where a clear distinction exists between the primary frame and the secondary structures.

Perhaps the most dramatic automotive design verification comes from actual vehicle collision tests. They not only bring perspective to everyday driving, but also make us more appreciative of the challenges that face vehicle designers. The dissipation of energy and the extent of deformation in collisions are often critical design considerations. A clear understanding of material behavior is essential to the design of structures and mechanisms that protect vehicle occupants. From the standpoint of a design engineer, vehicle impact simulation must meet three essential requirements: accuracy, versatility, and computational feasibility. The first two requirements usually translate into large, detailed finite element (FE) models that are usually not feasible for single-

processor workstations because of long computation times (around 600 CPU hours) and large memory requirements. Because the best vehicle models capture complex deformation during impact, it is not unusual for these models to have 50,000 or more FEs.

Over the past several years, the National Highway Traffic Safety Administration (NHTSA) has been developing an FE model of a midsize sedan. The model has been obtained by first disassembling the vehicle and then scanning the shape and measuring the mass and inertia of each component. The FE model is derived from the geometric model by discretizing each digitized part using FEs and connecting them into the final model. The separation of geometrical representation from the computational FE allows for flexibility in model modifications and the addition of complex constraints.

Fig. 1. Single-car offset impact with a rigid barrier, showing the results of a car crashing into and glancing off a rigid barrier such as a wall or post.

Research under way at ORNL in collaboration with NHTSA and George Washington University addresses essential requirements for developing detailed vehicle computational models. Vehicle models are combined with lightweight materials models and are used to analyze material performance in a wide variety of impact situations.

Several different impact situations are currently being investigated to optimize the vehicle models: single car offset impact with a rigid barrier (Fig. 1), two-car frontal offset impact (Fig. 2), and two-car oblique offset impact (Fig. 3). Simulations are compared with test data that consist of high-speed films of vehicle collisions and traces from accelerometers that are placed throughout the vehicles. In addition, the crashed vehicles are disassembled and analyzed so that the main mechanisms for the dissipation of impact energy can be identified and quantified.

Deformed parts are extracted and digitized so that they can be directly compared with simulation results.

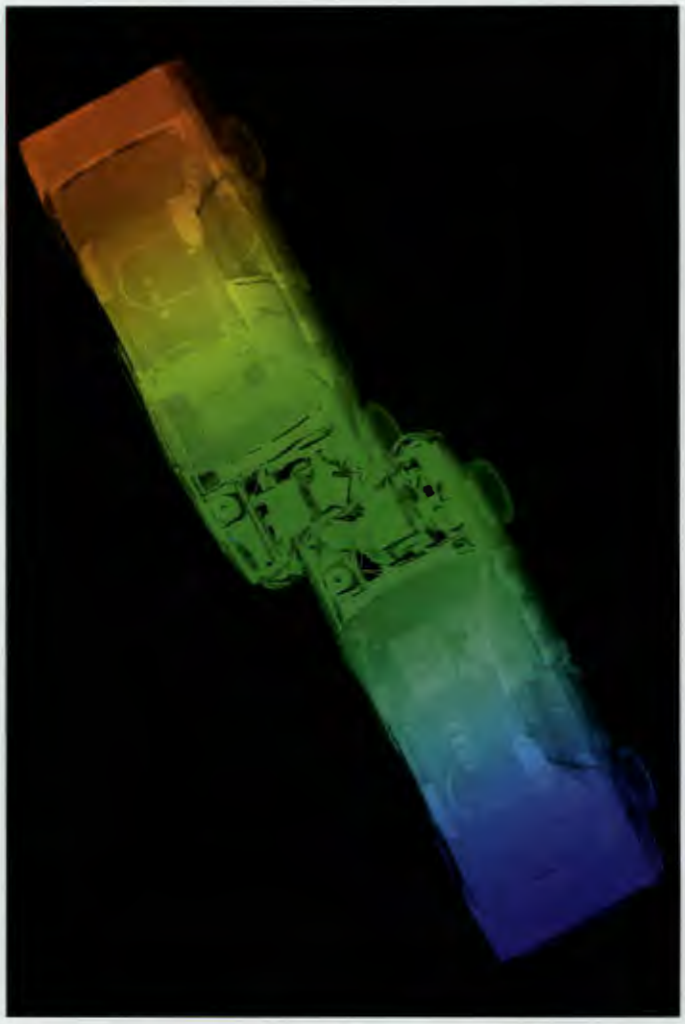


Fig. 2. Two-car frontal offset impact, showing the results of a head-on collision between two cars (in which the headlight of one car and the front center of the other collide).

Figures 4 and 5 show the deformed shape of the front underside of the vehicle after collision and the corresponding simulation result. In the comparison process, these images are scaled and overlaid to assess the quality of the model and to identify areas of the model that need further improvement. This well-organized and detailed approach provides credibility to the simulations and builds confidence in findings obtained by simulating new, not yet experimentally tested materials and impact conditions.

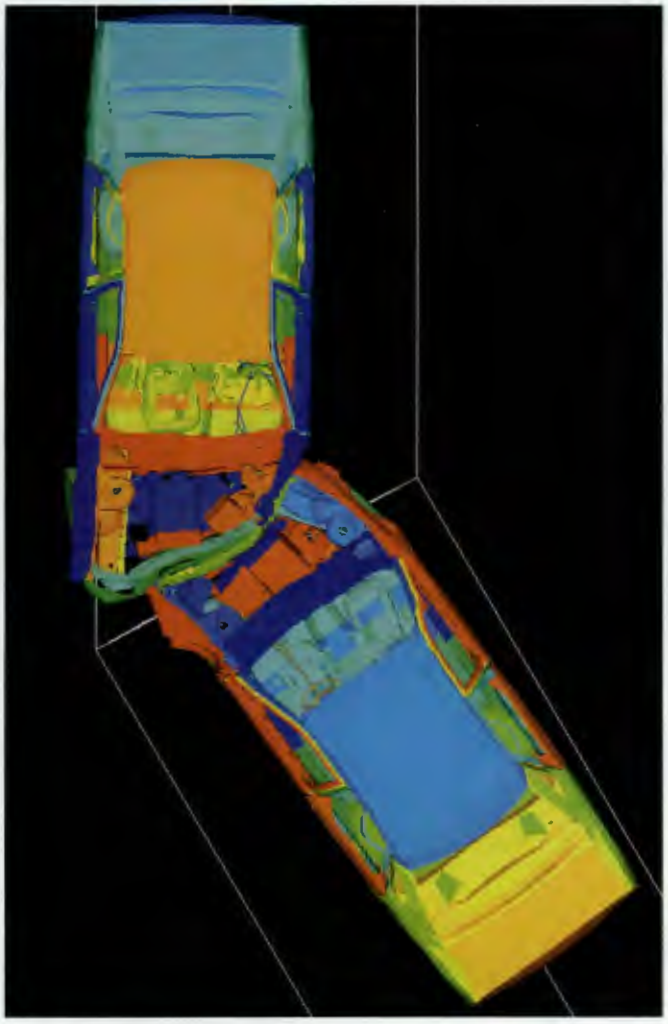


Fig. 3. Two-car oblique offset impact, showing the results of a collision between two cars in which the front of one comes in at an angle to the front of the other.

Fig. 4. Bottom view of test vehicle after two-vehicle crash.

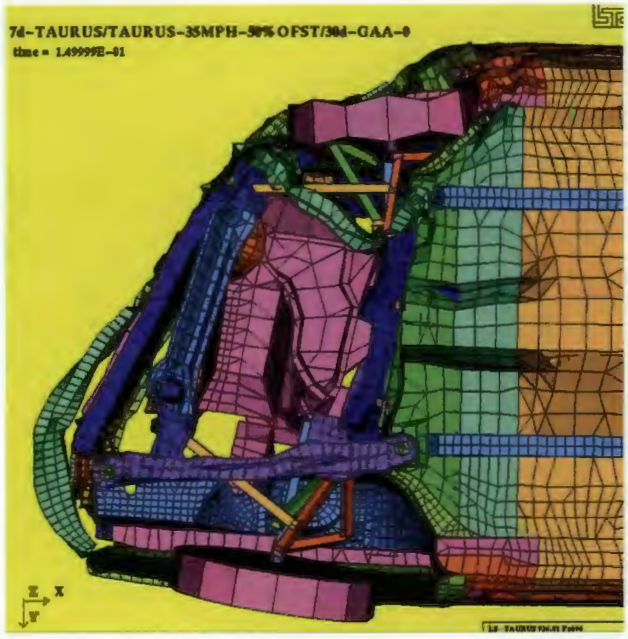


Fig. 5. Deformed shape of the front underside of the vehicle after collision—simulation result.

Parallel Computers and Crashworthiness Analysis

Crash simulations are being performed using the massively parallel version of LS-DYNA3D software. A research collaboration has been established between ORNL and the software vendor to improve the software performance on distributed-memory massively parallel computers. The program calculates accelerations, velocities, deformations of components, and forces acting on vehicles, taking into consideration variables such as different materials, impact interactions, complex constraints, and spot welds. The program employs an explicit time integration scheme with mass matrix diagonalization, thus making the matrix factorizations trivial without need for any significant interprocessor communication. The downside to this approach is that the computation is only conditionally stable. The stability condition requires that the time step increment within which the entire state of deformation needs to be computed be proportional to the size of the

smallest element in the FE model. For example, the simulation of a 120-millisecond-long collision of a car with a rigid barrier requires more than 130,000 such time increments. The FE model for the car used in this study involves 27,000 to 30,000 FEs, and approximately the same number of nodes. To process one FE during a computational increment, approximately 1000-floating point operations and several hundred "words" of memory are needed.

Fig. 6. An example of domain decomposition using RSB is shown here.

The domain decomposition approach has been employed in the program as the principal method for exploiting concurrent distributed-memory processing. Using this approach, different parts of the structure are assigned to different processors for computation of their deformation. At certain points in the program, information has to be exchanged between processors to account for interaction between the subdomains (adjacency and contact interactions) and to synchronize computation. The efficiency of the computation is influenced by the ratio between the balanced computational load assigned to the processors and the amount of communication that is needed between them. For a given size of the problem, as the number of processors used increases, the subdomains (and therefore computational load) decrease while communication becomes dominant. After the computation time becomes comparable to communication, the simulation time cannot be further reduced by increasing the number of processors. Three different decomposition methods can be used in the program: (1) recursive spectral bisection (RSB), (2) recursive coordinate bisection, and (3) greedy algorithm. An example of domain decomposition using RSB is shown in Fig. 6. The subdomain-to-processor assignment for the car above has been shown in exploded view to illustrate the domain decomposition approach. Usually, the average size of interfaces, or "cuts," between different subdomains is directly proportional to the communication that would be required in the program. Low communication resulting from RSB makes it a method of choice for parallel processing on distributed memory computers when there is no unilateral contact between the FEs. However, in situations where structural parts interact through contact and the spatial relations drastically change, the advantages of RSB may not be so apparent.

Vehicle impact simulation involves computing the deformation of vehicle parts as a result of their contact with impacting structures as well as with other vehicle parts. If two interacting parts reside on different processors, this interaction needs to be carried through interprocessor communication. Because it is very difficult to determine in advance which parts will come into contact, such information cannot be embedded into domain decomposition ahead of computation. In effect, this requires the application of geometrical reasoning, which is a global memory operation on a distributed memory environment, consisting of mainly independent entities (processors) having limited spatial scope. The contact algorithm employed in the program is based on frequent spatial sorting of the contact entities and redistribution of the sorted position information between processors. The problem space is divided into regular subdomains ("buckets") in x, y, and z physical directions. The process involves extensive communication between processors, and, if performed every time step, may create a computational bottleneck. Reducing the number of "bucket" sorts can speed up computations considerably; then, if errors in computation are noticed, the

sorting frequency can be increased to maintain accuracy.

The timing results for different numbers of processors simulating the offset impact of a car with a rigid barrier are shown in Fig. 7. The time axis represents average CPU time spent on the problem's time increment. In this case, the representative CPU time was averaged over a number of time steps and compared as it fluctuated, depending on simulation conditions and machine load. An example of CPU time per problem time increment throughout the simulation using 128 processors is shown in Fig. 8. When the representative CPU times for different numbers of processors are normalized with the CPU time needed for 16 processors (see Fig. 9), it may be noticed that there was a reasonable increase in computational efficiency up to 64 processors. A further increase in the number of processors did not significantly reduce the overall computational time as the communication between processors became dominant. In the case of the two-car crash, the efficiency increased up to approximately 128 processors. This efficiency increase could be attributed in part to the increase in the average size of computational subdomains assigned to processors with respect to required communication. Computational simulations for the single- and two-car impacts have been run numerous times to identify deficiencies of the existing models and to improve their performance.

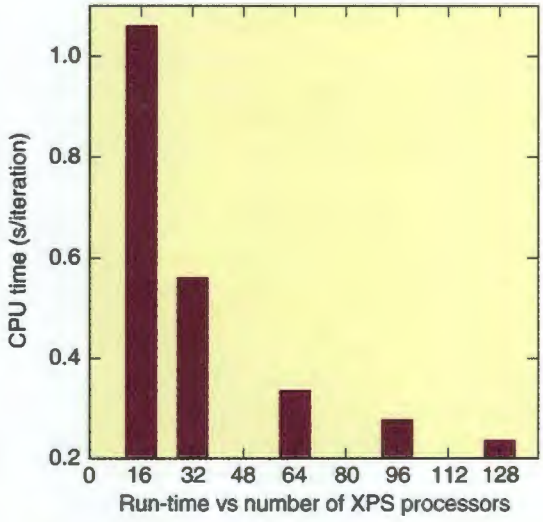


Fig. 7. Because the problem cannot fit on one processor, 16 processors were used as the base case.

Conclusions

Computational requirements for simulations are becoming more important as complex materials models for lighter materials are employed in new vehicle models. Ongoing research at ORNL will result in accurate vehicle and materials models that can be used for a host of applications, primarily the evaluation of the performance of lightweight materials in vehicles, especially those subjected to collisions. Massively parallel computing plays an essential role in this research because it allows for rapid development of these models. Scalability studies on current vehicle models indicate a threshold for the number of processors that can be efficiently used for a given simulation. This threshold can be related to the average number of finite elements that is assigned to each computer node of a massively parallel computer. **ornl**

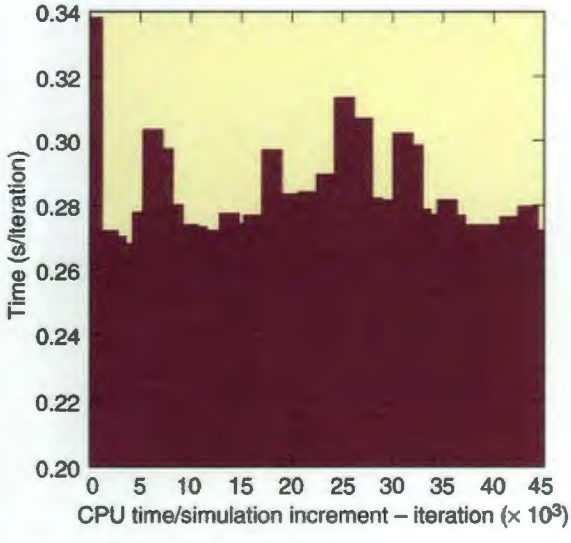


Fig. 8. An example of CPU time per problem time increment throughout the simulation using 128 processors.

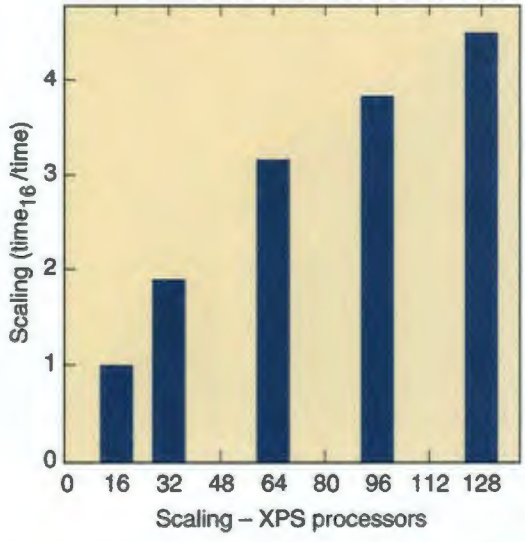


Fig. 9. When representative CPU times for different numbers of processors are normalized with the CPU time needed for 16 processors, computational efficiency increases to 64 processors.

Crunching Numbers vs Crunching Metal to Explore Vehicle Safety

A spanking new Ford Explorer delivered to ORNL has come apart, but studies of its parts should help ensure that tomorrow's automobiles meet or exceed established safety standards. Future cars and trucks will be made of lighter materials to help increase their fuel efficiency, so design changes may be needed to guarantee that lighter vehicles will be as safe in collisions as the heavier steel vehicles of today.

Researchers at the Laboratory dismantled one model of the nation's top-selling sport utility vehicle and weighed and measured each piece. As part of the project, they plugged that information into an ORNL computer program. A computer model was built which the Department of Transportation (DOT) can provide to U.S. automakers to help them improve future vehicles.

"Our role isn't to confirm or deny the safety of the Ford Explorer," says Thomas Zacharia of ORNL's Computer Science and Mathemathics Division. "We've built a computer model of the Ford Explorer and run simulated 35-mile-per-hour crash tests. Results from these simulations will be used to ensure that future, lighter vehicles meet safety requirements." ORNL, which performed similar tests on a Ford Taurus a few years ago, has gained expertise in automobile crash simulations using ORNL's powerful Intel Paragon XP/S 150 model supercomputer. That's why DOT is funding the current project.

"It's a lot less expensive to crunch numbers on a computer than it is to crunch metal in a crash test," says Zacharia. Once ORNL researchers validate their simulated offset, head-on crash with an actual controlled crash in Buffalo, New York, they will be able to perform a number of crashes and generate a variety of data. Simulated crashes will provide information identical to what researchers could gain from actual crashes that cost up to $75,000 per crash.

While ORNL is developing a vehicle model for the Explorer, other institutions are doing the same with other top-selling vehicles—the Chevrolet Lumina, Chrysler Concorde, Honda Accord, and the Dodge Neon.

ORNL's work is related to a national effort to develop a vehicle that gets 80 miles per gallon—triple the fuel efficiency of today's cars—without sacrificing performance, utility, cost of ownership, or the safety that consumers demand. "To achieve this goal, we're talking about a weight reduction of 40 percent," Zacharia says. "That dramatic reduction requires the use of lightweight metals, plastics, and composites that offer new challenges for automobile engineers."—*Ron Walli*

Thomas Zacharia examines a Ford Explorer during disassembly. Parts are measured and weighed to help researchers predict vehicle energy dissipation during collisions simulated by computer.

BIOGRAPHICAL SKETCHES

SRDAN SIMUNOVIC is a research engineer in the Modeling and Simulation Group of ORNL's Metals and Ceramics Division. He holds Ph.D. and M.S. degrees in structural mechanics from Carnegie Mellon University and a B.S. degree in civil engineering from the University of Split in Croatia. He joined the ORNL staff in 1994. His research activities include modeling of composite materials, automobile impact simulations using the finite element method, massively parallel computing, and modeling of casting processes. He is a member of the U.S. Society for Computational Mechanics and ASM International.

GUSTAVO A. ARAMAYO is a senior staff engineer in the Engineering Analysis Group of ORNL's Engineering Technology Division. He holds an M.S. degree in engineering mechanics and a B.S. degree in civil engineering from the University of Alabama at Tuscaloosa. He joined ORNL in 1974. His current activities involve the analysis and modeling of impact problems in fuel and weapons transportation packages and passenger vehicles, mechanical and thermal analysis of transfer rollers, modeling and simulation of refractories in kilns, and modeling and analysis of sheet metal processes. He is a member of the American Society of Civil Engineers, the Metals Society, the American Association for the Advancement of Science, and the American Institute of Aeronautics and Astronautics.

THOMAS ZACHARIA is director of ORNL's Computer Science and Mathematics Division. He received his Ph.D. degree from Clarkson University. He came to ORNL in 1987 to work on weld process modeling. His research interests involve advanced computational modeling and simulation of materials and processes. He played an active role in developing, establishing, and leading the Modeling and Simulation Group of ORNL's Metals and Ceramics Division. His research has resulted in several cooperative programs with industry and academia. He has chaired or co-chaired several international meetings and conferences in process modeling. He has presented invited keynote addresses for international conferences and serves as a committee member for several technical societies. Zacharia has received numerous awards for his research.

Optimization of Microstructure-Property Relationship in Materials

By Balasubramaniam (Rad) Radhakrishnan, Gorti Sarma, and Thomas Zacharia

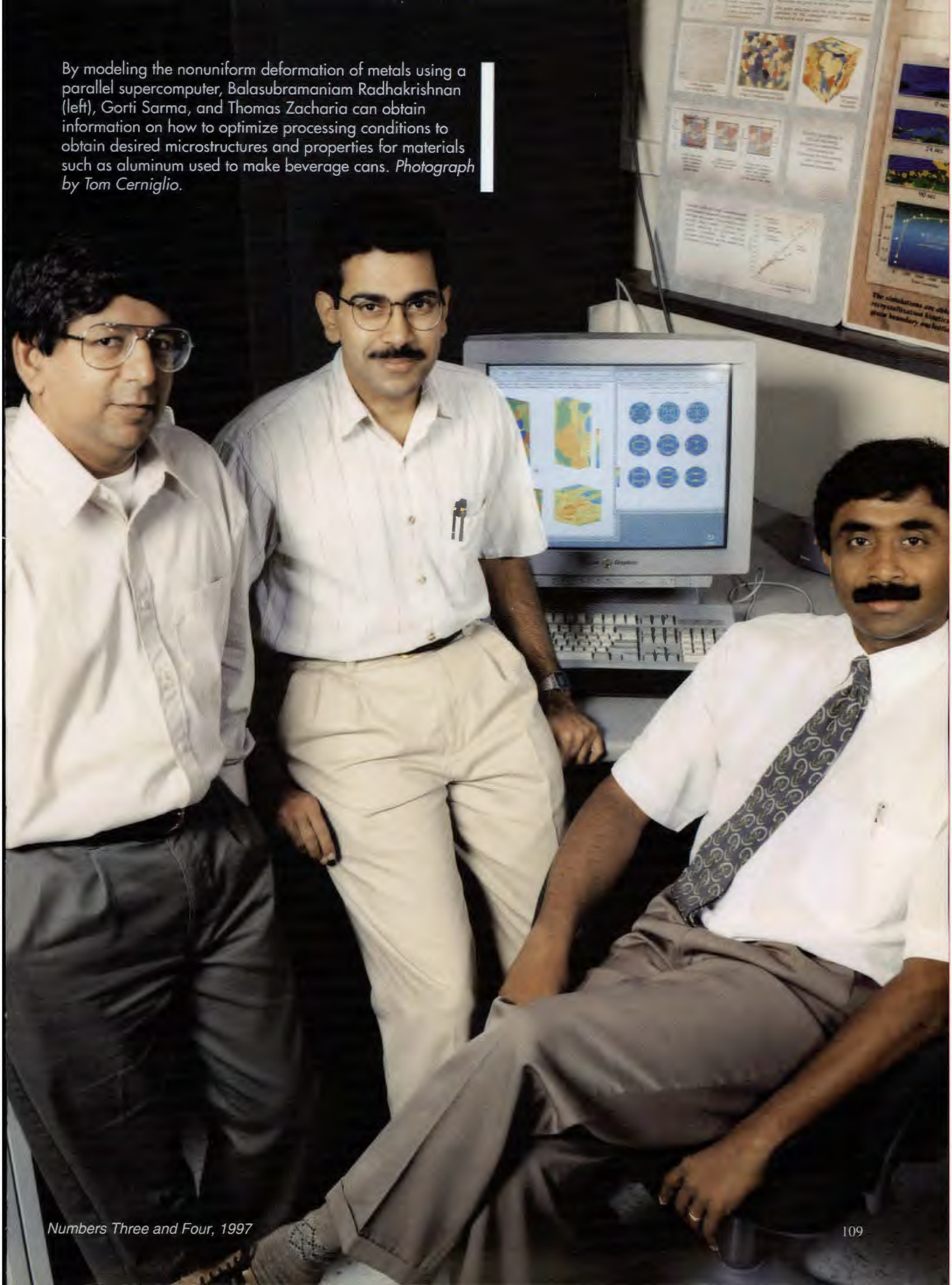
The production of aluminum beverage cans involves a number of thermal and mechanical processing steps, starting with the cast ingot. The reduction in thickness from the ingot to the final sheet is achieved by a series of rolling steps that reduce the aluminum ingot from a thickness of about 300 millimeters (mm) to 0.3 mm— the sheet thickness required for can making. The can is made by deep drawing, in which the sheet is held between a punch and a die and then drawn into the die by stretching. The success of the can-making operation depends upon the properties of the sheet, especially the orientations of the grains, referred to as texture. The texture control in the sheet depends on the proper choice of the processing variables during hot- and cold-rolling operations. Recrystallization is an important metallurgical phenomenon that influences the texture in the sheet during hot rolling.

ORNL researchers are using the Intel Paragon supercomputer to model the microstructural evolution of aluminum during thermomechanical processing. The models capture the rotation and elongation of the grains, the hardening of the material through the generation of dislocations by crystallographic slip during cold rolling, and the nucleation and growth of strain-free grains during annealing. The ORNL model can be readily used to develop the optimum processing window for producing controlled texture in aluminum to minimize scrap produced during can making.

Metals and alloys are made of crystalline grains whose characteristics and arrangements, which are visible in an electron microscope, can be altered by the application of heat (e.g., annealing) or mechanical action (e.g., compression). The microstructural features that determine the properties of a material include the size, shape, and orientation of the grains and their distribution in the microstructure. Optimizing the material microstructure for performance by designing and applying appropriate thermomechanical processing steps has been the prime role of metallurgists for decades. Until recently the study of processing-microstructure relationships has largely remained within the purview of experimental metallurgists because the mechanisms that contribute to these microstructural changes are very complex, and the changes occur either simultaneously or successively to varying degrees, depending on location within the material. The development of a computational model for predicting the overall response of the material to such a complex collection and sequence of metallurgical phenomena is extremely difficult. However, recent advances in high-performance computing have led to considerable progress in addressing this challenge.

Deformation Mechanisms

One of the basic deformation mechanisms in metallic crystals is crystallographic slip. Crystallographic slip involves the movement of dislocations in certain planes and directions in each crystal. A dislocation is an imperfection in the crystal structure of a metal resulting from an absence of atoms in one or more layers



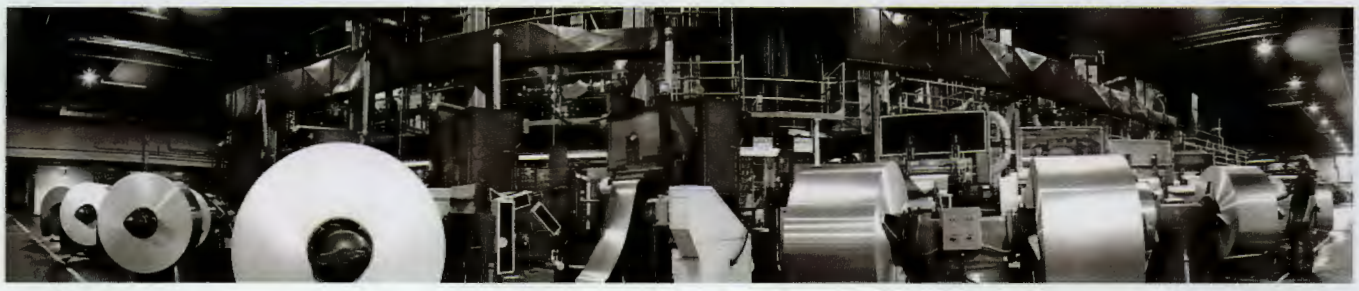
By modeling the nonuniform deformation of metals using a parallel supercomputer, Balasubramaniam Radhakrishnan (left), Gorti Sarma, and Thomas Zacharia can obtain information on how to optimize processing conditions to obtain desired microstructures and properties for materials such as aluminum used to make beverage cans. *Photograph by Tom Cerniglio.*

of a crystal. For a given crystal structure there are well-defined combinations of planes and directions in which slip occurs. For example, in the case of face-centered cubic materials, slip occurs on the {111} type of planes and in the <110> directions. There are four different kinds of {111} planes and three <110> type directions in each of those planes, giving a total of 12 slip systems.

The occurrence of crystallographic slip during plastic deformation gives rise to two other phenomena that are of technological importance. The first is the increase in dislocation density during deformation due to the presence of locks within the crystal that arrest further movement of dislocations. These locks are produced by the interaction of dislocations moving in different slip systems. Because the resistance to dislocation movement increases in the presence of the locks, the crystal requires additional stress in the slip system to move further dislocations, and the crystal is said to "work-harden." Work hardening is one of the mechanisms by which the deformation energy is stored within the crystal. The microstructure of the work- hardened material consists of a large number of cells, or subgrains, whose boundaries are essentially composed of a dense wall of dislocations. The second phenomenon that occurs is the rotation of the crystal during deformation. The crystal rotation is required for accommodating an arbitrary deformation because deformation by slip is possible only along a small number of slip systems. The crystal rotation accompanying arbitrary deformation is the underlying reason for the development of textures, or preferred orientations in materials, which results in anisotropic mechanical properties. The presence of texture is exploited in many industrial operations such as can making and other sheet-forming operations.

Beverage cans (above) are stamped out in the Coors Container Plant (below) in Golden, Colorado. ORNL is modeling the microstructure of rolled and heated aluminum before it is formed into cans.

So far we have discussed the deformation of single crystals. However, a material microstructure consists of several crystals, or grains, connected together. Each of the grains may have a random crystallographic orientation, or the grains may have a preferred orientation, depending on the prior processing history. The surfaces along which the grains are connected remain intact during deformation. Hence, the deformation of individual grains in a material microstructure should satisfy the condition that the displacements are continuous across grain surfaces. This results in the operation of different slip systems in the grain interior as opposed to regions in the vicinity of grain boundaries. As the extent of deformation increases, a



single grain breaks up into smaller "grains" of different orientations. Hence, formation of texture or preferred orientations during the deformation of a polycrystalline material depends not only on the orientations to which the grains rotate, but also on the orientation spread within each grain as different parts of the grain rotate to different orientations, as described above. Because the deformation of the grains is heterogeneous, the stored energy of deformation is also heterogeneous at the microstructural level. Both the heterogeneity in the stored energy of deformation and the orientation spread in the deformed microstructure are important variables that determine the further evolution of texture during thermal processing such as annealing.

Microstructural Events During Annealing

The microstructural events that occur during annealing of a deformed microstructure lead to a reduction in the stored energy of deformation by decreasing the dislocation density in the material. The two competing events that occur are recovery and recrystallization. Recovery is the process by which the stored energy of the material decreases continuously throughout the microstructure by the rearrangement of the dislocations into certain low-energy configurations. On the other hand, during recrystallization, there is a discontinuous change in the dislocation density because of the sweeping of the microstructure by certain surfaces that separate regions of high dislocation density and extremely low dislocation density. The resulting grain structure and texture depend on the orientation and the spatial distribution of the recrystallized nuclei that provide these surfaces. The relationship between the deformed microstructure and nucleation during recrystallization is a highly debated subject, and there is significant interest among researchers from both a fundamental and a technological viewpoint. Although several models have been proposed for the formation of nuclei during recrystallization, the extent to which these models apply to a real microstructure has not been quantified because of the lack of quantitative information on the deformed microstructure. The effect of simultaneous recovery during recrystallization is to diminish the driving force for the migration of the high-energy surfaces between recrystallized and deformed regions, with the result that the interface velocity decreases continuously and may even vanish before the recrystallization is complete.

Research at ORNL presented here shows how the use of massively parallel computing makes it possible to quantify the complex metallurgical phenomena that occur in aluminum during thermomechanical processing. For the first time, it is possible to model the deformation of a three-dimensional grain structure and quantitatively predict the development of not only the bulk texture but also the orientation gradients that exist in the deformed microstructure. In addition, the simulations also predict the heterogeneous distribution of the stored energy of deformation from grain to grain, as well as the intragranular variation of stored energy between sites at the interior of the grains and those sites in the vicinity of grain boundaries. The deformation simulation results have been mapped to a three-dimensional grid of regularly spaced points and used to predict the nucleation and growth of recrystallized grains, as well as the simultaneous recovery that occurs during subsequent thermal processing.

ORNL's Methodology

The simulations for predicting microstructural changes during thermomechanical processing of metals address two processes—deformation and recrystallization. Simulations of the plastic deformation of the material (aluminum, in this case) require computing the motion of the workpiece under applied boundary conditions. Balance laws for conservation of momentum, mass, and energy form the basis for solving the resulting initial-boundary value problem. In addition to the balance laws, it is necessary to prescribe the constitutive behavior of the material, which relates the applied stress to the rate of deformation and the microstructural state. The plastic deformation is modeled in incremental fashion: the displacement or velocity of the workpiece is determined keeping the material state fixed, and then the state is updated before moving to the next increment.

As discussed earlier, the deformation of the metal is assumed to occur by the movement of dislocations along specific directions in specific planes. The rate of shear on these planes is related to the shear stress through a constitutive relation, typically a power law. The rate of deformation of the grain is given by a linear combination of the shear rates on all the slip systems, while the shear stress on the slip plane is the projection of the stress applied to the grain. A constitutive law between the rate of deformation and the stress tensors for the grain can be derived by eliminating the slip system shear rates from the above-mentioned relations. This constitutive law is nonlinear in the stress and requires an iterative method to compute the stress for a given rate of deformation.

The governing laws lead to differential equations that must be integrated to obtain the motion or

deformation of the workpiece. The complex nature of the problems makes it necessary to use numerical methods for solving them, and the finite element method provides a suitable framework for this purpose. The domain of interest is discretized into several elements, and the balance laws are satisfied in an average sense over all the elements. The approach using finite elements for computing the motion of the workpiece consists of two main parts. The first task involves computing the stiffness for each element in the discretization, which represents a measure of the material response in that element. A stiffness matrix is set up based on the current material state by integrating the equations associated with the element. These stiffness matrices are then assembled in the second step to compute the discretized velocity or displacement field of the workpiece. The complexity of the two steps depends on the nature of the constitutive response and the size of the discretization.

The nature of the constitutive model based on crystal plasticity makes the stiffness computations extremely time-consuming. For a given rate of deformation with five independent components, a system of nonlinear equations must be solved to get the stress components. However, these computations can be carried out independently for each element, making them quite efficient on a parallel computer. It is this feature of the formulation which enables the treatment of fairly large-sized problems in a reasonable time frame. Although the stiffness computations scale fairly well with increasing numbers of processors, the assembly and solver routines are not so scalable. These parts of the program require communication between processors, which is an overhead that increases with the number of processors.

A finite element code capable of simulating the deformation of metals has been developed for the Intel Paragon at ORNL using High-Performance Fortran. A certain amount of optimization was achieved by making use of native NX message-passing calls. The code has been used to simulate the deformation of face-centered cubic metals in plane strain compression, and the resulting data on the distributions of stored energy and orientations have been used in modeling the subsequent recrystallization process.

The simulation of microstructural evolution during annealing is carried out using a Monte Carlo technique. The stored energy of deformation and the orientations of the elements in the deformed mesh are first mapped to a grid of regularly spaced points. As described previously, microstructural phenomena such as recovery, nucleation, and growth of recrystallized grains occur to varying degrees depending on the local deformation microstructure. In the Monte Carlo technique, each site in the grid is visited in a random fashion and each event is implemented on the basis of its probability of occurrence. The nucleation step is modeled by the growth of subgrains at each Monte Carlo site. In those sites where the stored energy of deformation is high and where there is also a monotonic increase in the misorientation of the subgrains during growth, the probability of forming a recrystallization nucleus is high. The quantitative description of the deformed microstructure allows, for the first time, the incorporation of a nucleation model based on subgrain growth at the mesoscopic scale which represents a collection of statistically significant number of grains. Hence, both the spatial distribution and the orientations of the nuclei can be obtained from first principles. The movement of a boundary separating a deformed region from the recrystallized region is driven by the elimination of the stored energy of deformation as the boundary advances. However, the driving force is constantly decreasing because of the recovery process. Also, the advancement of the boundary requires additional energy needed to create the new boundaries. The net energy change resulting from these processes is calculated, and the advancement of the boundary is allowed only if the net change in energy is negative.

Simulation Results

Figure 1(a) shows the initial microstructure and its finite element discretization. The different colors in Fig. 1(a) indicate different grains in the microstructure with a specific crystallographic orientation for each grain. The deformed mesh after a 50% reduction in height by plane strain compression is shown in Fig. 1(b). The nonuniform deformation of the mesh is seen clearly. Figure 1(c) shows the deformed microstructure without the mesh. A comparison of the grain structures in Figs. 1(a) and 1(c) shows that the grain deformation is also accompanied by a reorientation, the extent of which varies from grain to grain. In addition to an overall reorientation, there is also an orientation spread within each grain, which again varies from grain to grain. It is this orientation spread which gives rise to selective nucleation of recrystallized grains during annealing as discussed later. The deformation energy stored in the microstructure seen in Fig. 2(a) is shown in Fig. 2(b). Observe that the magnitude of the stored energy varies from grain to grain as well as within the grains. The stored energy is high at certain intragranular locations where there is an abrupt change in the grain orientation. These regions correspond to transition bands

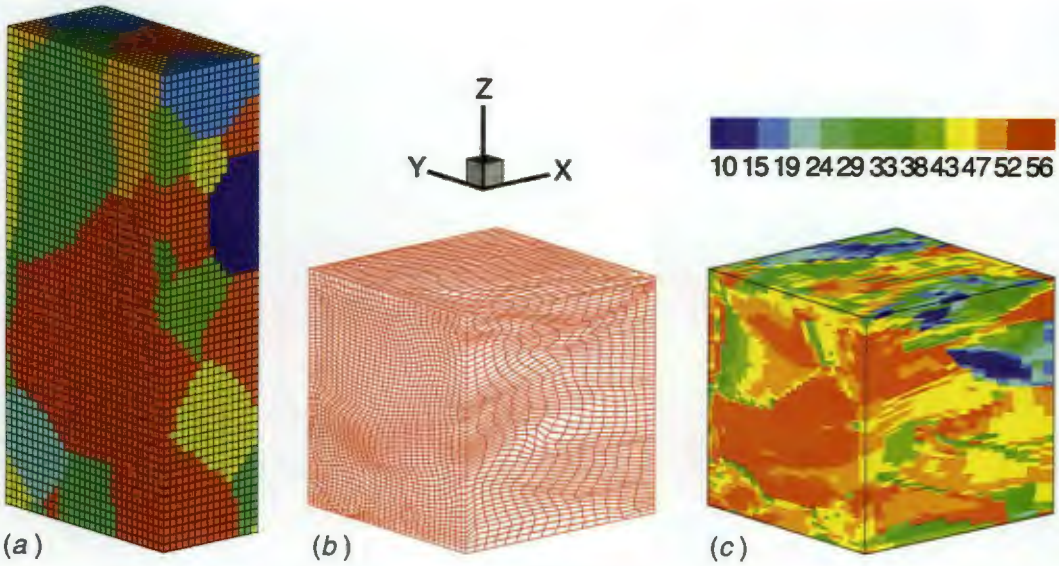


Fig. 1. (a) Initial microstructure with finite element mesh, (b) deformed mesh, and (c) deformed microstructure.

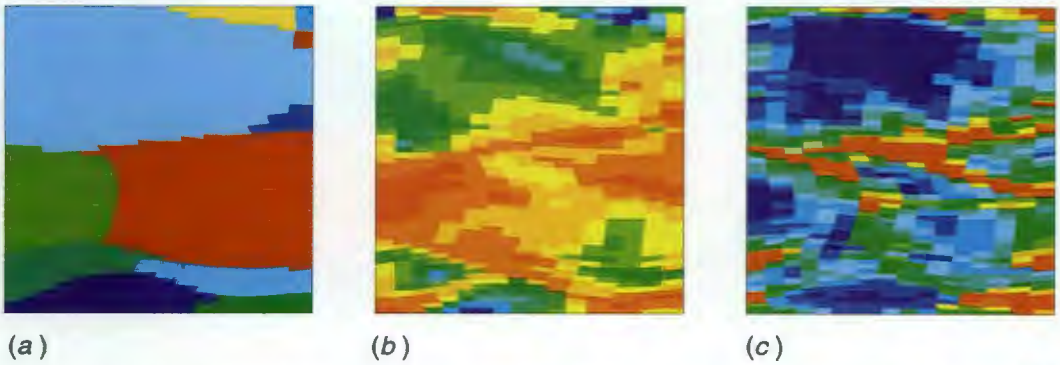


Fig. 2. (a) Deformed microstructure, (b) stored energy distribution, and (c) nucleation parameter for a section normal to the y-axis.

that are experimentally observed in deformed microstructures. The stored energy in the vicinity of grain boundaries as opposed grain interiors depends on the orientations of the surrounding grains. Hence, situations can be seen where the stored energy at the grain boundary is both lower and higher than in the grain interior.

Figure 2(c) shows the variation of a quantity called the nucleation parameter, which is the product of the stored energy and the misorientation of an element with respect to its neighbors, within the deformed microstructure. The nucleation parameter is an indicator of the probability of nucleation of the recrystallized grains on subsequent annealing. In regions where the stored energy is high, the dislocation substructure consists of a large number of small subgrains whose misorientation with the neighboring subgrains is fairly large. On the other hand, when the stored energy is smaller, the subgrain size is larger and the misorientation between subgrains smaller. Hence, the kinetics of subgrain growth is faster at those locations where the stored energy is high. However, a high value of stored energy alone is not sufficient for nucleation to occur. It is also necessary for the misorientation between subgrains to increase monotonically and to exceed the critical angle of 15° to form high-angle boundaries. This effect occurs in those regions where there is a significant local spread in the orientations, so that a given element has a large misorientation with respect to its surroundings. Hence, a site with a high value for the nucleation parameter also has a high probability for nucleation during annealing. The nucleation parameter is seen to have high values along certain grain boundaries and at triple points, as well as at certain intragranular locations where transition bands occur. It is important to note that the spatial distribution of the nucleation parameter is nonrandom.

Figure 3 shows the temporal evolution of the recrystallized microstructure on annealing. The locations where the recrystallized nuclei form coincide with those where the nucleation parameter [Fig. 2(c)] is high. The nonuniform spatial distribution of the nuclei results in early impingement of the adjacent recrystallization fronts, resulting in an overall decrease in the rate of recrystallization. This effect is

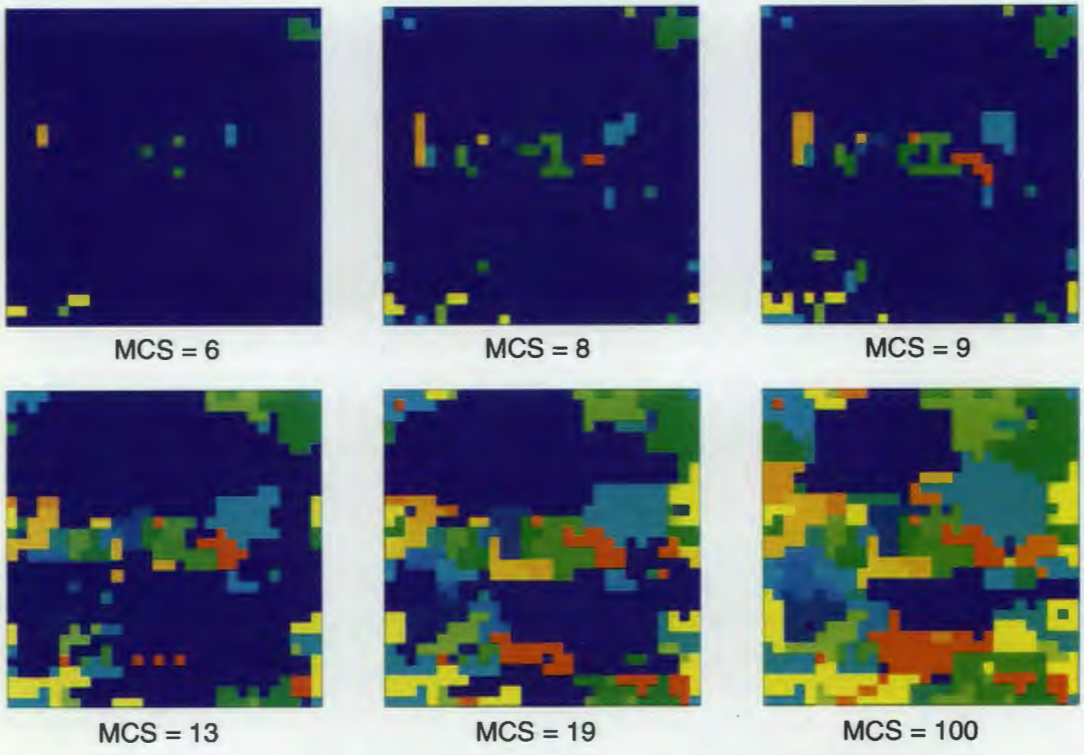


Fig. 3. Temporal evolution of recrystallized microstructure during annealing. "MCS" refers to time in Monte Carlo steps.

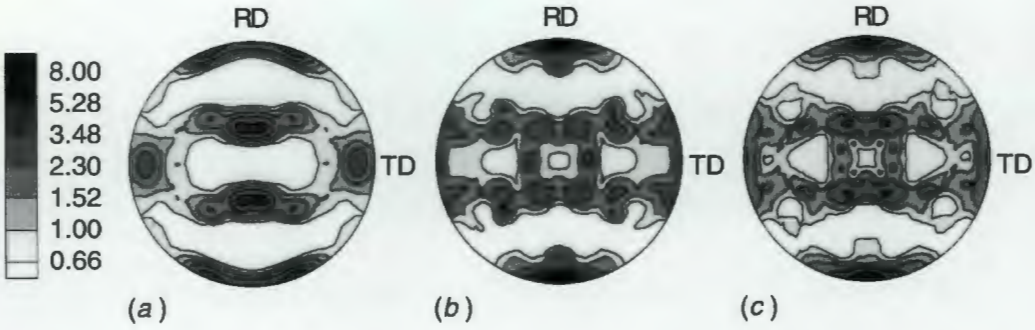


Fig. 4. <111> pole figures showing (a) the deformed texture, (b) the orientations of nuclei, and (c) the recrystallized texture.

accentuated by the occurrence of simultaneous recovery in the deformed locations. Hence, the material undergoes only partial recrystallization, with islands of recovered areas in the microstructure. This result has a significant influence on the mechanical properties of the annealed material.

Figure 4 shows the overall texture in the material in the deformed and recrystallized conditions. Also shown is the orientation distribution of the nuclei. Although recrystallization does not lead to the production of new orientations in the current simulations, it significantly redistributes the intensities of the texture components in the cold-worked material.

Conclusions

The work presented here (sponsored by DOE's Division of Material Sciences) is the first of its kind in the materials literature in which a quantitative description of the deformed microstructure has been used to predict the evolution of texture and microstructure during subsequent annealing. Although the present work is specifically concerned with face-centered cubic crystal structure, the modeling can be easily extended to handle body-centered cubic and hexagonal close-packed crystal structures. The availability of quantitative information on the cold-worked state has allowed, for the first time, the prediction of both the orientation and spatial distribution of recrystallized nuclei, thus enabling a more realistic simulation of the microstructure and texture evolution during annealing. **ornl**

BIOGRAPHICAL SKETCHES

BALASUBRAMANIAM (RAD) RADHAKRISHNAN received an M.S. degree in metallurgy from the Indian Institute of Technology, Madras, India, and a Ph.D. degree in materials science and engineering from the University of Alabama at Birmingham. Before pursuing his doctoral studies in the United States in 1986, he worked as a scientist at the National Aeronautical Laboratory in Bangalore, India. He joined the Modeling and Simulation Group in ORNL's Metals and Ceramics Division as a postdoctoral fellow in 1993 and became a staff member in 1994. His research interests involve the modeling of microstructural evolution during materials processing. He has developed and validated Monte Carlo–based simulation techniques for studying microstructural evolution during grain growth, recrystallization, Oswald Ripening, and solidification.

GORTI SARMA received his B.S. degree in mechanical engineering from the Indian Institute of Technology, Madras, and his Ph.D. degree in mechanical engineering from Cornell University in Ithaca, New York. He joined the Modeling and Simulation Group in ORNL's Metals and Ceramics Division as a postdoctoral research associate in September 1995. His main research interests are development of models to predict microstructural evolution during deformation processing, and application of the models to study problems in metal forming.

THOMAS ZACHARIA is director of ORNL's Computer Science and Mathematics Division and formerly leader of the Modeling and Simulation Group in the Metals and Ceramics Division. (For a more extensive biographical sketch, see p.107 in this issue.)

COMPUTATIONAL ENGINE MODELING

Osman Yaşar examines results of a computer simulation of a "cold-flow" experiment in which two pistons compress cold gas, slightly increasing its temperature in various regions. The study is part of a computational effort to design engines that use fuel more efficiently and produce lower emissions. *Photograph by Tom Cerniglio.*

By Osman Yaşar

The advent of massively parallel computers makes it possible to solve engine combustion problems in minutes, not months. ORNL has adapted the latest version of the KIVA engine simulation code for use on parallel computers. It should help American vehicle manufacturers design highly efficient and environmentally friendly cars more quickly.

American automakers must design more efficient, cleaner burning cars than ever, and quickly. The 1990 amendments to the Clean Air Act require a large reduction in pollutant emissions from U.S. cars and trucks by 2000, and the Comprehensive National Energy Policy Act of 1992 exerts pressure on vehicle manufacturers to improve fuel efficiency. At the same time, market competition demands a faster turnaround time than ever before for new vehicle designs.

Fortunately, American vehicle manufacturers are in a position to take advantage of new lightweight materials and better fuels, electronic controls, and ignition systems; and they have new tools to help them keep pace with government and market demands. One of these tools is computational engine modeling, in which manufacturers test new engine components on computers before creating expensive prototypes. Furthermore, the advent of massively parallel computers, such as ORNL's Intel Paragon XP/S 150, has now made it possible to solve car-crash and engine combustion problems in a reasonable time—in minutes and hours, not days and months.

Internal combustion engines, which power most vehicles, are extremely complex energy systems. An internal combustion engine burns fuel within a group of cylinders containing movable pistons; the gases formed in combustion push the pistons, which ultimately turn the car's wheels. The operation of these engines involves the coupled phenomena of combustion, turbulent fluid flow, turbulent flame propagation, radiative heat transfer, ignition and extinction, pollutant formation, and wall heat transfer—and in diesel and fuel injection engines, spray dynamics. Those phenomena are characterized by a number of different time and length scales.

Engine Simulation Codes Aid Efficiency

Because of the extreme computational demands, engine combustion modeling has been identified as a Grand Challenge problem (a complex, difficult problem that cannot be solved without the use of high-performance supercomputers). The goal of the modeling is to determine whether new designs will improve fuel efficiency and reduce emissions.

One of the most powerful multidimensional engine simulation codes is KIVA and its offshoots, KIVA-II and KIVA-3, which were developed by DOE's Los Alamos National Laboratory (LANL) originally for CRAY computers. The success of KIVA simulations has led to wide use of the code in the past decade, and it has been implemented on other platforms by various institutions. At ORNL we developed a scalable distributed-memory parallel version of KIVA-3 that is proving to be very useful.

One typical KIVA simulation of just one engine cycle takes about 30 hours on mainframe supercomputers such as the CRAY Y-MP system. A processing time this long is not acceptable to the engine industry. Many medium-sized companies do not even have access to such computers. They typically do all of their engine development using simplified, zero-dimensional tools on PCs or workstations. It is hoped that ORNL's parallel implementation of KIVA-3 on distributed-memory parallel computers or a cluster of workstations will reduce the time required for these simulations. Such parallelization would not only allow modelers to introduce more variables into their calculations to achieve higher grid resolution, but also provide them a scalability in performance and memory that is important to tackle large-scale, complex problems.

Involving a great deal of physics, KIVA analyzes coupled fluid dynamics, fuel spray dynamics, combustion and pollutant formation reactions, and heat transfer in an engine cylinder. It allows engine designers to see the effects of alterations to an engine's geometry without actually building the engine. The user can combine the results with a computer graphics package to visualize the combustion process. The user can see how the fuel-air mixture is initially ignited and how the flame grows from the initial ignition point, spreading throughout the combustion chamber. Predictions of nitrogen oxide levels or other hazardous emissions can be obtained for optimum engine conditions.

KIVA has been a subject of much research and constant improvement since its first release in 1985. Besides the work by KIVA's original authors, new submodels have been developed by other groups such as the Engine Research Center at the University of Wisconsin at Madison. Efforts are also under way at ORNL to add highly accurate spark-ignition, radiation heat transfer, and turbulence models.

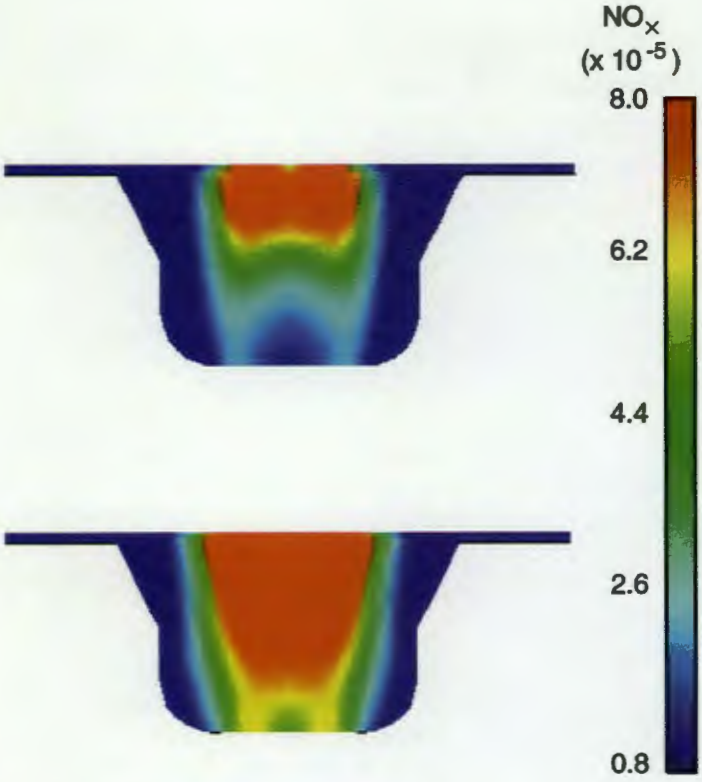


Fig. 1. Display of the effect of spark energy on the nitrogen oxide (NO_x) concentrations (g/cm^3) for a baseline engine after ignition. Higher spark-energy deposition leads to an increase in the NO_x level.

The latest version, KIVA-3, addresses the inadequacies of earlier versions. It uses a block-structured grid, allowing modeling of more complex geometries. It also handles both intake and exhaust flows, permitting the computations to proceed simultaneously in the intake and exhaust manifolds as well as in the engine cylinder itself, both when each component is in physical contact with the other and when the flow paths are closed off by valve and piston motion. Using this new version, scientists from national laboratories and the automotive industry have demonstrated good agreement between the computations and actual experimental data. Thus, the new version can help the auto industry design cars that deliver increased fuel efficiency and reduced emissions.

KIVA is helping to enhance the competitive position of the U.S. automotive industry. Practically every major automotive and engine manufacturer has requested a copy of the KIVA computer code. One of the biggest users of the KIVA model is General Motors (GM), which has been heavily involved in its development since the beginning. To our knowledge, other users of KIVA include not only engine manufacturers such as Cummins Engine, Ford, Chrysler, Caterpillar, and John Deere, but also companies that make and use utility boilers in which coal is burned. In the United States, coal currently supplies 56% of our electricity and 17% of our total energy needs. KIVA is being used for coal combustion modeling needed to develop the next generation of utility boilers.

Although the United States is a world leader in combustion technology, it is being challenged by aggressive new programs in Europe, Japan, and elsewhere. The health of the U.S. automotive industry is clearly critical to the overall economic health of the nation. The industry is faced with increasingly stringent emission and safety standards and strong overseas competition for its markets.

The international KIVA users group, which is headed by Rolf Reitz of the University of Wisconsin at Madison, holds its annual meetings in conjunction with annual meetings of the Society of Automative Engineers (SAE) Congress in Detroit.

To further strengthen the U.S. automotive industry's competitive position, there are ongoing cooperative research and development agreements to advance state-of-the-art computer modeling to complement the experimentation. Participants include national laboratories (including ORNL), universities, and major car companies such as General Motors, Chrysler, and Ford. The enhanced capabilities in computer modeling using massively parallel computers are expected to help in designing new products and bringing them to market more quickly. The availability of such industrially important software tools is an indicator of the success of the federal High Performance Computing Program.

Computer Tools for Emission Control

Developing better tools not only will help the auto industry improve fuel efficiency, but also will help it design engines with lower emissions of harmful by-products. During the past two decades, controlling emissions of nitrogen oxides (NO_x) has become an issue of national importance because NO_x contributes substantially to acid rain and photochemical smog. As a consequence, NO_x emissions present the most widely spread detrimental impact on air quality, vegetation, and human health of any regulated emission. Current technologies to control NO_x emissions either (1) modify the combustion zone in an effort to control the temperature, residence time, or stoichiometry, thereby lowering NO_x emissions, or (2) use a reducing agent

that reacts with the oxygen in the NO_x molecule after combustion, producing nitrogen and water.

Other solutions could be developed by carefully studying the effect of input parameters on the emission, and the KIVA model might be useful in doing that. It should be noted, however, that there might be technological difficulties in controlling some of the input parameters, such as the spark energy. A recent spark-control experiment at ORNL's Life Sciences Division (LSD) has been a source of new interest in using KIVA to study the effects of input spark energy characteristics on emissions (see Fig 1). Isidor Sauers and his colleague David Paul have recently been able to stabilize the spark breakdown voltage dramatically.

We are all familiar with a spark discharge. You've felt one jab your hand after walking across a carpet. A more dramatic example is a lightning strike, which occurs when voltages become so high that the air can no longer sustain them so it starts to conduct electricity. In an automobile engine, a spark from the spark plug causes the same effect in the air-fuel mixture. The high voltage (up to 20,000 volts) from the ignition coil, which is generated in a very short time (on the order of millionths of a second), causes the electrical breakdown of the gas. The by-products of the breakdown depend not only on the intrinsic gas properties but also on random events such as the location and concentration of charged particles in the gas.

In an engine the energy from the ignition coil is transferred to the air-fuel mixture through a spark. How that energy gets dissipated (e.g., current and duration of the spark) in the air-fuel mixture can significantly affect the combustion process. Incomplete combustion leads to undesirable by-products such as paraffins, olefins, aromatics, aldehydes, ketones, carboxylic acids, acetylene, ethylene, polycyclics, carbon monoxide, hydrogen, nitrous oxides, sulfurous oxides, lead oxides (from impurities), various oxidants, and soot. To study the evolution of by-products to assess the accuracy of computational models, it is important to control in a systematic way the breakdown voltage and, hence, the energy delivered by the ignition coil to the gas.

Until now, it had not been possible to study the breakdown characteristics systematically because the randomness of the breakdown process results in breakdown voltage values that vary widely from spark to spark. Thus, determining the relationship between the input energy characteristics and output emissions has not been a topic of research. A joint effort among ORNL's Center for Computational Sciences (CCS), Engineering Technology Division (ETD), and LSD is under way for improving KIVA-3 to probe this untapped field. This effort involves a close marriage of plasma physics and automotive engineering. Developing a new, highly accurate spark ignition model and validating it through experiments are among our primary goals. The experimental effort targets research engines employing the spark control mechanism developed earlier at ORNL.

The collaboration involving ETD (headed by Ron Graves), LSD (headed by I. Sauers), and CCS (headed by the author) is just one of the examples of ORNL's multidisciplinary efforts in high-performance computing and high-precision spark-plug and engine diagnostics. A collaboration with General Motors and Cummins Engine on spark ignition modeling is also under consideration. As ORNL's focal point for DOE's high-performance computing program, CCS offers industrial researchers a mechanism through its outreach component—Computational Center for Industrial Innovation (CCII)—for taking advantage of ORNL's modeling efforts on massively parallel computers.

Parallel Implementation of KIVA-3

KIVA-3 is a package consisting of the main code, a preprocessor, and a postprocessor. The preprocessor uses a block-structured mesh to discretize the physical domain and generates an input file for the main code. This input lists the grid point locations and the connectivity arrays that identify neighboring grids in all six directions. Each block is initially created independently using a tensor-product grid, but they are all patched together at the end with connectivity arrays describing the surrounding points for each mesh point. Because of connectivity information for each cell, the grid points do not have to be stored in any order in data arrays, making it possible to sort out the active and nonactive (ghost) cells and leading to shorter vector lengths in the computational loops.

The use of ghost cells, connectivity arrays, and cell-face boundary conditions in all directions creates a general recipe for physics, numerics, and boundary conditions that can be applied to a part of the domain as well as the whole domain, thereby providing for a convenient block-wise domain decomposition. In a block-wise distributed implementation, the ghost cells match the real cells of outer layers residing on other adjacent processors.

Spatial dependencies in the code extend only one layer in each direction and the presence of ghost cells and cell-face boundary arrays in the code is important in storing the neighborhood information that processors depend on. No dependency seems to be created through temporal differencing because variables are computed on the basis of

quantities from the previous iteration or time step. Spatial differencing requires estimating variables and sometimes their gradients (diffusion terms) on the cell faces, leading to communication between adjacent processors sharing the cell face in question. Momentum cells around the boundary vertices are split between processors, requiring each to compute only their share of the vertex momentum contribution. Advection of mass, momentum, and energy involves fluxing through regular and momentum cell faces. Cell-face values that are evaluated via upwind differencing require physical quantities and their derivatives on both sides of the face. Spray dynamics requires some communication, and nonuniform distribution of particles and combustion could lead to load-balancing problems for some problems. Particles that cross processor boundaries must be created or destroyed, depending on the direction in which they move. The grid points on the shared faces between processors must have the same structure for predictable communication patterns.

Parallel implementation of KIVA-3 is done on the Intel XP/S 150 Paragon at ORNL. Although KIVA-3 uses the native NX Message Passing Library, the communication interface is kept modular and easily portable to other communication packages such as PVM and MPI. High parallel efficiencies (90%) have been measured for a baseline engine test case. The baseline engine problem has been successfully run on up to 1024 processors on the Paragon without any major input/output or communication bottlenecks. Each processor uses multiple input/output files. The speedup on a large number of nodes depends on the problem size, so it is necessary to keep the 100 grid-points/processor ratio of divisional work to operate on a high parallel efficiency. Though our tests so far involve relatively small problems, an advantage of the distributed-memory implementation would be the ability to run large problems. Solving a problem requiring 6 gigabytes of memory (millions of mesh points) is certainly feasible on our 1024-node Paragon, and our future work will attempt to demonstrate that.

Conclusion

Recommendations to develop advanced predictive capabilities for combustion and emission processes have come from recent workshops on the design of next-generation vehicles and environmentally responsive technologies. The available simulation software has been limited in its ability to represent the detailed physical processes and the complex geometries of engines and other industrial combustion systems. Trends such as increasing fuel economy and lowering emissions often conflict, so a balance must be achieved through careful optimization. Designers must address various parameters (i.e., piston bowl geometry, swirl, fuel injection pressure and rate, nozzle geometry, number of nozzles, compression ratio, spark ignition time and energy) to arrive at an optimized engine design that meets their targets.

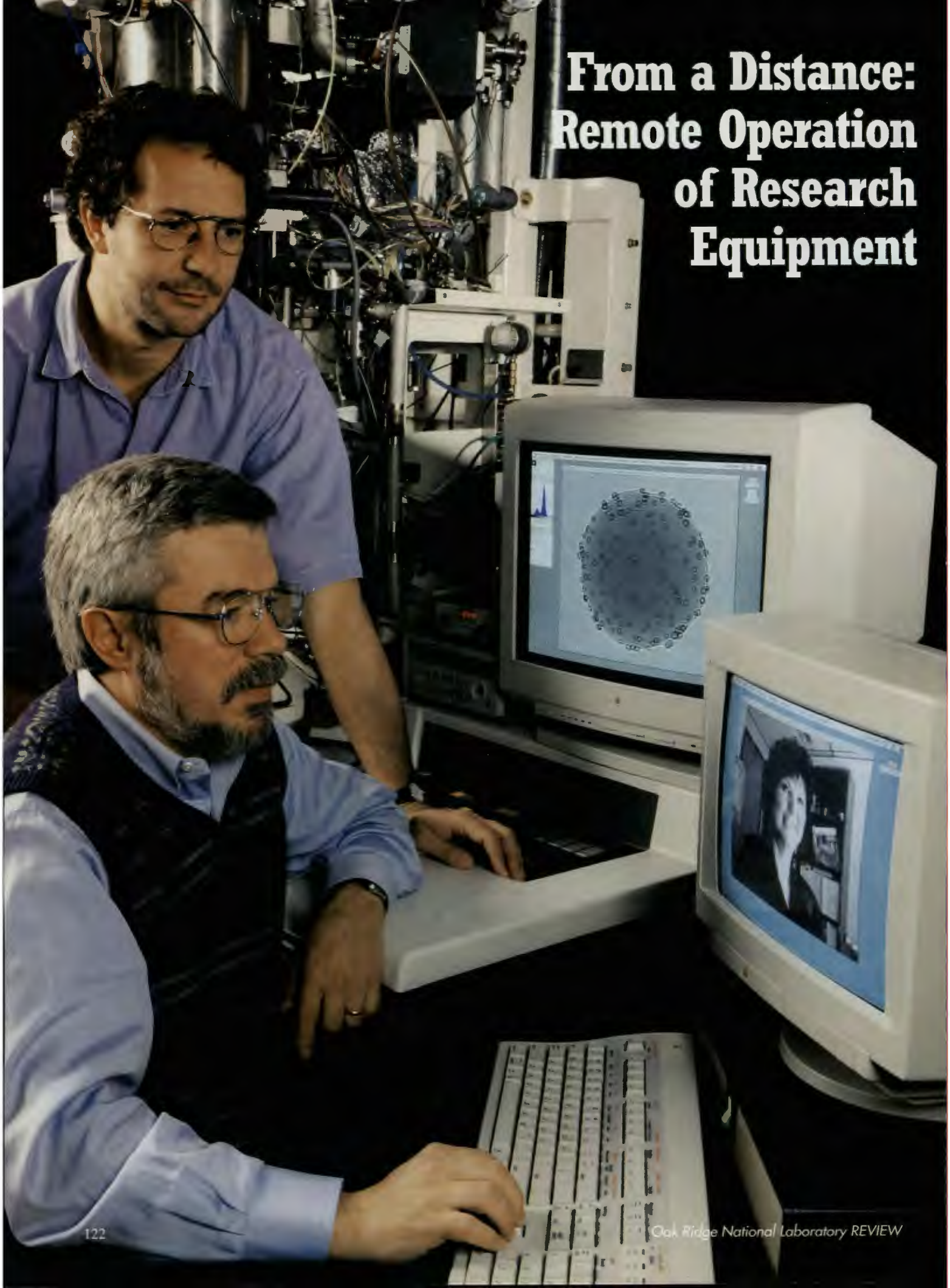
Computational models not only provide tools for such a design study, but also might lead to a better understanding of the physics of engine combustion. New insights into the physical processes might lead to new ways of dealing with them. Our large-scale computational capabilities, based on a parallel implementation of KIVA-3 on a scalable system such as the Intel XP/S 150 Paragon, are expected to create a testbed for industrial optimization studies. As a result, more efficient and environmentally friendly automobiles may be designed and brought to market more quickly. ornl

Isidor Sauers (standing) and David Paul examine results of a spark control experiment they developed at ORNL. They were able to stabilize the spark breakdown dramatically, opening new possibilities to lower emissions and engine cyclic variations.

BIOGRAPHICAL SKETCH

OSMAN YAŞAR is a staff scientist at ORNL's Center for Computational Sciences and an adjunct associate professor at the Applied Mathematics Department of the State University of New York at Stony Brook. Before he joined the ORNL staff in 1994, he worked as a research staff member and a manager for the Parallel Computing Laboratory at the University of Wisconsin—Madison, where he earned his M.S. degrees in nuclear engineering and computer science and his Ph.D. degree in engineering physics. He also has taught at Inonu University and Hacettepe University (his alma mater) in Turkey. His areas of expertise are parallel computing, computational fluid and particle dynamics, engine combustion modeling, spark ignition, plasma and radiation hydrodynamics, and adaptive mesh refinement. He has served as publication manager, conference chair, vice chair, and general chairman of the international Intel Supercomputer User's Group (ISUG), and is currently the advisory chair of ISUG. He is the founder and chairman of the international High-Performance Computing Users (HPCU) Group, a guest editor of the *Journal of Computers and Mathematics with Applications*, chief editor of the web-based *Journal of High-Performance Computing Users*, and an organizer of the High-Performance Computing Simulation conference. His Web site is at *http://www.ccs.ornl.gov/staff/yasar/yasar.html*.

From a Distance: Remote Operation of Research Equipment



By Carolyn Krause

ORNL has received DOE 2000 funding to conduct experiments involving collaboration by electronic means among geographically separated researchers, including the remote operation of research equipment, such as electron microscopes and neutron diffractometers at a research reactor. This equipment can be operated over the Internet by researchers at other facilities, thus bringing the user facility to the user. The collaboration also includes researchers at LBNL, ANL, NIST, the University of Illinois, and industry. To help scientists share and record their observations over the Internet, ORNL has also received funding to continue its development of electronic notebooks.

In an era of shrinking research funds but rising demand for rapid research results, managers in the DOE system face several problems.

- How can research and development be done more efficiently, safely, and productively?
- How can scientists at DOE's national laboratories collaborate more effectively with each other and with researchers in industry and academia to solve DOE's complex scientific problems?
- How can access to DOE resources be increased for both DOE's personnel and its R&D partners, even when travel budgets have shrunk?
- How can institutional barriers to research be lowered or eliminated?

DOE believes that many of these challenges can be met if scientific research involving dispersed but interacting collaborators can be done—from a distance.

Enhanced R&D collaborations are thought to be achievable through use and development of new computational, communication, and distributed computing technologies that connect researchers across the nation, even around the world. The Internet is the best known vehicle of computer connectivity that gives people access to various computer technologies. The DOE philosophy was published in late 1996 in a document entitled *Department of Energy DOE 2000 Initiative*. DOE's objectives are to conduct research, promote the development of new computing technologies for simulations of experiments, and establish two or three "collaboratory" pilot projects. A collaboratory is defined as "an open laboratory spanning multiple geographical areas where collaborators interact via electronic means—'working together apart.' " It's a virtual place in cyberspace that enables researchers to collaborate and even conduct experiments remotely. According to the DOE document, the "vision for the collaboratory projects is to develop and demonstrate within three to five years the tools that allow remote workers and facilities to be electronically linked so closely that it is 'better than being there.' "

Researchers at ORNL, particularly C. E. (Tommy) Thomas of the Instrumentation and Controls Division, have helped shape DOE thinking about remote operation of research equipment by world-class scientists using the Internet's World Wide Web. Thomas was on assignment in 1996 to assist with the National Collaboratories / Virtual Laboratory project (Distributed Collaborative Environments and Facilities Online), sponsored by DOE's Office of Energy Research, Office of Computational and Technology Research, Mathematical, Information, and Computational Sciences Division.

According to David B. Nelson, DOE's associate director of Energy Research for Computational and Technology Research, "The goals of the DOE 2000 initiative are to develop and demonstrate collaborative tools that will help integrate R&D program activities, introduce new paradigms for the remote use of DOE science facilities, and accelerate the development of new communication, computational, and distributed computing capabilities to enhance R&D collaborations." To help meet DOE's vision of what its laboratories should be doing after 2000, DOE's Mathematical, Information, and Computational Sciences Division funds winning proposals for R&D partnerships for pilot applications of collaboratory technologies.

In March 1997, ORNL received $850,000 in DOE 2000 funding to begin work on four projects. Four ORNL electron microscopes are now among nearly a dozen microscopes at DOE facilities that will be remotely

Larry Allard (seated) and Edgar Voelkl demonstrate the remote operation of an electron microscope. *Photograph by Tom Cerniglio.*

operated as part of the new Materials MicroCharacterization Collaboratory pilot project supported by the DOE 2000 initiative. The other ORNL project receiving DOE 2000 initiative funding is the development of electronic notebooks (see sidebar on p. 129).

DOE's approach in FY 1997 is to provide $8.5 million for three project areas: Advanced Computational Testing and Simulation (ACTS), Technology R&D Projects, and National Collaboratories (including secure online facilities, infrastructure and tool research and development, and collaboratory pilot projects). ACTS might include large computer simulations of airline explosions; nuclear weapons for "science-based stockpile stewardship"; and environmentally hazardous plumes in air, surface water, geological layers, and groundwater. Many of these simulations would deal with scenarios for which experimental data will never be available. However, for researchers to receive funding for such simulation work, the software they develop for a specific simulation must be generic and reusable by the scientific community for other types of computational problems. ORNL's Computational Center for Industrial Innovation may receive funding for such activities.

Secure online facilities is another area for which ORNL is well positioned. At a DOE conference in March 1996 in Reston, Virginia, two demonstrations of online facilities were presented to Secretary of Energy Hazel O'Leary and conferees. The presenters were researchers from Argonne National Laboratory (ANL) and ORNL. Larry Allard, Ted Nolan, and Edgar Voelkl, all of ORNL's Metals and Ceramics Division, showed that an expensive electron microscope at ORNL's High Temperature Materials Laboratory (HTML) can be operated remotely from Reston. O'Leary saw the magnified image of the sample on the computer screen and watched as Allard tapped a key to change the magnification and position of the sample. (See section below for details on remote operation of the microscope and other ORNL instruments.) Although they were not presented to Secretary O'Leary, ORNL's Online Harsh Environment Laboratory and Remote Experimental Environment for Fusion Experiments (described later in this article) also were demonstrated at Reston.

After the conference, an ORNL group formed the Secure Online Facilities (SOFA) committee, chaired by Michael Wright, a nuclear physicist in the Instrumentation and Controls Division. The committee consists of more than 30 ORNL staff members from 10 divisions. The committee meets biweekly to foster cooperation among researchers, develop skills and ideas, and prepare joint proposals for funding.

"One reason ORNL got DOE's attention in Reston is that we pitch low-cost tools for online facilities," Wright says. "We have shown that you can remotely operate an electron microscope or a harsh environment laboratory using commonly used hardware, such as a personal computer with browser software and an Internet connection; inexpensive hardware, such as small cameras that cost less than $100 apiece; and inexpensive or free software for video, audio, and computer control. We are looking for recipes—the right combinations of hardware and software that produce an illusion of presence and control in a remote area. Of course, the tools are primitive, so we are not yet ready for prime time. But, we have demonstrated that these tools, once refined, offer the potential of giving the user the feeling of being there."

Because the World Wide Web is so accessible and easy to use, Wright says that ORNL researchers are writing special software (e.g., Java applets) so that remote operation of research equipment can be Web-based. For example, Java applets (miniprograms written in the Java programming language developed by Sun Microsystems) are being written to simulate pushbuttons on a microscope or in a control room; all the user has to do is click on a button to change the microscope's focus or to alter the angle at which a sample is placed in a neutron beam from a reactor. Other applets can be used to plot data.

One of the jobs of the SOFA committee is to get experimental devices hooked up to the Web. An equally important job of the committee is to ensure that these online facilities are secure.

"Security of online facilities is the number one concern for the DOE 2000 managers," Wright says. "Computers linked through the Internet are vulnerable. For example, someone could attack your computer by flooding it with invalid e-mail messages. Your user name and password alone do not guarantee that your computer is protected from attack. Hackers can sniff out passwords. So, the password should be encrypted so that only a specific code, or key, can restore the original data, or decrypt the message. More sophisticated security measures, such as public key encryption, digital signatures, and certificates, may be needed. Encrypted passwords will be needed to ensure that only authenticated users use online facilities."

For online facilities, in FY 1997 DOE spent $3 million for computing infrastructure—building a high-speed network and developing application programming interfaces so that generic programs can interact with each other and with the operating systems of different types of computers.

Also in FY '97, DOE spent another $3 million for collaboratory pilot

projects. Funding for subsequent years is expected to equal or exceed these amounts. The collaboratory projects are expected to involve geographically separated personnel and facilities and to address a problem of national significance related to DOE's missions in energy resources and technology, environmental science and technology, and national security. Such studies will include demonstrations similar to the following ones performed in 1996 at ORNL.

At a press conference in March 1997 in Washington, Martha Krebs, director of DOE's Office of Energy Research, announced DOE 2000 support for the Materials Micro-characterization Collaboratory (MMC) pilot project. In the materials collaboratory, ORNL researchers will be working with researchers from ANL, Lawrence Berkeley National Laboratory, and the DOE-funded microscopy center at the University of Illinois at Urbana—Champaign. Contributing partners in the research will be the National Institute of Standards and Technology (NIST) and six manufacturers of microscopes and control systems: Philips, JEOL, Hitachi, R. J. Lee, Gaton, Inc., and Emispec. This 3-year, $11-million effort includes matching funds from DOE Energy Research's Basic Energy Sciences, Division of Materials Sciences and from DOE Energy Efficiency's Office of Transportation Technologies, Office of Heavy Vehicle Technologies, as well as in-kind contributions from NIST and industry.

ORNL facilities and principal investigators involved in the first year of the collaboratory are electron microscopes in ORNL's SHaRE program (Kathi Alexander) and at HTML (Allard, Voekl, and Nolan), the Neutron Residual Stress Facility at the High Flux Isotope Reactor, or HFIR (Wright and Cam Hubbard), and ORNL-supported X-ray beam lines at the Advanced Photon Source at ANL and the National Synchrotron Light Source at DOE's Brookhaven National Laboratory (Gene Ice). Additional ORNL facilities will be included in later years.

Thanks to DOE 2000 funding, four ORNL electron microscopes will be available to authorized outside users through the Internet. They are the Phillips CM 200F field emission transmission electron microscope, the Phillips XL30 scanning electron microscope (both in Building 5500), the Hitachi S-4500 scanning electron microscope, and the Hitachi HF-2000 cold-field emission transmission electron microscope (both in HTML).

The collaborators will try to make these user facilities more user-friendly. They will automate routine functions as much as possible and provide an easy, effective mouse-driven user interface. They will also add features to ensure data security and keep unauthorized users off the system.

Collaborative research projects among scientists at the participating laboratories will concentrate on critical problems involving surfaces and interfaces, which are important in controlling the behavior of advanced materials. Specific microscope research will focus on catalysts used to control emissions from automobiles and diesel trucks as well as interfaces between substrates and the coatings designed to protect them against corrosion.

Ed Oliver, associate director for Computing, Robotics, and Education at ORNL, says, "Collaboratories would make expensive facilities like the electron microscopes in HTML much more usable and much more productive. Our massively parallel computers run 24 hours a day. We would like for the tools in the user facilities to be that busy, too. That's why ORNL projects for remote operation software development are being supported by our Laboratory Directed Research and Development Fund. By making it possible for a researcher far away to use some of these tools remotely, we can greatly enhance our user facilities' practicality and affordability and possibly have them working around the clock, too. It's more bang for the buck."

REAL-LIFE SCENARIOS AT ORNL

A Million-Dollar Microscope

Larry Allard sits beside a sophisticated and unusually powerful electron microscope at HTML. The microscope, one of the few such instruments in the world, brings up on a computer screen a clear digital image of a sample of fullerene carbon material, magnified 400,000 times. Suddenly, the magnification and angle of the sample in the microscope's electron beam change. However, neither Allard nor anyone else in the room is at the controls. A colleague, Edgar Voelkl, is adjusting the instrument from San Diego, California—far away from the Tennessee laboratory.

Three years ago, Voelkl wrote the software to operate HTML's Hitachi HF-2000 field-emission transmission electron microscope from a computer keyboard. The software also allows automated processing of images of magnified samples captured by charge-coupled device (CCD) cameras instead of film.

In 1995, a $200 commercial software package from Farallon called TimbuktuPRO became available. A user who has TimbuktuPRO on his computer can remotely control a distant computer, such as the one controlling a research instrument. This

remote operation program enables researchers to run the $1.6-million microscope by computer remotely through the Internet. Any researcher with this software, an appropriate personal computer, an Internet link, and proper authentication can operate the ORNL microscope from practically anywhere.

Though hundreds of miles apart, Voelkl and Allard can see each other because, on the top of each computer is a $90 Connectix QuickCam camera. Through the "telepresence" mode, they can talk to each other much like scattered participants in a teleconference who "see" each other on a computer screen as they converse, using speakerphones or computer sound cards for voice contact. Operators can also send electronic messages instantaneously via keyboard using "flash" mail.

The microscope is controlled by Farallon's TimbuktuPRO remote operation software. On his remote computer screen Voelkl can see the local microscope and the image of the magnified sample. By pressing computer keys, he can control the microscope focus and the sample position and magnification, and he can scan the sample with the electron beam. A user can then remotely operate the microscope with the mouse by clicking on an appropriate screen button that changes the microscope's focus or sample position or sample magnification.

Once the user sees the digital image of the sample on the screen, he can download it and save it on his own computer, as well as on the file servers in HTML. Collaborating scientists who are authorized to access the file servers can view the image and discuss the results over the Internet. Such remote control of the ORNL microscope has been demonstrated by ORNL researchers in Washington, D.C.; Nashville; and Detroit, where participants at Focus Hope (which puts unemployed people to work making parts for automobiles and diesel trucks) also operated the electron microscope during a Partnership for a New Generation of Vehicles demonstration in March 1996 at ORNL. In November 1996, students in an electron microscopy class at Lehigh University in Pennsylvania operated the ORNL microscope remotely and had live audio and video contact with their ORNL collaborator using teleconferencing tools. In the future, Voelkl says, his group will write software to allow the microscope to be controlled over the World Wide Web. Al Geist of ORNL's Computer Science and Mathematics Division is writing Java applets that generate an array of icons, or pushbuttons, on the computer screen. These controls will be linked to real controls on the microscope, and images will be returned to the remote user in the form of Web pages.

Because user facilities like HTML allow visiting researchers from U.S. industries and universities to take advantage of ORNL's expensive, state-of-the-art equipment, such a remote operation capability opens up tremendous possibilities. A scientist in another city could simply send a sample to ORNL and analyze it on a million-dollar microscope without ever leaving the office. This strategy reduces researcher time, travel costs, and the need to give users training in using the microscope. Remote operation brings the user facility to the user.

Remotely Operated Reactor Instrument

Until recently, a scientist who wanted to conduct an experiment on a research reactor had to undergo safety training and risk exposure to low-level radiation. Now, widely scattered scientists can remotely measure the angles and intensities at which reactor neutrons are scattered from a target material to determine its structure. These scientists can do a neutron-scattering experiment at a research reactor without being there.

Thanks to the Web Virtual Laboratory (WeVL) project at ORNL, scientists will remotely monitor and control the DIXIE double-crystal small-angle neutron-scattering spectrometer at ORNL's HFIR, which is a DOE user facility. The WeVL, or Web interface for a small-angle neutron-scattering experiment at ORNL, was developed by Royce Sayer and Richard Ward of the Computational Physics and Engineering Division; Mohana Yethiraj of the Solid State Division; A. S. (Buddy) Bland of the Center for Computational Sciences; and Al Geist.

If you are a scientist authorized to access the WeVL home page on the Web, you will first see the title, "Welcome to the DIXIE Virtual Laboratory." Then at the top right corner you will see a photograph of the spectrometer. The home page offers you a chance to click on icons so you can remotely select a crystalline sample to place in the neutron beam, remotely control the angular range of the neutron detector (which measures neutron intensities at different angles), and select the intervals at which the neutrons scattered from the sample are counted.

Sitting at your computer at work, you remotely maneuver the crystal in the neutron spectrometer, positioning it at a specific angle with respect to the incoming neutron beam. You get video display of the apparatus, so you can see it and the sample move as you control them with the mouse. You wait for new results to appear on the screen. Soon the data—the numbers of neutrons that are scattered at a variety of angles—are displayed in tabular

Mohana Yethiraj checks a small-angle neutron scattering spectrometer that will be operated remotely for neutron science experiments at ORNL's High Flux Isotope Reactor.

and graphical form. The number of neutrons is plotted against each angle at which neutrons are scattered when the neutron beam struck the target.

You go home at 6:00 p.m. to eat dinner with your family. By 11:00 p.m., you want to know whether the crystal and detector are properly positioned to produce good data. So you turn on your computer and camera system and log in. A video display of the apparatus shows that the detector is aligned at a good angle. You view the graphical display of the data. You check the "electronic notebook" (see sidebar on p. 129) to see the comments of other researchers viewing the data and analyzing data plots. All this gives you a warm feeling.

The ORNL researchers started the project using LabVIEW, a commercial software package that was installed for instrument control, monitoring, and data analysis. LabVIEW stores data and plots neutron counts for each scattering angle to provide information on the structure of a crystal in the neutron beam.

The researchers then set up a user interface between LabVIEW and ORNL's Web server because the Netscape Navigator browser works with LabVIEW. They then implemented the prototype Web user interface and tested it with the hardware. Finally, they set it up for facility security so only authorized researchers (with approved user names and passwords) could access the HFIR instrument through the WeVL home page.

DOE officials say that WeVL is needed to increase use of the HFIR beams and facility, expand the user community, reduce travel costs, encourage multi-institutional collaborations, and minimize low-level radiation exposure (some scientists don't want to be exposed to any radiation from reactors). The DIXIE experiment was chosen for the pilot project because the neutron count rates are low, the chance of damage to hardware through remote control is minimal, and data sets are small (limited to detector angle, number of neutrons counted, time, monitor counts).

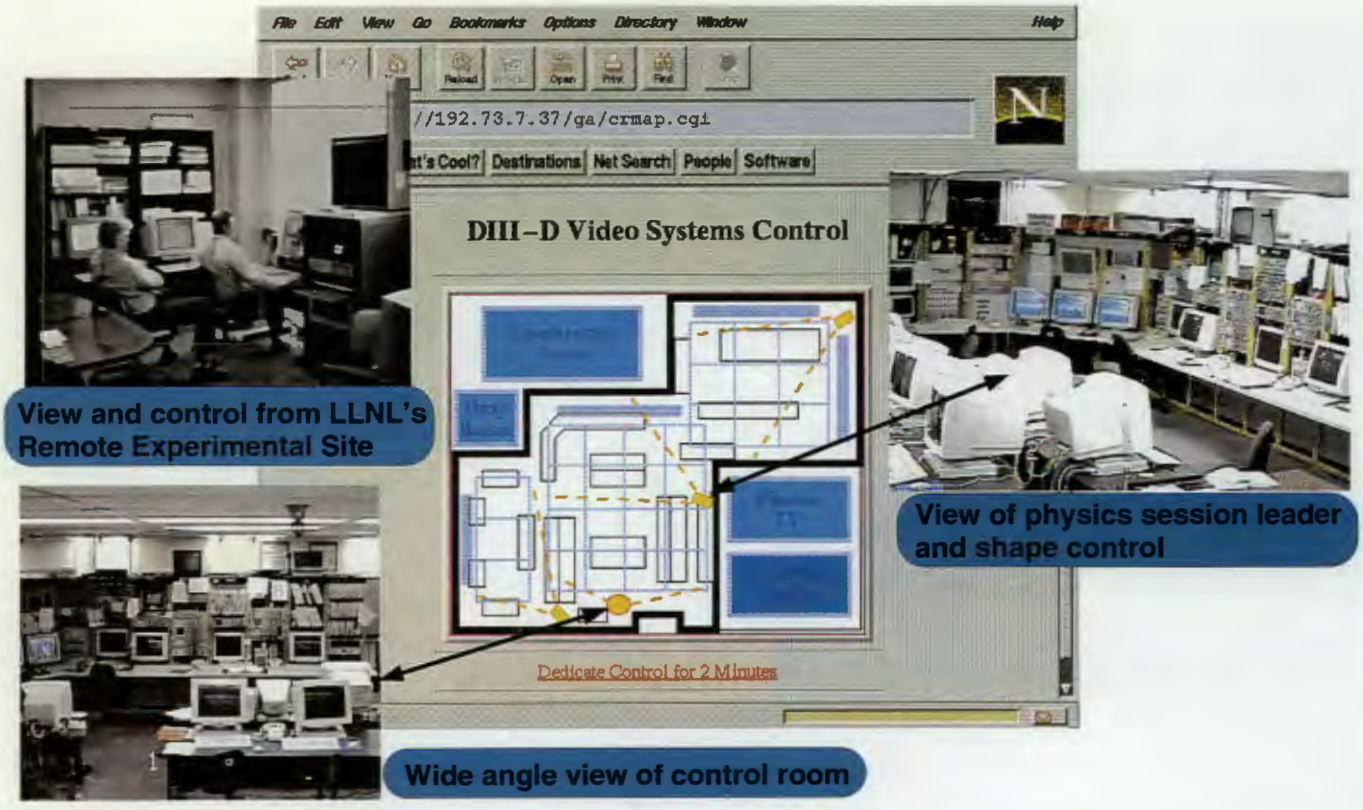
Remotely controlled experiments will be carried out at HFIR in 1998, thanks to DOE 2000 funding. The first experiments will be similar to the ones performed in 1996 by Cam Hubbard, a researcher in the Metals and Ceramics Division, who monitored and controlled a neutron-scattering instrument at HFIR from his office 3 miles away in HTML. Hubbard and Wright have adapted the HFIR facility for remotely operated residual stress studies, and such experiments are expected to be carried out in 1998 by researchers at facilities outside Oak Ridge.

Remote Participation in Fusion Experiments

What makes you feel like you're there even though you're not? It's "telepresence," a term that may soon become common in our vocabulary.

David Greenwood of Information Technology Services, Lockheed Martin Energy Systems, has experience with a crude telepresence arrangement that "sort of gives you the feeling of presence in the control room of an experimental fusion device." The project is called the Remote Experimental Environment for Fusion Experiments.

Greenwood, who has worked with ORNL's Fusion Energy Division for 19 years, interacts with fusion researchers at ORNL, Princeton Plasma Physics Laboratory, Lawrence Livermore National Laboratory, and General Atomics, which operates the DIII-D



Controllable view of the control room of the experimental DIII-D fusion device seen remotely through a World Wide Web site. Users in Oak Ridge and Livermore, California, can observe and control actions at the San Diego fusion device.

tokamak for fusion energy research. Some of these researchers are located at the previously mentioned labs and others are working on an experiment at the San Diego tokamak, but all the researchers involved in the experiment can interact with and view operations in the tokamak control room.

"We started out with a Web home page so we could review our scientific proposals, read reports, and archive all our mail," Greenwood said. "Then we decided we'd like to participate in remote planning meetings and watch experiments in progress. We also wanted to know if an experiment was active or if our fellow researchers had gone to lunch."

Four cameras were set up in the DIII-D control room and one camera was placed in the conference room. Microphones were also set up in these areas. MBONE (a free software) was installed for audio and video monitoring. The name stands for "multicast backbone." Electronic mail is an example of unicasting—the message travels point to point, from computer to computer. In multicasting, the message is sent out to everybody, and those who want it reach out and receive it.

White Pine's CU-SeeMe software (originated at Cornell University), which, like MBONE, provides audio and video monitoring, was also installed so that remote participants could use whichever software was more convenient. Java applets were developed by Princeton for the Web page so that the movable camera in the control room could be controlled remotely by clicking on buttons on the computer screen. The home page for the fusion researchers features a photograph of the DIII-D control room and a map showing the location of cameras as part of the video system control.

"To avoid having multiple users try to move the camera at the same time, Greenwood said, "we decided to schedule camera control according to who is doing the experiment that day. If Princeton is doing the experiment, Princeton gets to control the camera. If Oak Ridge is running the experiment, the camera is controlled by Oak Ridge."

In a recent talk, Greenwood discussed the sociological aspects, or human factors, of telepresence. "There are some problems with our early

Electronic Notebooks for Scientists

Scientists traditionally use paper notebooks to keep track of their ideas for experiments and notes on experimental setups, observations, and research results. These notebooks are kept on bookshelves or in file cabinets.

Is there a more efficient alternative in the age of computers and the Internet? Why manually copy documentation into a paper notebook when you can cut and paste it electronically and later do searches to quickly find a special entry?

ORNL's Al Geist recommends the recordkeeping tool of the imminent future—the electronic notebook. A notebook accessed by computer offers scientists all the features of the traditional paper notebook, along with the capability to accept multimedia input (audio and video clips) and computer-generated images, tables, and graphs placed by drag-and-drop.

Geist and Noel Nachtigal, researchers in ORNL's Computer Science and Mathematics Division, have developed a prototype for an electronic notebook that is being used by a dozen different groups around the country (and further development of the prototype is continuing in 1998, thanks to DOE 2000 funds earmarked for Collaboration Technology R&D projects). It is particularly useful for collaborating scientists involved in remote operation of research equipment for conducting experiments.

"Right now," Geist says, "the biggest obstacle is the legal acceptance of the electronic notebook. Once this happens, electronic notebooks will soar in popularity—not only for collaborating groups but also for private users."

An electronic notebook is a repository for objects that document scientific research. It can be used to enter, retrieve, or query objects such as text, sketches, images, tables, and graphs. "Electronic notebooks are not calculators, nor are they chat spaces," Geist explains. "They hold a static record of ideas, experiments, and results."

Electronic notebooks have many advantages over paper notebooks. "They can be shared by researchers, even those collaborators separated by distance," Geist says. "They can be accessed remotely through the Internet. They can't be lost or destroyed. It is easy to incorporate not only computer files and experimental data but also multimedia into an electronic notebook. It can easily be searched for information. It can contain hyperlinks to other information, such as a reference paper stored elsewhere on the Internet."

ORNL is collaborating with researchers from DOE's Lawrence Berkeley National Laboratory and Pacific Northwest National Laboratory (PNNL) to design a common notebook architecture that will allow interoperation of the different groups' notebooks.

"What that means," Geist explains, "is that I could use ORNL's notebook interface to view entries that were written by my friend at PNNL using his own notebook. Also, we could share input tools we each develop."

A demonstration version of ORNL's notebook is available on the Internet's World Wide Web (*http://www.epm.ornl.gov/~geist/java/applets/enote/*). It can be accessed by any authorized user from any type of computer (platform) that has a Web browser.

In developing the Web-based electronic notebook architecture, the ORNL researchers are focusing on ensuring the security of the notebook. Electronic notebook entries can be digitally authenticated and signed, individually or collectively. They can be electronically time-stamped and notarized. While entries cannot be modified once signed, the pages can be annotated and forward-referenced. Entries can be secured by encryption, both in transit and in storage. All these securities can be performed transparently to the users, thus adding no complexity to the user interface.

The research was initially supported by ORNL's internal Laboratory Directed Research and Development Program. Funding now comes from DOE's Mathematical, Information, and Computational Sciences Division.

The ORNL prototype uses Common Gateway Interface scripts to access notebook pages. The researchers are developing Java applets to enter objects in the notebook, such as a pen-based sketch pad. Of course, their ideas for making improvements and their progress on this project are recorded in their electronic notebooks.

Al Geist demonstrates the electronic notebook for Vice President Al Gore during his recent visit to ORNL. Photograph by Tom Cerniglio.

attempts at telepresence," he said. "The vocabulary differs among sites, especially with foreigners involved in our international experiments. Time differences can be a problem; some collaborators may want to sleep when others want to meet online to discuss an aspect of the experiment. We found that DIII-D operators were initially uncomfortable with the cameras and microphones in the control room. Even though time conflicts and other issues will always be present, many other problems are being reduced as people become more familiar with the technologies and embrace the need to improve communications.

"Although collaborators are encouraged to work more together, there is still stiff competition among them, making them resistant to sharing information. However, one surprising thing has come out of this experimental telepresence arrangement. The pressure to improve communication between groups actually improved communication within groups."

Greenwood said that Livermore and MIT have used MBONE to control fusion experiments and that Princeton has posted information on sessions of fusion meetings. "It's difficult now to see viewgraphs on MBONE," he noted, "but that will change as people learn to make viewgraphs that are visible on this medium." It's also difficult to recognize some people on the computer screen using CU-SeeMe because they are shown in black and white. But this problem may be solved, Greenwood said, by the color version of CU-SeeMe.

To make telepresence more user-friendly, Al Geist is developing Java applets and electronic notebooks (see sidebar) to improve interactions among the dispersed researchers.

The Remote Experimental Environment for Fusion Experiments project recently received national recognition. The project was selected as one of the 60 finalists in the 1996 National Information Infrastructure Awards program, chosen from a field of more than 850 nominees. The project was a finalist in the Next Generation Award category. The awards program seeks to recognize the nation's most creative and beneficial uses of communication technologies in 10 different categories that touch on all areas of America's work, play, and community life.

Online Harsh Environment Laboratory

ORNL has a test bed that simulates a harsh industrial environment. It's not the type of bed you'd want to lie on; in fact, while you might want to know what's going on in the test bed, you'd prefer to be far away from the action.

The test bed has steam vents that can produce up to 100% humidity and a temperature of 500°F. The conditions in the bed are measured by a humidity sensor, a hydrogen sensor, a pH monitor, carbon dioxide and carbon monoxide monitors, and thermocouples. These data are relayed electronically to a computer loaded with LabVIEW software, which provides video control and real-time data acquisition.

Users can have Internet-based remote access to data acquisition and control of the test bed, as well as real-time video and video conferencing. They can remotely control the experimental setup and parameters and view the control parameters, data, and graphs plotted from the data on the computer screen.

"The client requests data from our server when needed," says William Holmes, an engineer in ORNL's Instrumentation and Controls Division. "The first one to ask for control of the facility gets it. Those who ask later are denied. That way we don't have two different people trying to control it at the same time."

ORNL's test bed is a test case for Michael Wright's SOFA Committee. It shows that low-cost computer tools can create a secure online harsh environment laboratory. It was also the first secure online facility to have an outside user. Recently, a researcher from the Electric Power Research Institute in California viewed data from a hydrogen sensor at the test bed.

Besides LabVIEW, the tools used for the test bed include Farallon's TimbuktuPRO remote operation software, an ISDN link or a 28.8-kilobaud modem, video cameras, and White Pine's color-enhanced CU-SeeMe (color, chat box, white board), which makes possible teleconferencing. Remote control, data acquisition, and video conferencing can be accomplished using either an Internet link, an ISDN link, or a 28.8-kilobaud modem over a standard telephone line. Thanks to these tools, you can grasp the situation without actually being there. And someday, improved tools should make you feel as if you are really there even though you aren't.

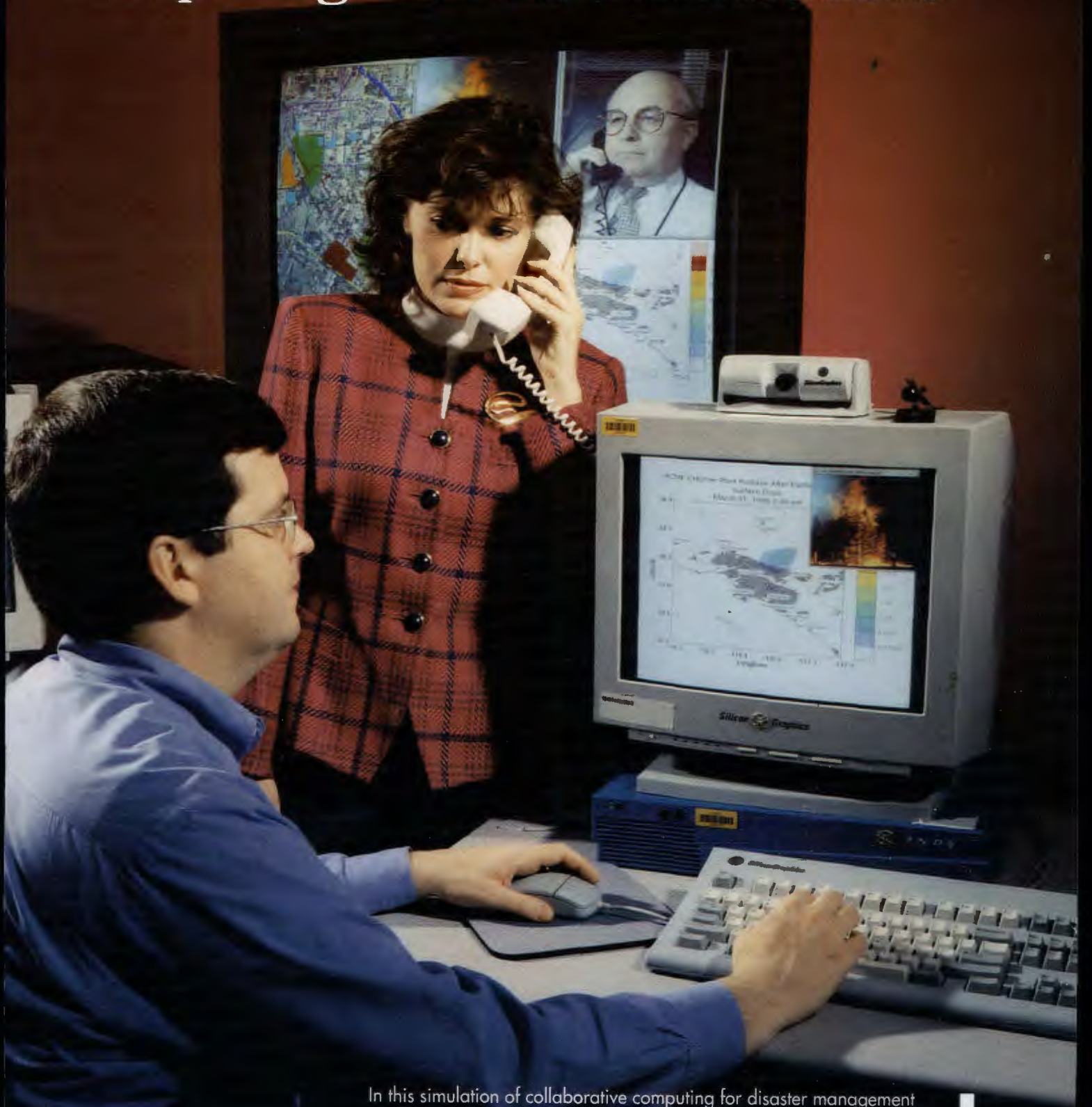
"We're pitching our ideas for improving these tools to other potential sponsors as well as DOE," Wright says. "With enough research and development work, remote control of research equipment should be ready for prime time." ornl

Carolyn Krause is editor of the *Oak Ridge National Laboratory Review*.

CORRECTION

In the article "Breast Cancer Treatment Proposed" on pp. 24-25 in the Vol. 30, Nos. 1&2, 1997 issue of the *Review*, it was incorrectly stated that ORNL licensed the technology described to a local company, Photogen Inc. In fact, Photogen Inc. owns this technology subject only to a license to DOE.

Crisis Management and Collaborative Computing: ORNL's Contributions



In this simulation of collaborative computing for disaster management involving a chemical plume, John Cobb checks the information on the computer screen while Kimberly Barnes confers by phone with Ed Oliver (ORNL's associate director for Computing, Robotics, and Education), seen on upper right of big screen. *Photograph by Tom Cerniglio.*

By Kimberly Barnes, John Cobb, and Nenad Ivezic

ORNL researchers have been combining software engineering, computational science, and collaborative technologies to respond to many domains such as enterprise management, disaster management, education, banking and finance, and engineering design and manufacturing. Collaborative technology environments will provide rapid, on-demand interoperability of autonomous legacy applications and tools within new and evolving environments.

A scenario of the near future: In the middle of the night, an earthquake of magnitude 7.1 on the Richter scale violently shakes the ground and buildings near a large metropolitan area. A few people are killed, some property is damaged, water and gas pipes are broken, and power and phone lines are down. However, public safety is threatened most by events following the quake. Because of leaking gas from severed lines, fire breaks out in parts of the city center, and the conflagration grows because of the lack of water for firefighting. At the same time, a toxic plume is spreading from a badly damaged chemical plant. At least 350,000 people living within 5 miles of the plant worry that their homes and even their lives may be endangered by the plume.

Nenad Ivezic, developer of the Rapid Integration for Disaster Management collaborative information system, is shown in his office.

The situation is critical. Crisis management efforts in the first few hours after the quake will determine the total extent of losses. The toll may be as high as 5,000 dead, 20,000 injured, 100,000 homeless, and $35 billion worth of damage. However, optimal crisis management strategies may be able to reduce it to as low as 15 dead, 250 injured, and $500 million worth of damage. Critical decisions must be made fast. Where will the dangerous plumes drift? Where is the fire danger greatest? Which neighborhoods should be evacuated? How will emergency crews be alerted? Where will fire and police personnel be deployed? How will risks to safety be communicated to the public at large?

Fortunately for this stricken area, the Rapid Integration for Disaster Management (RAPID-DM) collaborative information system developed by Nenad Ivezic of ORNL's Computer Science and Mathematics Division (CSMD) is deployed as part of the city's emergency management preparedness. RAPID-DM, within minutes, identifies, activates, and allows a dozen logistic, transportation, plume transport prediction, and evacuation systems and resources to work together, or interoperate, to help scores of end users responsible for making critical decisions.

Remarkably, these complex systems have never previously been assembled in exactly the same configuration. Quick interoperation mechanisms for weather feeds, geographic information system (GIS) databases, transportation planning tools, and plume movement prediction systems allow decision makers to accurately predict the direction that a toxic plume will move and evacuate population from the areas expected to be affected. Quick coordination of rescue forces from the city's police and fire departments and from the National Guard is possible only because of the RAPID-DM capability, which enables communication among these teams

and geographically dispersed decision makers.

Collaborative Decision-Making Environments

Researchers at ORNL are accepting the challenge of addressing problems of national importance such as disaster management. The ultimate goal, much like the scenario described, is to allow geographically dispersed decision makers to respond quickly in a collaborative decision-making environment. Disaster management is only one example of the applicability of current and proposed research that combines software engineering, computational science, and collaborative technologies.

To enable a collaborative decision-making environment, many complex issues must be investigated and plausible solutions identified. In a collaborative decision-making environment, unlike traditional approaches, information is extremely varied and in a multitude of formats. Software programs historically written to solve a single problem without the requirement to interoperate with other software programs must be adapted to work in concert with many other software programs. Diverse end users with very distinct educational backgrounds and use of professional jargon are required to work in an environment of common understanding. The information needed goes beyond data on the status of the infrastructure; it includes not only inventory, finance, and accounting data but also detailed, predictive, interactive "what-if" calculations that involve large-scale scientific computation, visualization, and steering to answer near-term questions of dramatic importance. For example: Will the flash flood affect this neighborhood? Will the plume cloud move over this neighborhood, that neighborhood, or away from all population centers? Where will the hurricane make landfall?

Collaborative computing is the paradigm of choice for solving large, complex scientific and managerial problems. The use of collaborative computing to establish a rapid, on-demand interoperability of autonomous legacy applications and tools within new and evolving environments requires researchers to go beyond current software integration approaches. New initiatives, such as DOE 2000 (see previous article in this issue), establish an aggressive research agenda to "...fundamentally change the way scientists work together and how they address the major challenges of scientific computation." To accomplish this change, DOE 2000 plans to "develop and explore new computational tools and libraries that advance the concept of 'national collaboratories' and Advanced Computational Testing and Simulations (ACTS). The vision of DOE 2000 is to accelerate the ability of the DOE to accomplish its mission through advanced computing and collaboration technologies. DOE 2000 ushers in a new era of scientific collaboration that transcends geographic, discipline, and organizational boundaries."

Collaborative Computing Advances at ORNL

In collaborative computing, two or more computer users work in concert across time and space by using interoperable software so they can simultaneously solve a problem. ORNL computer scientists have broken new ground in collaborative computing, spanning the scientific and administrative computing spectrum. Each step contributes to the foundation upon which real collaborative environments are built.

In scientific computing, DOE 2000 efforts at ORNL include the Materials Micro-Characterization Collaboratory (MCC), CUMULVS, and the electronic notebook projects. In the MCC project, the goal is to join several centers of excellence into a single on-line interactive collaboratory in which electron microscopes can be operated remotely (for more details, see the article in this issue starting on p. 122). CUMULVS is designed to support remote computational steering of parallel applications and includes features such as interactive visualization and fault tolerance (for more details, see the article in this issue starting on p. 54). In distributed, collaborative environments, projects like ORNL's electronic notebook provide a mechanism for scientists to record information such as the usage of instruments and experimental results (for more details, see the article in this issue on p. 131).

Other ORNL information and computer science efforts also contribute to enabling collaborative computing. In the Computer Science and Mathematics Division (CSMD), researchers are developing the Collaborative Management Environment (CME) and other technologies such as Netsolve and data mining techniques. Researchers in the Center for Computational Sciences (CCS) are also contributing to advancements in data mining.

- The **CME,** led by Kimberly Barnes and T. E. Potok (both of CSMD), is a joint research project among Oak Ridge, Ames, Lawrence Berkeley, Los Alamos, and Fermi National Laboratories to establish a robust, scalable, and secure virtual management system for the DOE complex. The focus is on comprehensive integration of information within

DOE and tools to enable management of inter-laboratory collaboration. The objectives are to create an enterprise model that unifies disparate legacy databases, adapts to changing environments, and rapidly synthesizes and presents information on thousands of research projects where the information is distributed in a multi-platform environment.

- **"NetSolve,"** according to Jack Dongarra, ORNL–University of Tennessee Distinguished Scientist, "is a network-enabled solver that allows users access to computational resources—both hardware and software—distributed across a network. Its development was motivated by a need for easy-to-use, efficient mechanisms for remotely accessing computational resources. Ease of use is obtained via four different interfaces—Fortran, C, MatLab, and Java."
- **Data mining,** or knowledge data discovery, is a field in which a collection of sophisticated techniques is used to retrieve needed information from data. The techniques represented within this discipline allow new patterns and rules to be discovered that may not have been previously considered. Nancy Grady is leading the CSMD data mining effort.

CSMD researchers are combining existing techniques and new approaches to mine transportation, financial, scientific, and medical data as part of a project funded internally by ORNL's Laboratory Directed Research and Development Program. Working with banking industry data, researchers developed a prototype system to predict personal bankruptcy. This system is expected to be used by one of the largest banks in the nation. The approach combines decision-tree capabilities with neural networks (to allow for handling the categorical account records on an off-line basis, such as monthly) and with the time-series transaction data in real time.

CCS is collaborating with the Connecticut Healthcare Research and Education Foundation (CHREF) to perform data mining on Medicare-Medicaid patient encounter data collected by the Health Care Financing Administration (HCFA), a branch of the U. S. Department of Health and Human Services. Hundreds of gigabytes of anonymous inpatient, outpatient, home health care, hospice, and physician-supplier data have been stored in the High-Performance Storage System (HPSS), developed by IBM and DOE national laboratories including ORNL. These data will be analyzed to develop quality care indices based on HCFA data, which could be used to influence public health and health-care delivery policies.

Crisis Management Advances at ORNL

In the quest to address problems of national concern such as disaster management, researchers in ORNL's Computational Physics and Engineering Division (CPED) have laid new groundwork through development of large, single-purpose software applications such as the Joint Flow and Analysis System for Transportation (JFAST), the Police Command and Control System (PCCS), and Hazardous Assessment for Consequence Analysis (HASCAL). In addition, researchers in the Energy Division developed the Oak Ridge Emergency Management System (OREMS), and researchers in the Environmental Sciences Division developed the Ecological Model for Burning in the Yellowstone Region (EMBYR).

- **JFAST,** initiated by Brian Jones of CPED, is a multimodal transportation analysis model designed for the U.S. Transportation Command (USTRANSCOM) and the Joint Planning Community. JFAST is used to help the armed forces determine transportation requirements, perform course-of-action analysis, and project delivery profiles of troops and equipment by air, land, and sea. JFAST was used to guide deployment of troops and equipment in Bosnia and Haiti, and its predecessor, ADANS, was used for the Persian Gulf War.
- **PCCS,** led by Bob Hunter of CPED, is an information management system that was used to assist the Atlanta Police Department in providing security for the Summer Olympic Games in 1996. Vice President Al Gore described this system as "pioneering technology" in his report to the president on the preparations for the Atlanta Olympics. Before the Olympics, the system assisted the Atlanta Police Department in planning for the Olympics. During the Olympics, the system gave the Atlanta Police Department a critical response advantage as it exercised responsibility for security of the area during the games. Currently, the PCCS helps the Atlanta Police Department in managing their resources on a daily basis.
- **HASCAL,** led by Brian Worley of CPED, stimates the health hazards from atmospheric releases of nuclear, biological, and chemical materials. For example, it is used to predict the transport of a hazardous cloud, the effects of hazardous material at geographic locations, and the geographic distribution or cross section of the atmosphere. HASCAL is currently used by the Department of Defense.
- **OREMS,** initiated by Ajay Rathi and John Sorensen, both of the

Energy Division, is a simulation and analysis model for evacuation strategies based on the detailed network traffic flow simulation model. OREMS is currently used by the Department of Defense and the Federal Emergency Management Agency (FEMA).

- **EMBYR** is a computer fire-simulation tool used to investigate the causes and consequences of large-scale fires such as those in Yellowstone National Park during 1988. This tool will be used to investigate "what-if" scenarios related to possible landscape-scale effects of variations in fire frequency, fire management, and global climate regimes over time scales ranging from complete fire seasons to millennia. William Hargrove of CPED participated in the development of EMBYR.

A New Center at ORNL

To build a collaborative environment by combining advances in computing and information science with many software applications, fundamental research in semantic modeling, object technologies, software engineering, and data fusion and analysis is necessary. In addition, the process to build a collaborative environment, and the process to establish a collaborative session must be researched and standardized.

The Collaborative Technologies Research Center (CTRC) was recently established in CSMD to perform this fundamental research with the goal of enabling adaptive tools, languages, and problem solvers to be brought together across time and space for a vast array of domains: enterprise management, disaster management, education, banking and finance, and engineering design and manufacturing. CTRC partners with groups from government, industry, and universities to accomplish its core research.

As a part of the core research, semantic modeling provides the "glue" necessary for establishing and maintaining collaborative environments and warrants the most explanation. Semantic modeling attempts to provide a more capable structure to software objects than is provided by traditional software engineering approaches. These models provide for definitions of interobject connectivity, behaviors, and information in a way that supports expressive and powerful manipulation, organization, querying, and searching for information. An important trait of semantic modeling is that it is designed to support the building of (1) a shared understanding of problem domains by humans, and (2) unified models of application domains that are transferable across multiple software components. This trait is very important when multiple software components need to interoperate, yet have not been designed for interoperation or cannot be designed by a tightly interacting design team.

CTRC researchers are leading the RAPID-DM effort described in the introductory scenario and are partnering with ORNL's disaster management software developers and Carnegie Mellon University. (To find out more about CTRC activities, please visit our World Wide Web home page at *http://www.epm.ornl.gov/ctrc*.

Building a Collaborative Environment

How is a collaborative environment really built and how does it work? Consider what must be done to enable rapid communications and coordinated responses to the disaster management scenario outlined at the beginning of this article. Figure 1 illustrates a collaborative disaster management environment that enables such rapid communication and coordinated response. However, this environment

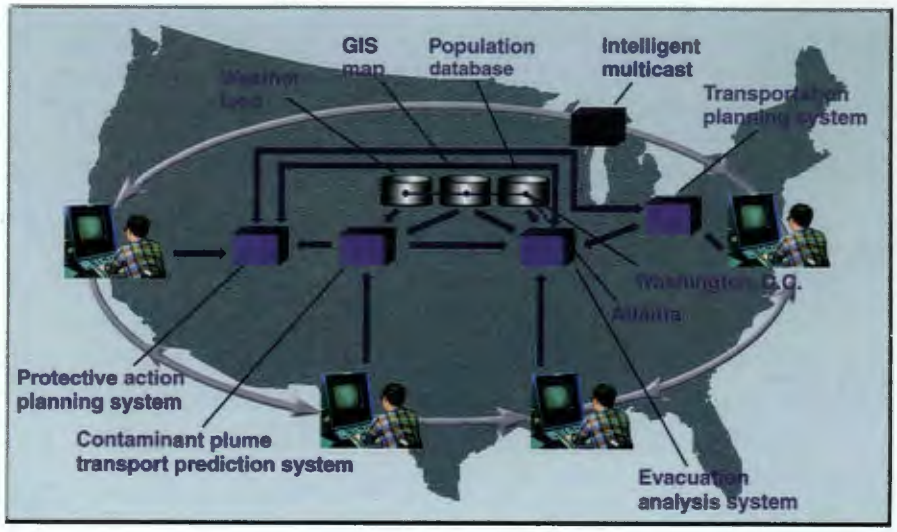


Fig. 1. The envisioned ORNL collaborative disaster management environment will make interoperable a number of ORNL-developed software systems to provide transportation planning and scheduling (JFAST), evacuation analysis (OREMS), toxic plume movement prediction (HASCAL), and police command and control (PCCS).

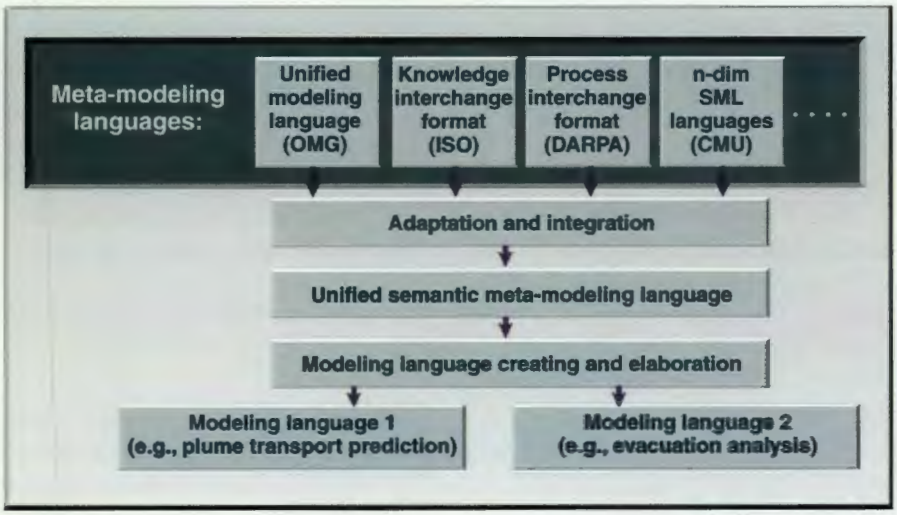


Fig. 2. ORNL's approach to crisis management is based partly on semantic meta-modeling. Development of semantic meta-modeling language provides a common basis for software and domain languages and an approach for building shared meaning and evolving languages.

assumes a significant collection of interoperating legacy systems. To understand the complexity of the building task, keep in mind that the software developers never designed or interacted to make the software interoperate in the first place. Hence, legacy software makers and collaborative tool developers create and publish models of their software so that others may understand the intended behavior and function of the software. The emergence of standards in the software engineering community is enabling development of common problem domain-specific languages. These languages are derivable from common metalanguages (e.g., Unified Modeling Language), making development of shared, agreed-upon languages a distinct possibility. Figure 2 illustrates this situation.

The domain experts negotiate models of the domain with the software developers to ensure proper interaction between the software models and collaborative tools and models of the domain. This creation, negotiation, and publishing of models will be done using tools provided by CTRC, which include:

- a software modeling and wrapping tool to enable independent modeling and code-wrapping of component software by software developers;
- a domain modeling tool to enable development and management of models that capture the properties of the problem domain;
- a modeling support workbench that helps an integration engineer support application and domain modeling through intelligent user interfaces (so that, for example, the integration engineer can use the support workbench to discover, retrieve, and compare software patterns from a repository of software models);
- a communication language that provides a medium for interaction with and querying of software models; and
- a systems configuration interface builder to enable building application-specific interfaces for end users to configure new collaborative environments.

Before users can rapidly establish a collaborative session during the planning process or the actual event of a disaster by employing the tools described, the environment must be built. As a feasibility study for this research, ORNL scientists are building a test environment. The disaster management tools (e.g., HASCAL, OREMS) are modeled by ORNL software developers, and the disaster management model is defined by an integration engineer working with disaster management experts. The models are published in a repository from which they can be retrieved as needed for a collaborative session.

Using a Collaborative Environment

Having built a collaborative environment so that many software-application and communication mechanisms can now interoperate, how is the environment used? Consider this disaster management scenario. A biologically contaminated plume is discharged into the atmosphere in the Atlanta region. Upon learning about the crisis, a representative from FEMA searches for services to provide information about road accessibility in a biological atmospheric hazard in the Atlanta region. HASCAL, one of the computational systems that deals with this type of problem, predicts the directions in which the contaminant plume will move. The FEMA representative examines the performances and requirements of the candidate systems (e.g., overall response time,

required data feeds, and administrator requirements) before selecting a system. In this instance he selects HASCAL, calls up a virtual conferencing link with the HASCAL administrator, and communicates the requirements for the service.

The HASCAL administrator establishes the data feeds necessary for the application. She issues a request to the disaster management information broker to identify alternative data sources in the Atlanta region that are capable of supplying field measurement data for the specified biological disaster, weather feeds, and a GIS map of the region. The administrator then selects and interconnects the optimal services from the broker-provided list. This process allows the HASCAL application to operate with the latest local data to make predictions about the plume's toxicity and movement given the current situation.

In the meantime, the FEMA representative establishes connection, via an intelligent multicast tool from the repository of collaborative tools, with the regional disaster relief headquarters, the police department, the fire department, and the medical emergency squad. In addition to the visual and textual link with the team members, the representative chooses to communicate that certain roads are closed because they are in the area of the expected plume flow. This communication is done by broadcasting the information about the inaccessible roads and using a shared geographical map of the region. Next, the FEMA representative searches for evacuation planning services and identifies alternative systems to handle evacuation planning for the affected area. The representative chooses the OREMS system and brings it into the collaborative environment in a manner similar to the HASCAL system with its output overlaid onto the shared geographic map.

This scenario demonstrates how two applications, HASCAL and OREMS, and collaborative tools such as the intelligent multicast are rapidly combined in an environment to allow remotely located decision makers from various agencies and departments to define an evacuation plan using the latest available information. The ultimate goal is to provide a mechanism for many applications, tools, and experts to work in concert to solve complex problems. For example, one can easily imagine adding to and/or deleting from the collaborative session other software applications and invoking additional collaborative tools as the situation evolves.

"The ORNL disaster management technologies provide a grassroots opportunity to test the use of collaborative technologies in solving a real-world problem."

Conclusion

Although much research is still required, the advances being made by ORNL researchers push collaborative computing to the leading edge. In DOE 2000, important discoveries are being made with regard to the remote control of instruments, steering of computational simulations, and electronic storage (in a shared or private manner) of important findings from experimental results. All of the technologies resulting from DOE 2000 efforts will enable scientists from around the world to work in collaboration as if they were in the same laboratory. Other efforts such as CME, Netsolve, and data mining contribute to collaborative environments. CME enables collaborative management of thousands of research projects. Managers and researchers can use a combination of technologies developed from this and DOE 2000 efforts to collaborate much in the same way that scientists use the technologies in the laboratory. Netsolve provides the capability to find and manage hardware and software resources needed for a collaborative session. Data mining and storage capabilities aid in validation, knowledge discovery, and efficient storage of very large amounts of data found in computationally intensive problems. Advances in semantic modeling, object technologies, and software engineering provide the "glue" to enable the software, hardware, and users to work together in a common environment. The ORNL disaster management technologies provide a grassroots opportunity to test the use of collaborative technologies in solving a real-world problem. As more insight is gained, the hope is that such technologies can be used by researchers from around the world to jointly study and solve many complex problems that are otherwise insolvable. **ornl**

BIOGRAPHICAL SKETCHES

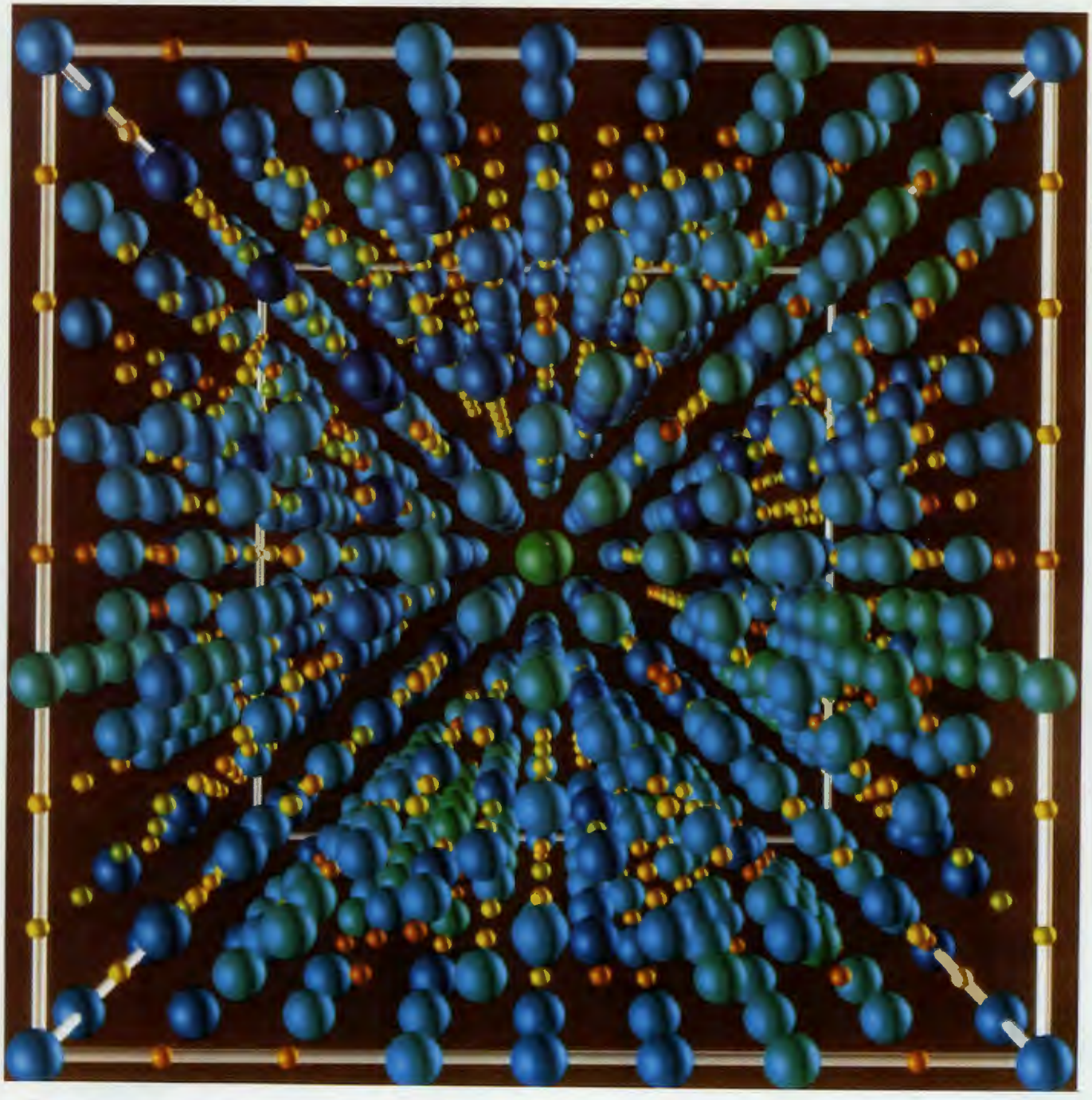
KIMBERLY D. BARNES is director of the Collaborative Technologies Research Center in ORNL's Computer Science and Mathematics Division. She has an M.S. degree in accounting from the University of Tennessee at Knoxville and a B.S. degree in business administration from Tennessee Technological University. Her research interests are accounting information systems, data mining, information technologies, and electronic commerce. The center's research projects include development of the Financial Automated On-line User System, Collaborative Management Environment, Financial Services Technology Consortium (FSTC) Electronic Check, FSTC Bank Internet Payments System, Mining Large Multimedia Data Sets, and Gas and Oil National Information Infrastructure.

JOHN W. COBB is chief information officer and technical assistant for the Spallation Neutron Source project managed at ORNL. Previously, he worked in the Computing, Information, and Networking Division as the ORNL scientific computing coordinator and user advocate. He has a Ph.D. degree in physics from the University of Texas at Austin. His dissertation concerned computational and theoretical research on advanced fusion power concepts. He came to ORNL to work on a Fusion Energy Division project to build predictive computational simulation models for semiconductor processing tools. His research interests include plasma physics, plasma astrophysics, high-performance computing, and fusion energy. He is a member of the American Physical Society, American Vacuum Society, Materials Research Society, and the Association of Computing Machinery.

NENAD IVEZIC is a research staff member at the Collaborative Technologies Research Center of ORNL's Computer Science and Mathematics Division. He received his Ph. D. degree in 1995 in computer-aided engineering from Carnegie Mellon University. His interests are in the areas of software engineering, machine learning, engineering design, and collaborative technologies. He has been involved in the research and development of machine learning applications for a number of engineering decision support systems. He is investigating technologies that enable collaborative work including semantic modeling, ontology engineering, and shared work environments

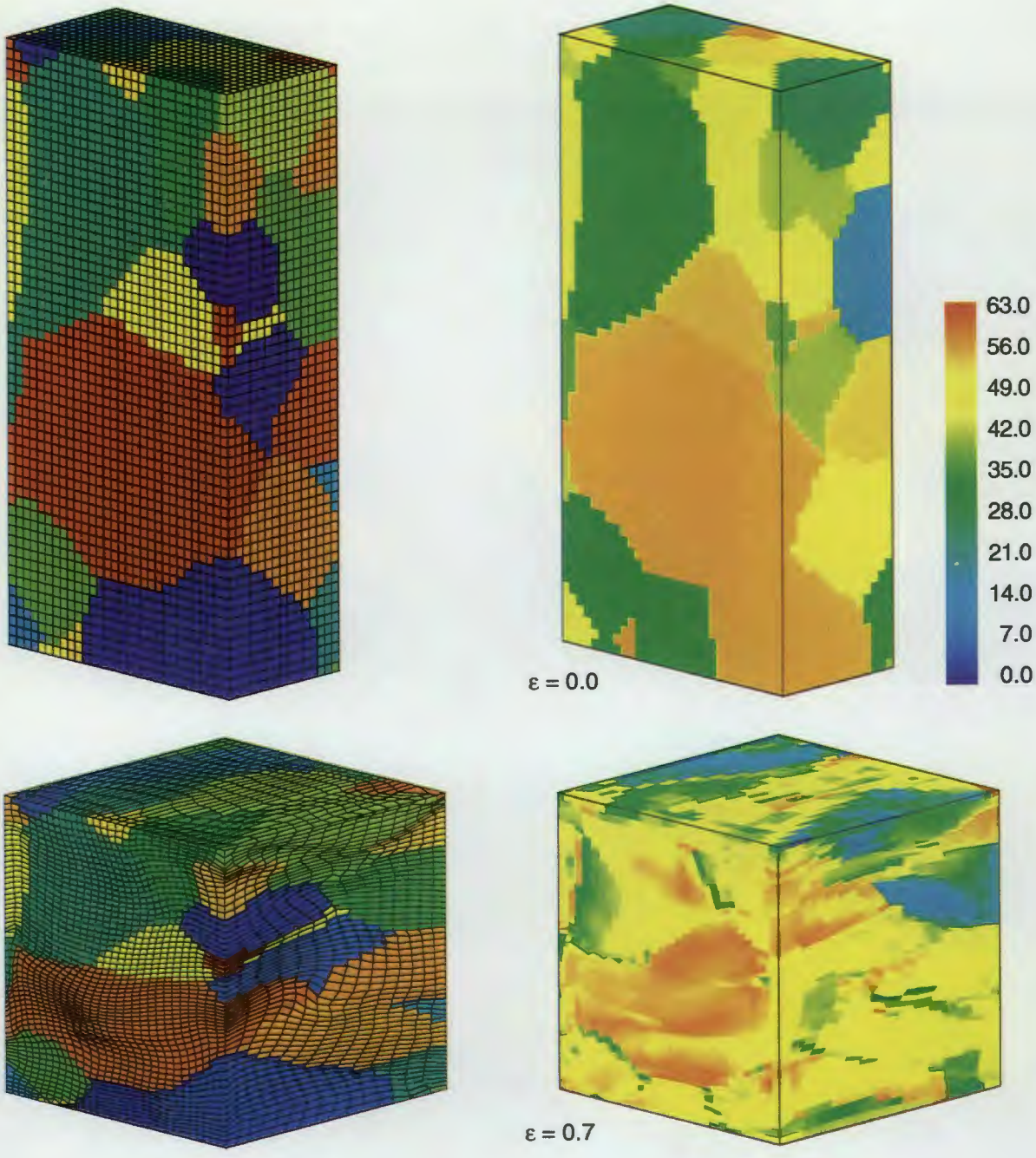
Computer Art

Crunching numbers and applying visualization techniques using a massively parallel computer can generate colorful images. Such computer art in which colors have mathematical meaning can provide insight into scientific phenomena. Examples are provided on the following pages and the back cover.

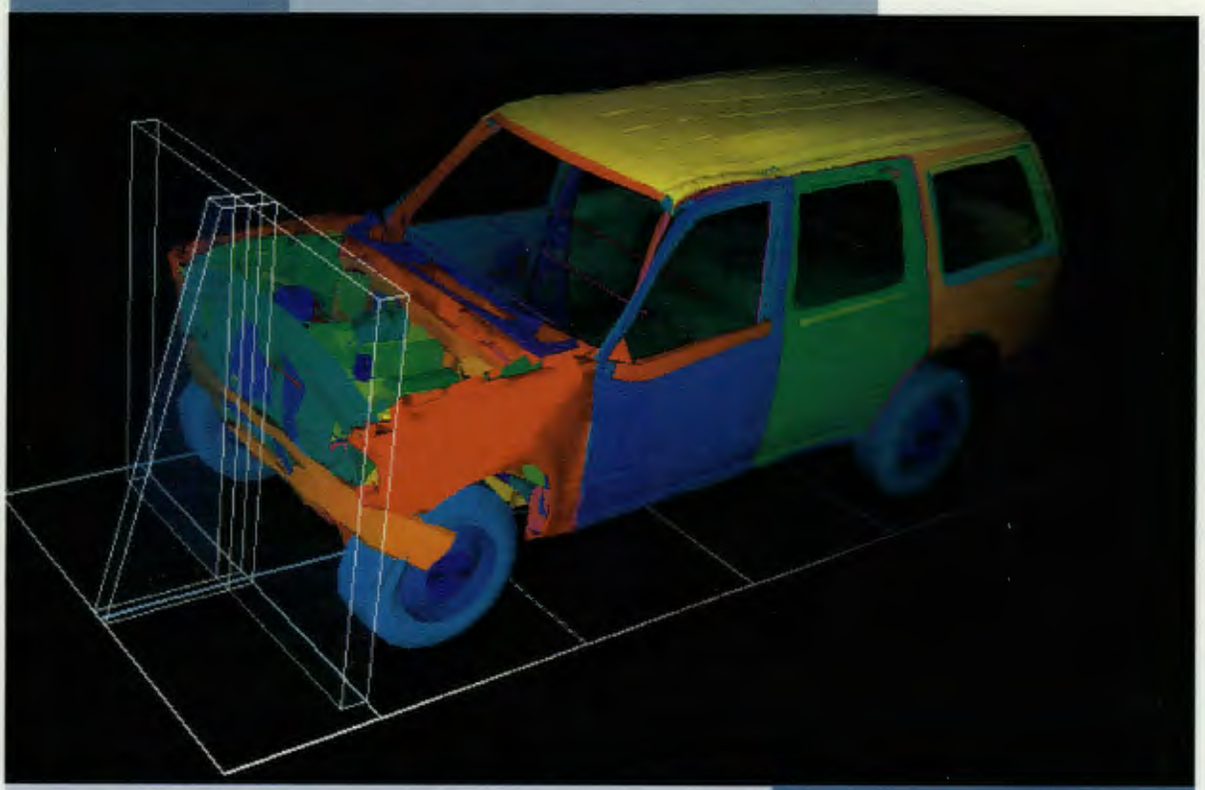


Computational methods have been developed to calculate the physical properties of crystalline materials at the microscopic level, where the crystal is made up of atoms in a periodic arrangement, as shown in this visualization. For more information, see p. 70. *Electronic image by Ross Toedte.*

Numbers Three and Four, 1997



When a sheet of aluminum is deformed, its polycrystalline microstructure changes. These images obtained by modeling the nonuniform deformation of the metal show the structural changes at the atomic level. The information helps researchers optimize processing conditions to obtain microstructures that give the metal improved properties. For more information, see pp. 18 and 113. *Electronic images by Gorti Sarma.*



ORNL computer simulation of a Ford Explorer crashing into a rigid barrier. For details, read the article starting on p. 100. *Electronic image by Srdan Simunovic.*

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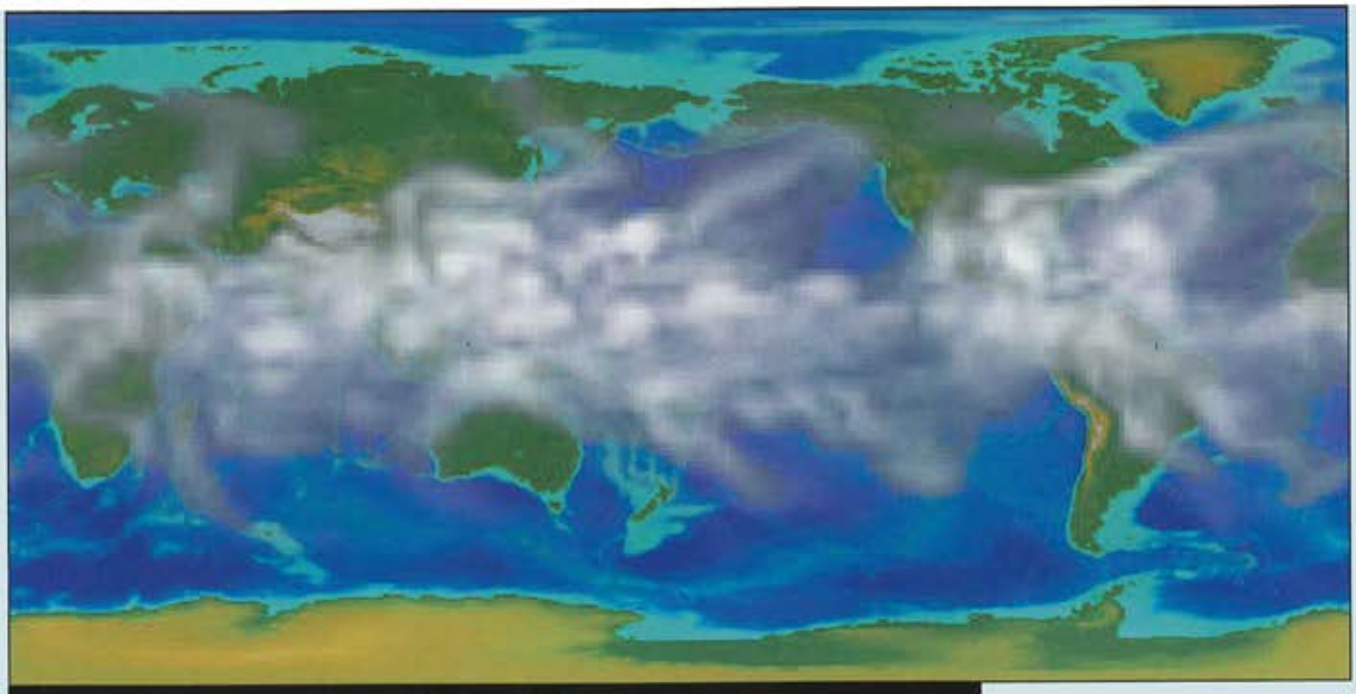

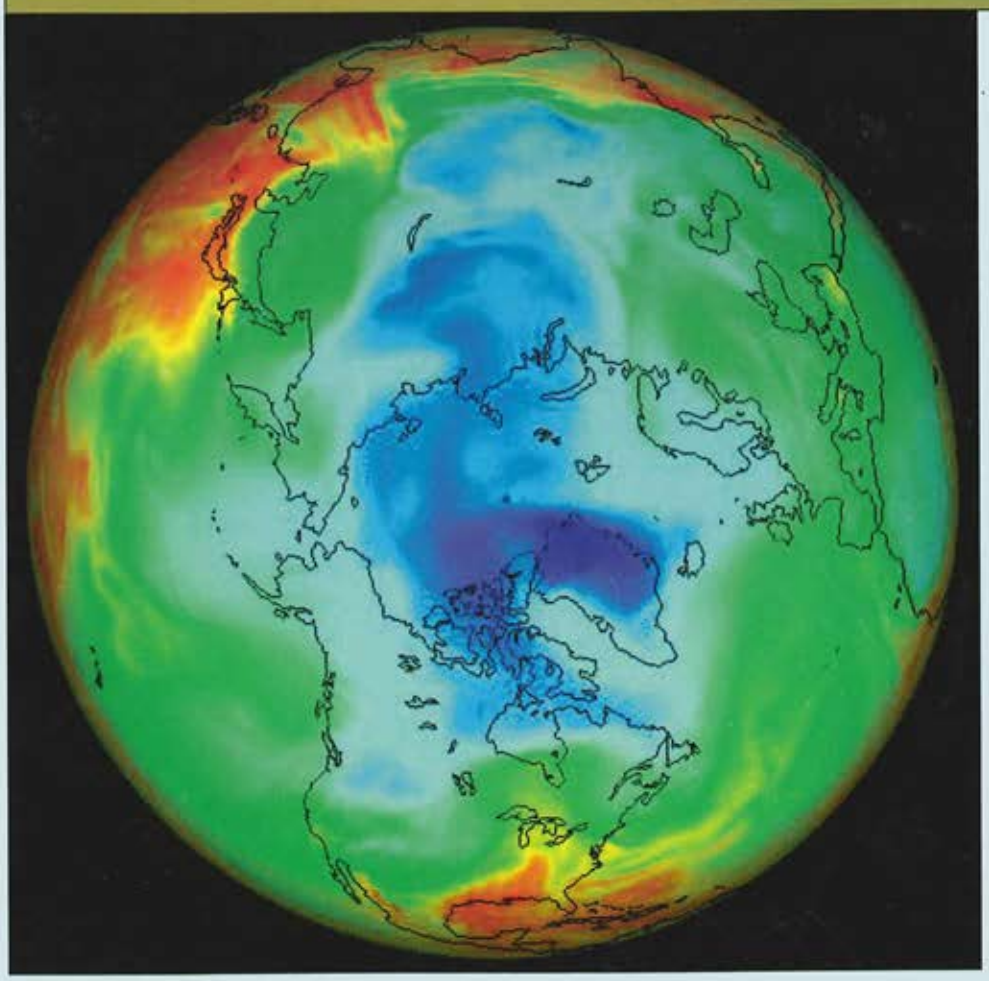

Simulating the atmosphere and ocean using coupled general circulation models requires world-class computational resources. Energy policy and the science of climate change depend increasingly on the reliability of these models to predict the effects of increased levels of carbon dioxide and other greenhouse gases. ORNL has pioneered the use of massively parallel computers for climate modeling. A snapshot from a simulation of the current climate shows the amount of moisture in the atmosphere. In a warmer climate the circulation is likely to carry more moisture from the tropics into the mid-latitudes, increasing the transfer of heat toward the poles. Models are continually improving by comparing results with observed data. The precipitable water field can be compared directly with satellite measurements. See discussion on p. 32.