Oak Ridge National Laboratory

REVIEW

Vol. 21, No. 3, 1988

REVIEW

Volume 21 *Number Three 1988*

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in the physical, chemical, and life sciences; in fusion, fission, and fossil energy; and in energy conservation and other energy-related technologies.

ON THE COVER

This computer graphic (produced by Paul T. Williams of the Martin Marietta Energy Systems, Inc., Computing and Telecommunications Division) is a "finite elements" model developed for vibrational analysis of part of a scanning tunneling microscope being built at ORNL. Color variations indicate the degree of surface change (see page 9 for the full story). A special section of this issue is devoted to the applications of supercomputers, particularly the local Cray X-MP, in research and in visualizing scientific results at ORNL.

Editor
Carolyn Krause

Associate Editor
Luci Bell

Consulting Editor
Alex Zucker

Designer
Vickie Conner

Technical Editing
Lydia Corrill

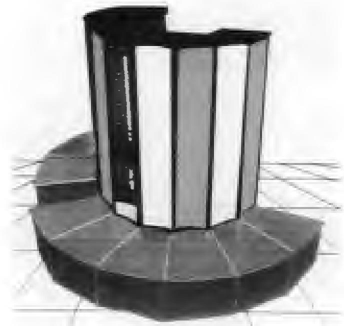
Photography,
Graphic Arts, and
Printing and Duplicating
departments

The *Oak Ridge National Laboratory Review* is published quarterly and distributed to employees and others associated with ORNL. The address of the editorial office is Building 4500-South, M.S. 6144, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6144. Telephone: internal, 4-7183 or 4-6974; commercial, (615) 574-7183; or (FTS) 624-7183.

ORNL is operated by
Martin Marietta Energy Systems, Inc.,
for the Department of Energy
under Contract No. DE-AC05-84OR21400

ISSN 0048-1262

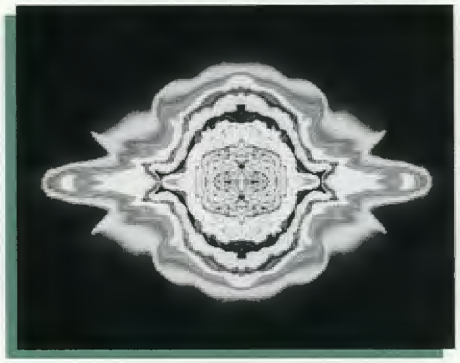
Features



Departments

Supercomputers in Scientific Research

By H. Richard Hicks



This image is a supercomputer simulation of an astrophysical explosion between two colliding neutron stars. The image (originally in color) was created by Donna J. Cox, artist and color software designer, and Charles R. Evans III, astrophysicist. Cox used this in a seminar at ORNL in January 1988 to illustrate the use of supercomputers in scientific data visualization.

Supercomputers are powerful machines used to predict the weather, model the climate, design buildings and vehicles, and locate oil reserves. At Oak Ridge National Laboratory they are used for scientific research in areas such as fusion energy, chemistry, physics, metallurgical theory, and reactor simulations.

The term supercomputer simply means one of the most powerful computers available at any given time. This working definition avoids any controversy about "How fast is fast?" and reflects the expectation that more powerful supercomputers will evolve.

Supercomputer also usually means a machine that is not embedded. Embedded computers are those built into devices such as cars or rockets and having fairly specific roles. Usually, supercomputers are thought of as being general-purpose machines, although some have been designed to solve narrow classes of problems.

The term "powerful" refers to the arithmetic or logical processing speed of the computer. Supercomputers normally have other resources, such as memory size, communication speed, and storage capacity that are commensurate with the processing speed, but these factors are usually not considered to be primary measures of power. Sometimes the maximum hardware speed, in millions of instructions per second (MIPS) or in millions of floating-point operations per second (MFLOPS), is quoted as a measure of power. A floating point operation is an arithmetic operation between two real numbers. However, the speed of computation on most modern supercomputers bears little resemblance to this maximum number, because programming techniques and compiler optimization play an important role in determining the actual speed achieved. Compiler optimization refers to the degree to which a computer program is translated into machine instructions that permit efficient execution of the program.

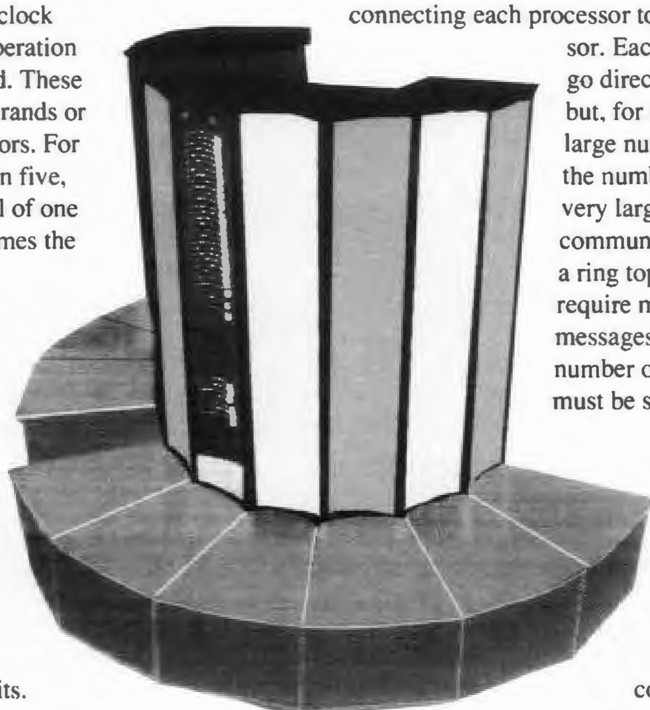
Because supercomputers are near the leading edge of technology, some prototypes or research machines are not widely available to end users. These machines are of great importance but are not generally relevant to the typical supercomputer user.

When more "capability" (ability to process bigger jobs in the same time) is needed, then a faster computer may be the only answer. When more "capacity" (ability to process more jobs in the same time) is required, it can be achieved either by a faster computer or by simply adding more computers. As one author put it, the difference between a faster computer and a host of computers working together is like that between a Saturn-V rocket and a fleet of automobiles. They may have the same total power, but the rocket and the cars are optimized for different purposes.

Vector Processing

In the early 1970s, the computer industry realized that the speed of electronic switching in computers was not increasing as rapidly as it had in the previous decade. It was also recognized that floating-point arithmetic operations generally took a lot longer to complete than most other operations. This recognition prompted an architectural advance called vectorization.

This is how it works. Suppose that five clock periods are used to multiply two numbers together. It is possible to design a multiplier in the form of a five-segment "pipeline." The first segment is busy during the first clock period, the second during the second clock period, and so forth. This arrangement does not provide any advantage for a single operation. However, consider the case in which a sequence of pairs must be multiplied to produce a sequence of products. If all of the pairs are known in advance (that is, if none of them depend on any of the products), then, when the pairs are fed through the pipelined multiplier, the first product will appear after five clock periods. After that, one product will appear per clock period because a new operation begins each clock period. These sequences (of either operands or answers) are called vectors. For vectors much longer than five, one approaches the ideal of one result per cycle—five times the scalar speed.



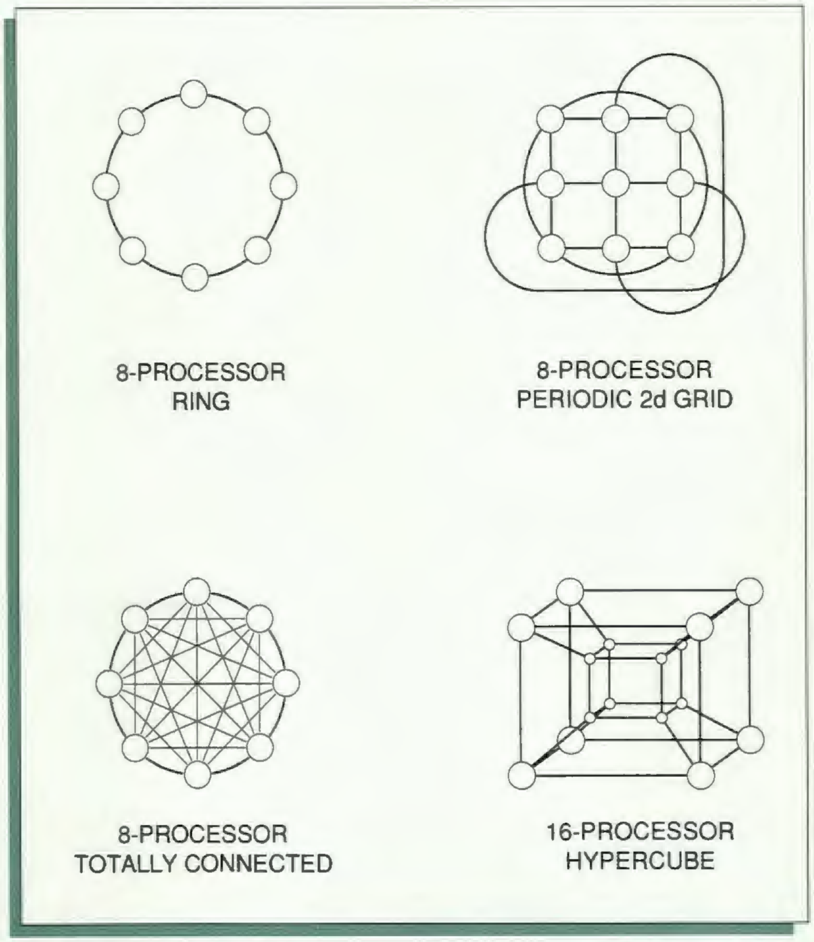
The computer drawing of the Cray X-MP was done by Gail Finch of the Energy Systems Computing and Telecommunications Division.

Parallel Processing

In a limited sense, vectorization allows several operations to be in progress at once. In contrast, the term parallel processing is applied to computers that have several fairly complete processing units. (See article on parallel computing on page 21.) When these units are allowed to process different instruction streams and different data streams simultaneously, the machine is classified as a multiple-instruction, multiple-data (MIMD) machine. In contrast, the older, standard, serial processor would be a single-instruction, single-data (SISD) machine, and a machine that operates in parallel on arrays of data using a single stream of instructions would be a single-instruction, multiple-data (SIMD) machine.

Even these categories barely scratch the surface in describing this rich class of computers. The memory's organization plays a very important role in the operation of a parallel computer. At one extreme are computers that store all data in a common memory that can be accessed by all processors. Any data to be passed between processors must go through this memory. At the other extreme are computers in which each processor has a local memory. A communications network is used to move data between processors. In local-memory multiprocessors (sometimes called distributed-memory machines), the topology of the internal communications network is the key. Maximum communication is provided by directly connecting each processor to every other processor. Each message can then go directly to its destination; but, for computers having a large number of processors, the number of connections is very large. The minimum communication is provided by a ring topology, which may require many hops for some messages. (A hop is the number of times a message must be sent from processor to processor to reach its final destination.) Another natural topology is a two-dimensional rectangular grid. Perhaps the most elegant, and the best compromise between minimizing connections and minimizing hops, is the hypercube topology, which requires the number of processors to be a power of two, 2^d. The total number of connections between processors in this configuration is $d \times 2^{d-1}$, and the maximum number of hops a message will take is d.

By far the largest installed base of supercomputers is of those manufactured by Cray Research, Inc. In the early 1970s, Seymour Cray, the developer of the CDC 7600, left Control Data Corporation to found his own company, Cray Research, Inc., which focuses exclusively on building supercomputers. In the mid-1970s, this company marketed the Cray-1, which was about a



Various configurations for connecting the processors in different types of multiprocessor supercomputers.

factor of 4 faster than the CDC 7600, the premier supercomputer at the time. The Cray-1 achieved this speed because of its vector architecture. Although Seymour Cray specializes in hardware design and packaging, Cray Research also provides its customers with the software to allow standard FORTRAN programs to take advantage of this vector capability.

Cray has also developed and marketed the Cray X-MP, Cray-2, and Cray Y-MP computers, which have provided incrementally greater processor speed and which allow up to eight processors per computer. The ability to harness these processors for a single job requires effort on the part of the programmer, because each processor usually works on a separate job. Thus, more processors provide increased capacity, but only with programming effort does this provide increased capability. In fact, although maximum theoretical processing speed has increased, no dramatic increases in the actual processing speed for most typical calculations here occurred since the introduction of the Cray-1.

The primary difference between the Cray X-MP and the Cray-2 is in memory size. The X-MP offers up to 16 megawords (memory units consisting of one million 64-bit words). The Cray-2 offers up to 256 megawords of memory, allowing calculations using large amounts of data to be executed more efficiently. ETA, a spin-off company of Control Data, has produced supercomputers having greater theoretical speed than the Cray machines, but to achieve this greater speed, the calculations must use very long vectors. Recently, IBM and a number of Japanese companies have entered the supercomputing arena.

A number of "minisupercomputer" vendors now claim 10 to 40% of the speed of a Cray-1 for, at most, a few hundred thousand dollars. (Cray computers usually cost several million dollars.) Hence, the days of Cray's virtual monopoly in the supercomputer market are past.

Although the large commercial vendors have concentrated on shared-memory machines having a small number of fast processors, universities and a few small companies have focused on hypercubes and other computers having large numbers of processors. One limitation of having multiple processors is the conflict over access to a shared memory. Hence, these machines usually have a local memory for each processor and a means to communicate between processors. Major efforts are under way at ORNL and elsewhere to design algorithms that will execute optimally in this environment and to develop tools to help the programmer utilize the computer's inherent parallelism.

Who Needs Supercomputers?

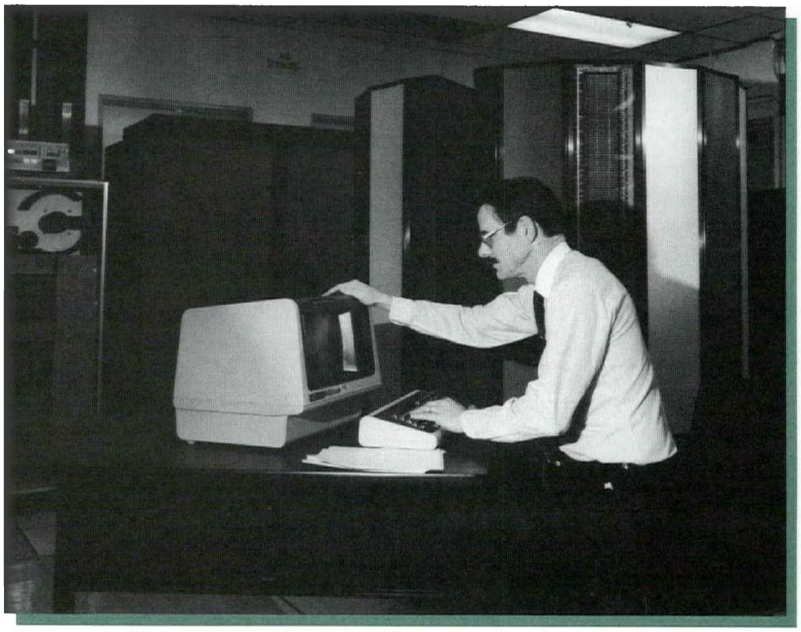
Several years ago, the National Science Foundation (NSF) began to recognize that U.S. university professors and students needed supercomputer access and training. To achieve this goal, the NSF established five supercomputer centers, which are now operational: The National Center for Supercomputer Applications (University of Illinois), the San Diego Supercomputer Center (University of California, San Diego), the John Von Neumann Center at Princeton, the Pittsburgh Supercomputer Center, and the Cornell National Supercomputer Facility. They employ Cray, ETA, IBM, and Floating Point Systems (FPS) products. Although this initiative has had the undesirable short-term effect of making programmers for supercomputer systems somewhat scarce, a generation of students and scientists is receiving valuable training. Some 6000 researchers around the country have shared computer time at these centers. The NSF plans, as the next step, to establish a higher-speed communication network between these centers.

U.S. industry is now beginning to recognize the importance of supercomputers for performing geologic calculations, engineering design, high-quality animation, and even large, mundane business tasks. Thus, the commercial market for supercomputers is also growing.

Historically, the DOE defense laboratories, Lawrence Livermore and Los Alamos, have led the way in purchasing supercomputers and in developing software to run them. As supercomputers become more widely used, vendors will be able to provide more of the necessary software.

Today, using all the capabilities of highly parallel machines such as hypercubes cannot be done without incurring considerable added programming costs. To do it economically will require software advances and, probably, programming languages that are designed to incorporate parallelism. Some studies suggest that parallel computers will not be used as general-purpose computers within the next ten years because of the programming costs.

Increasingly, supercomputers will be considered merely another resource that can be accessed from a personal workstation. With the advent of reliable, high-bandwidth telecommunications, it is possible for workstations to route work invisibly to the most effective resources for execution. Work-stations are now starting to provide real-time animation of simulations produced by supercomputers, such as the operation of a reactor or the aerodynamics of an airplane.

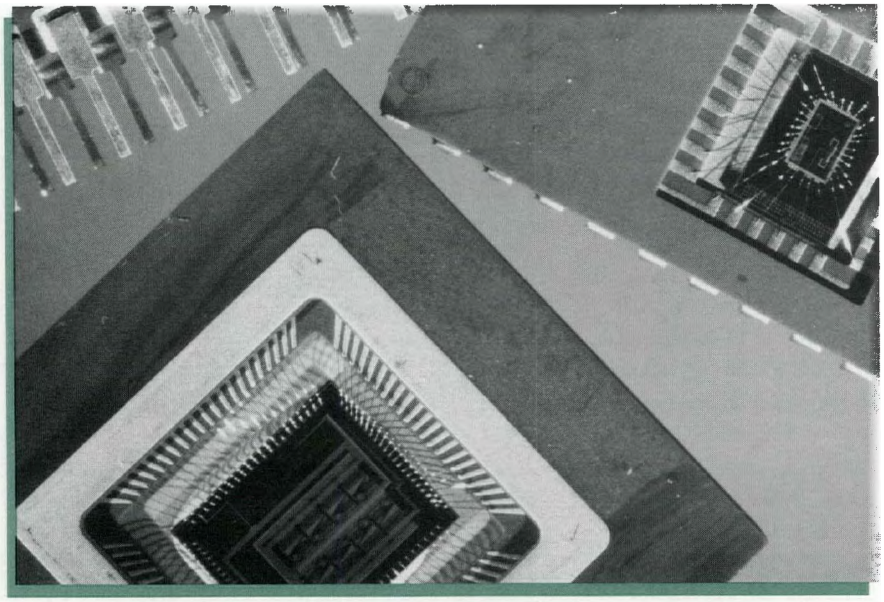


The Cray X-MP (shown in the background) is controlled by researchers like Richard Hicks, working at an ordinary computer terminal.

Oak Ridge's Cray X-MP

The Cray X-MP, located at the Oak Ridge Gaseous Diffusion Plant (ORGDP), was acquired to handle uranium enrichment calculations in a classified environment. Just as the machine was obtained in 1985, that work disappeared because the plant was placed on standby, and the gas-centrifuge enrichment project was terminated. The computer was retained, however, to satisfy other computing needs within Martin Marietta Energy Systems, Inc., and is now operated for classified use during part of each week and unclassified use for the remainder. Most of the unclassified time is used for ORNL projects, while the classified time is used primarily by ORGDP and the Oak Ridge Y-12 Plant. When the Cray is unclassified, most Energy Systems employees may access it.

At ORNL, this Cray and other supercomputers are used for the simulation of complex physical systems and for large engineering studies to provide numerical results that augment theoretical, heuristic, and probabilistic approaches. In this context, the supercomputer is a useful tool for problem solving. The level of resolution (detail)



An arrangement of computer chips and microcircuits typical of the electronics that drive a supercomputer.

of the solution is usually limited by the power of the computer available. Doubling the linear resolution in a three-dimensional simulation, for example, can require a factor-of-eight increase in computer run time.

Ten years ago, the validity of numerical simulations was not widely accepted in the scientific community. Because of verified successes during the last decade and the money saved by performing computer, rather than laboratory, experiments, numerical simulations in many fields are considered as acceptable as other theoretical and laboratory techniques. (See the following articles for some detailed examples of supercomputer uses by ORNL researchers.)

Even before installation of the local Cray, some ORNL researchers used remote supercomputers, primarily those at the defense laboratories. For example, the researchers in ORNL's Fusion Energy Division have historically used the largest annual amount of computer time at the National Magnetic Fusion Energy Computer Center at Livermore.

ORNL researchers have also been investigating better ways to design and use computers. They have explored the use of parallel processors in robotics and have optimized some numerical algorithms for parallel processors. Significant progress has been made in the effective use of parallel architectures for certain classes of scientific problems.

Future of Supercomputers

Even if the next-generation supercomputer is only slightly larger than today's personal computer, it is likely to cost millions of dollars. But, as the desktop power available for thousands of dollars increases dramatically, so will the power available in a supercomputer increase. Many of the problems being solved today on supercomputers will be studied economically on much faster machines. Today's computerized physical simulations have by no means exhausted all possibilities. They incorporate numerous assumptions that can be refined, yielding further understanding. The study of nonlinear phenomena, geometrically complex systems, and problems involving diverse time or space scales, real-time animation, and a high degree of dimensionality will strain the capabilities of supercomputers for some time into the future. Scientific problems that require even more computer power than can be delivered will persist.

If software can be developed to facilitate the effective use of many parallel processors, then the widespread use of massively parallel machines could enormously increase the effective computing capability available. This assumption, however, implies that compilers will also recognize and utilize parallelism.

Many researchers are also investigating the possibilities for significantly increasing processor speed. Today's computer chips are based on macroscopic electronic technology. Atomic- or

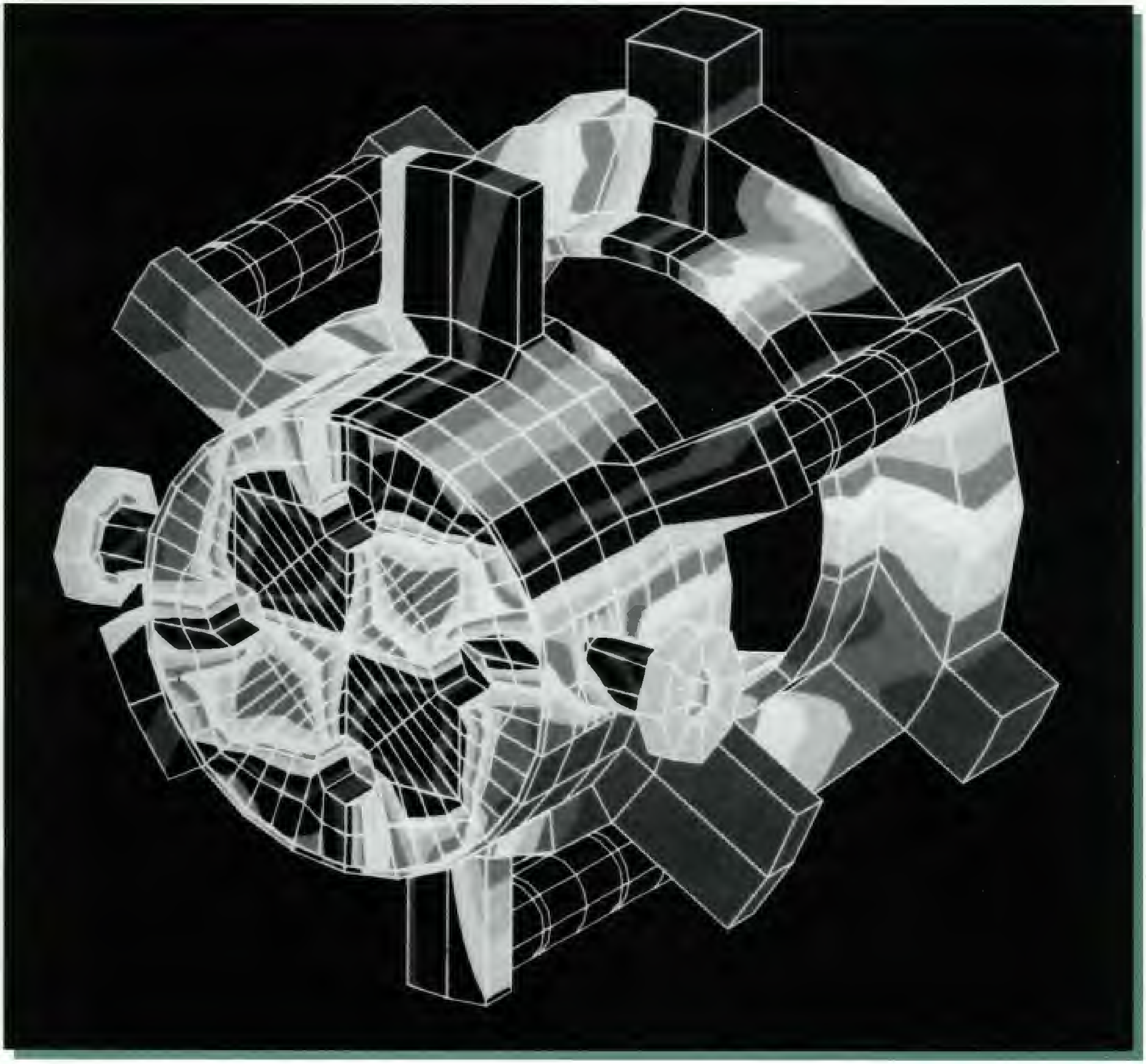
View of the Cray X-MP's multiple connections.

molecular-based circuit elements could shorten the signal path lengths, and thus the cycle times, by several orders of magnitude. Some of these approaches may decrease heat buildup, thus allowing the development of more-compact computer architectures. If these developments succeed, the trend toward heavy reliance on parallel computing may reverse. ornl

Richard Hicks has used a Cray X-MP for studying the dynamics of fusion plasmas.

Biographical Sketch

H. Richard Hicks is the program coordinator for the Office of Scientific and Technical Computing in the Energy Systems Computing and Telecommunications Division. He has worked for this division since 1972. He holds a Ph.D. degree in physics from the University of Illinois. An overall theme of his scientific work has been the study of nonlinear problems through computer simulation. For a decade, Hicks worked in the magnetohydrodynamics (MHD) project of ORNL's Fusion Energy Division. Project researchers, headed by Ben Carreras, pioneered techniques to perform efficient MHD computations for better understanding the dynamics of fusion plasmas. Hicks, formerly one of the largest users of supercomputer time in the world, developed the computer program RSF. In the early 1980s, this and other computing tools helped to lay the theoretical groundwork for the design of ORNL's Advanced Toroidal Facility, which achieved its first plasma in early February 1988. Hicks has been involved in design discussions for one of the earliest parallel computers, the ILLIAC IV, as well as projects to "parallelize" existing computer programs for Cray supercomputers and hypercubes. Hicks is an editor of *Journal of Computational Physics*.



Cray X-MP Aids Visualization of STM Geometry

This "finite-element" model of part of a scanning tunneling microscope (shown in black-and-white here and in full color on the cover) aids the visualization of the surface geometry. A rapid change in color indicates high curvature, while uniform color represents a flat surface. The Cray X-MP was used in a vibrational analysis with the goal of controlling vibrations to ensure accuracy in the STM's imaging of materials with atomic-scale resolution. The STM is being built by John Noonan of ORNL's Solid State Division.

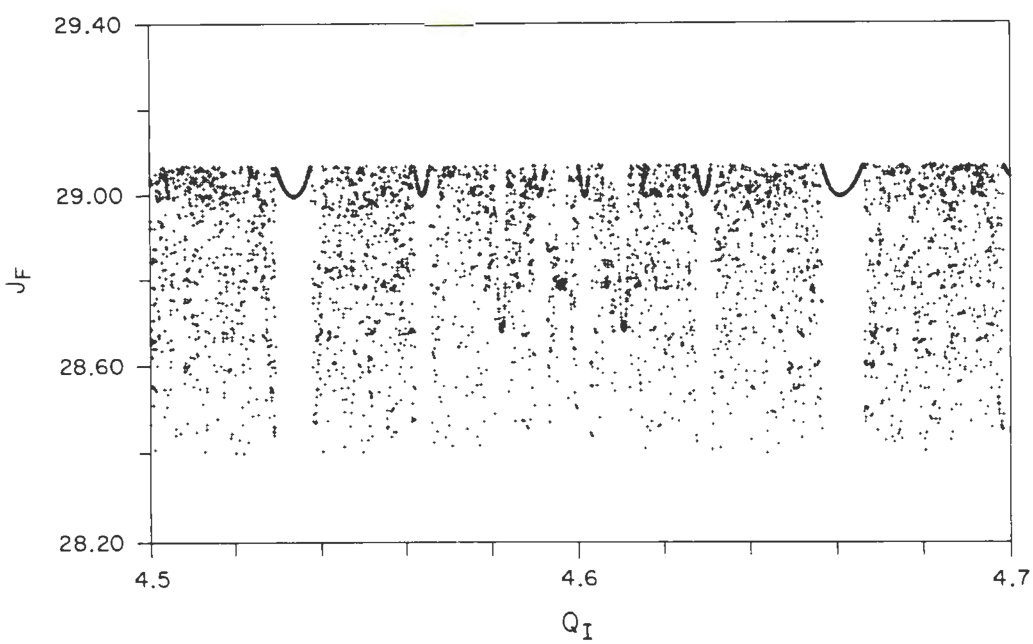
Using a Supercomputer for Theoretical Chemistry

Describing the motions within atoms and molecules is a goal of chemistry and physics. A detailed understanding of these "nonlinear dynamical systems," which have received much attention since the late 1970s, could provide insights into how they are affected by molecular collisions, laser irradiation, and other perturbations.

"Chaos, currently a hot topic in science, has been found in almost every dynamical system ranging from nuclei to planets."

Almost every molecular or atomic system has been found to exhibit two very different types of motion. In the ground state, there is a stable, or quasiperiodic, motion. However, if a certain amount of excitation energy is deposited in the system as a result of molecular collisions or absorption of a laser photon, the motion becomes random, or chaotic. This chaotic motion was unknown until 1964, when high-speed digital computers were first used to simulate the motions of a set of objects believed to be governed by classical mechanics, such as the solar system. Before then, analytical methods always revealed only quasiperiodic motion. Chaos, currently a hot topic in science, has been found in almost every dynamical system ranging from nuclei to planets. (See the book review of *Chaos* on page 62.)

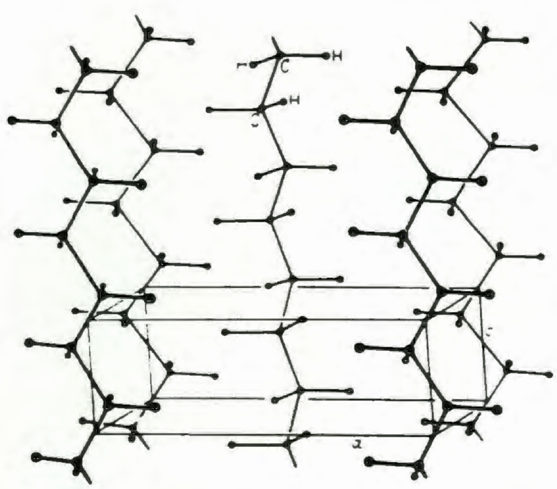
During the past 15 years (10 of them at ORNL), I have studied quasiperiodic and chaotic behavior in the infrared (IR) multiphoton dissociation of molecules, molecular collisions, atomic dynamics



This fractal region of the energy-transfer map for a helium atom colliding with a diatomic molecule of iodine (I_2) was produced by the author in collaboration with S. D. Gray and S. A. Rice of the University of Chicago.

in strong magnetic fields, nuclear dynamics of the gamma-ray laser, and dynamics of polymers (complex chemical compounds consisting of repeating structural units). I have pioneered several of the methods used for these studies in collaboration with M. L. Koszykowski of Sandia National Laboratories and R. A. Marcus of the California Institute of Technology.

Most analyses of dynamical systems require the use of a supercomputer to solve large sets of coupled, nonlinear differential equations or to diagonalize large matrices. Recently, we have used the Cray X-MP at ORGDP to study chaos in molecular collisions. Using 10 h of computing time, we generated an energy-transfer map (shown on opposing page) of an atom colliding with a



Drawing of a polyethylene crystal.

diatomic molecule. This map is an example of a function called a fractal (i.e., any further magnification, or finer grid, of the map would show a similar set of scattered points). The extensive Cray calculation was needed to show that this function has a dimension greater than the normal Euclidean dimension of a line and is a result of classically chaotic motion.

Investigating both the physical and chemical properties of polymers is a related new initiative in the Chemistry Division. As part of that effort, we have started to develop a computer model for the dynamics of large polymer molecules. Our current goals are

- To conduct large-scale simulations of macromolecular motion, using molecular dynamics models, and
- To develop better methods to make these calculations routine.

We plan also to extend our understanding of nonlinear dynamics and chaos in simple systems to the more complicated (many-body) structural problems of polymers.

Our projects will investigate the detailed process by which a poly-ethylene chain melts on a surface and the energy flow in polymers irradiated by a beam of IR light. We also plan to calculate the various spectral properties of polymers and to study the Condis crystal, a conformationally disordered phase in polymers discovered by Bernard Wunderlich, a University of Tennessee-ORNL Distinguished Scientist. Because of the larger number of atoms to be simulated and, consequently, the much larger number of numerical calculations required, we are fortunate to have available to us the capacity of the Cray X-MP and the support from staff members of the Energy Systems Computing and Telecommunications Division.—*Don W. Noid, Chemistry Division*

"Recently, we have used the Cray X-MP at ORGDP to study chaos in molecular collisions."

Supercomputing and Reactor Safety

The 100 commercial nuclear power plants currently operating in the United States generate about 17% of the total electricity produced annually. Forty of these plants employ the boiling water reactor (BWR) design. Thus, the continued safe operation of BWR plants is a matter of great national importance and public concern.

> **"The scope of phenomena that must be considered in these analyses is, perhaps, without parallel in any other field of simulation."**

Since 1980, ORNL has made significant contributions to the improved safety of all commercial BWR power plants through work conducted in the BWR Severe Accident Technology (BWRSAT) Program for the Nuclear Regulatory Commission (NRC). This work, centered in ORNL's Engineering Technology Division, is providing new insights into the physical phenomena and processes that likely would occur in the event of a severe or "core-melt" accident in a commercial BWR power plant.

Accident scenario. One scenario for such accidents assumes the complete failure of all normal and emergency core-cooling systems, an extremely unlikely event. The failure of these systems, coupled with the continued boiloff of water in the reactor, would gradually reduce the reactor's water inventory and eventually expose the hot nuclear fuel. Once uncovered, the fuel temperature would increase significantly, leading to melting of the reactor core and subsequent breach of the reactor vessel.

After reactor vessel failure, the hot core debris would fall onto the concrete floor of the primary containment, causing complex chemical reactions that release a mixture of combustible gases (hydrogen and carbon monoxide), aerosols, and fission products. These reaction products would heat and pressurize the primary containment, which could ultimately fail, releasing fission products, aerosols, steam, and combustible gases (cumulatively referred to as "blowdown") into the surrounding reactor building or secondary containment. The aerosols and fission products would migrate through the reactor building, driven by primary containment blowdown and combustible gas deflagrations (combustion of hydrogen and carbon monoxide gases inside the reactor building). Some of the radioactive fission products could eventually be released to the surrounding environment.

The goal of the BWRSAT Program is to provide best-estimate analyses of all of the phenomena in the scenario described above. Particular emphasis is placed on predicting the timing of key events (e.g., the time lags between the initial loss of coolant and events such as reactor vessel and primary containment failures) and on estimating the environmental releases of fission products.

The scope of phenomena that must be considered in these analyses is, perhaps, without parallel in any other field of simulation. These phenomena include neutronics, thermodynamics, heat transfer, mass transfer, fluid flow, metallurgy, chemistry, aerosol transport, combustion phenomena, and structural mechanics. This is obviously a formidable challenge for both analyst and computer.

New codes for the Cray. The basic simulation tools employed in the BWRSAT Program are a new generation of computer codes (BWRSAR, CONTAIN, and MELCOR), which incorporate state-of-the-art simulations of the appropriate phenomena, and the Cray X-MP supercomputer at the Oak Ridge Gaseous Diffusion Plant, which enables engineers to use these new codes realistically and economically.

The BWRSAT work uses these tools in combination with detailed plant descriptions (models) to provide analysis capabilities undreamed of just a few years ago. ORNL researchers have pioneered studies of the ability of reactor buildings to retain fission products released from the primary containment during severe accidents. This capability has recently become the focus of much attention within the NRC and the nuclear power industry.

Current ORNL investigations are evaluating the ability of BWR reactor buildings to withstand the pressures and temperatures generated by the combustion of hydrogen and carbon monoxide in the reactor building following primary containment failure. The computer code used for these studies is MELCOR—a 500,000-line FORTRAN code developed by Sandia National Laboratories for the NRC. Although MELCOR simulates a wide variety of phenomena (including core heatup, fuel melting and relocation, reactor vessel failure, core-concrete interactions, primary and secondary containment response, and fission product and aerosol transport), only the containment analysis capabilities of the code are exercised in the present studies.

A typical ORNL MELCOR secondary containment model might consist of 26 computational cells or control volumes that represent the various regions within the reactor building. MELCOR performs mass and energy balances for each cell; calculates cell pressures and atmospheric and structural temperatures; simulates hydrogen and carbon monoxide deflagrations; and tracks the flow of gases, aerosols, and fission products through the reactor building. Within the MELCOR model, the primary containment blowdown can be assumed to enter one or any combination of cells.

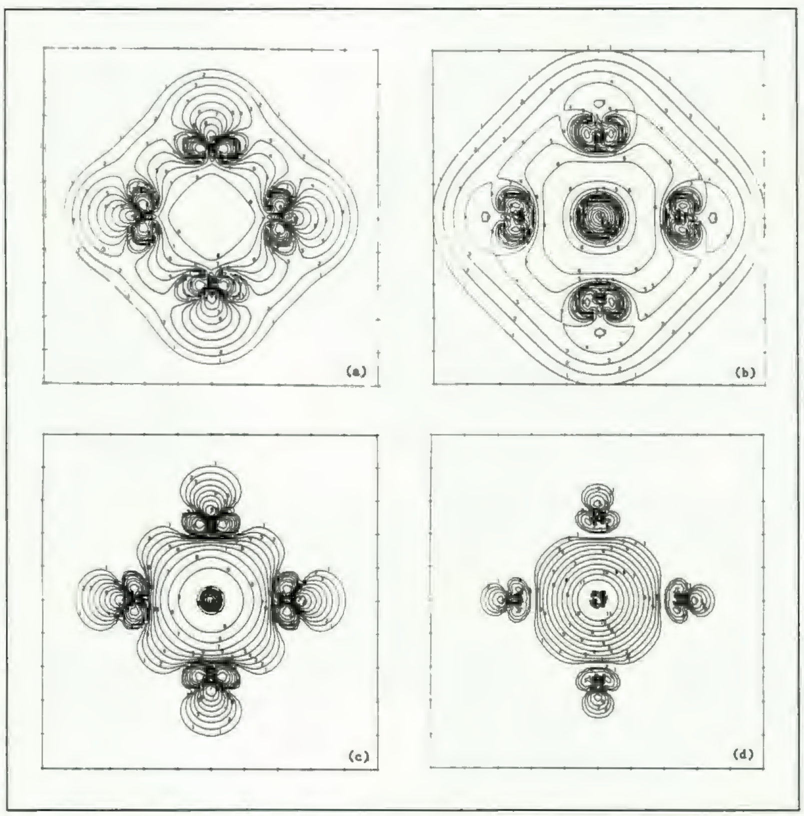
The accident analysis period of interest for these calculations typically ranges from 1 to 10 h, and the computation time depends on factors such as model formulation and the physical phenomena chosen for investigation. Computing time on the Cray generally ranges from 30 min to 10 h. A recent series of calculations required 6 h of computing time for simulation of a 2-h transient event. Such simulations would not be feasible on less powerful computers. In fact, codes such as CONTAIN and MELCOR typically execute 5 to 100 times faster on the Cray X-MP than on the IBM-3033 system.

Reactor buildings contain releases. In some scenarios, as much as 98% of the aerosols released into intact reactor buildings may be retained, never reaching the surrounding environment. The results of recent analyses indicate, however, that the structural integrity of reactor buildings may be challenged in some accident sequences. Much work remains to be done in this field, and many uncertainties persist. However, ORNL's resource triad of experienced and skilled personnel, state-of-the-art severe accident simulation software, and the Cray X-MP ensures our future as a national center for BWR severe accident research.—*Sherrell R. Greene, Engineering Technology Division*

"Codes such as CONTAIN and MELCOR typically execute 5 to 100 times faster on the Cray X-MP than on the IBM-3033 system."

Supercomputers in Materials Science Theory

It has been recognized for over half a century that the physical and chemical properties of materials ultimately depend upon the electronic bonding interactions among the component atoms, as described by quantum theory. But understanding the cohesive properties of materials remained a challenge to theorists, until the breakthroughs in theoretical technique and computer performance achieved during the past decade and a half. As a result, the total energy of most crystalline solids can now be calculated, greatly advancing scientists' understanding of the cohesive properties of such materials.



Contour plots of orbital charge density for strongly bonding states in octahedral nickel clusters: (a) bare nickel and clusters containing (b) lithium, (c) carbon, and (d) fluorine atoms. The plot plane bisects the octahedron intersecting four nickel atoms and the impurity atom at the center. Adjacent contours differ by a factor of 2, with initial value = 0.0001 (contour 1).

There are two important factors underlying these advances. One is refinement of the local spin density approximation (LSDA), a theoretical concept that relates the total energy of an atomic system to the electronic charge density. The second is great improvement in computer capacity and performance. The LSDA provides a reliable and tractable framework for describing the interactions between electrons during bonding, while recent advances in computer design have provided the means to carry out the complex calculations involved in first-principles studies.

Using these advanced tools—the LSDA concept and supercomputers—materials scientists have made great progress in understanding cohesion in materials where the atoms occupy ordered sites on an underlying crystal lattice. However, some of the most interesting materials science problems have remained beyond the scope of contemporary theoretical techniques, because most materials contain impurities, defects, and areas of structural disorder. Only in the last few years have the advanced computer programs and computer power been developed to treat such problems. Materials science theorists are now beginning to understand the atomic-level factors that are important in designing materials with specific improved mechanical properties.

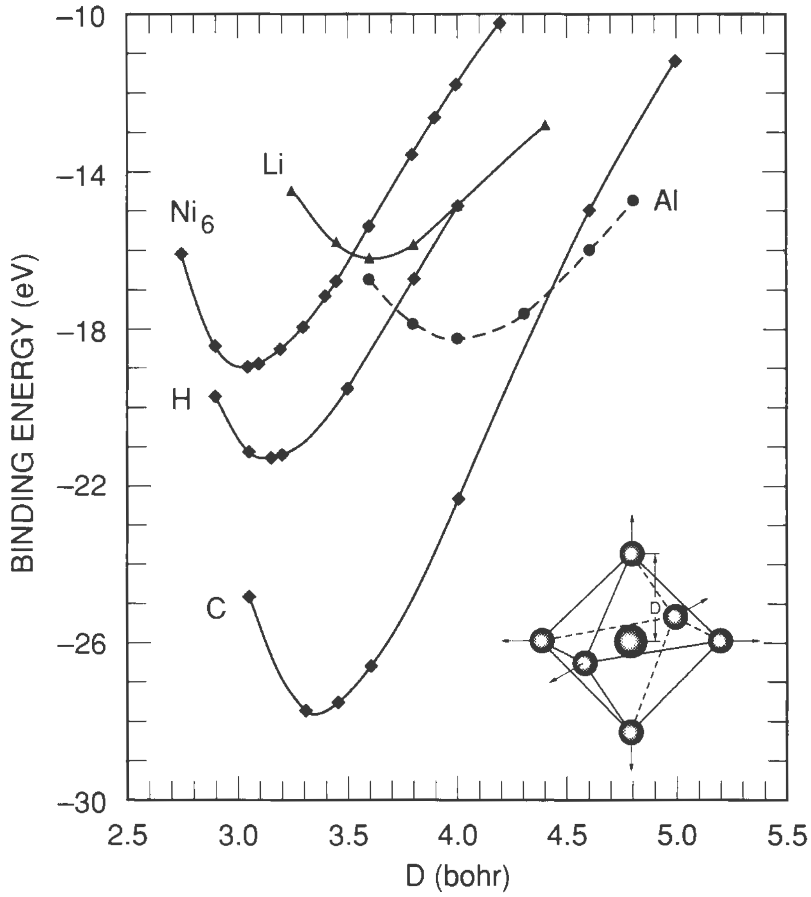
Modified nickel aluminide alloy. An outstanding example of an ORNL development in this area was the design of a strong, ductile, new nickel aluminide alloy for high-temperature service. This superior material was developed, using microalloying procedures, by the Alloying Behavior and Design Group of ORNL's Metals and Ceramics Division. The leader of this group, C. T. Liu, recently received a 1988 E. O. Lawrence Memorial Award from the U.S. Department of Energy for his work in alloy development.

Before this recent work was done, $L1_2$-phase nickel aluminide alloys had very limited applications, because the materials are intrinsically too brittle to be fabricated into useful structures. The grain boundaries (interfaces between grains in the solid material) are structurally disordered regions that attract impurities from the bulk material, causing embrittlement and severely affecting performance. The key to controlling this grain boundary brittleness in the ORNL nickel aluminide alloy was the discovery that minute additions of boron to the correct alloy composition resulted in strong interfacial cohesion. The new ORNL-designed material is ductile and can be easily fabricated. Five companies have already obtained nonexclusive licenses for the commercial use of the improved aluminide alloy.

Why boron? At first the question of *why* boron enhances interfacial cohesion in grain boundaries of the alloy seemed beyond the scope of conventional theoretical techniques. However, I have recently developed, collaboratively with Frank Averill of Judson College, Illinois, a new atomic-cluster theoretical approach called the augmented Gaussian orbital method, which solves the LSDA equations for model atomic clusters of arbitrary composition and structure. This approach had the potential for explaining why boron produced this remarkable enhancement of cohesion (whereas most impurities cause embrittlement). With our new technique, we addressed the problem of explaining the effects of boron and other impurities on the properties of nickel aluminide. First using various atomic clusters to model the grain boundary region of the nickel aluminide alloy, we then calculated the effects of various impurities on the binding energy and interatomic forces in the clusters.

Value of the Cray X-MP. Great care and accuracy are required in all phases of our work, because the energy differences of interest are in the parts-per-million range. Supercomputers such as the Cray X-MP are extremely useful in performing these intensive calculations. To understand how various impurities affect the cohesive strength of grain boundaries in nickel aluminide alloys, we first calculated the binding energy as a function of interatomic separation for several bare-host clusters (nickel, aluminum, and mixed metal) as reference systems. The calculations were repeated for impurity-containing clusters to determine the effects of inserting impurity atoms in octahedral host clusters representing the open sites where impurities bond in grain boundaries (see figure above).

Our research showed that the effects of various impurities on the cohesive and mechanical properties of the host material are profoundly



Binding energy curves for various impurity atoms in nickel host clusters.

different. The figure shows the binding energy curves we calculated for various impurity atoms [hydrogen (H), carbon (C), lithium (Li), and aluminum (Al)] when they occupy the interstitial octahedral site in a Ni_6 host cluster. The curve labeled Ni_6 represents the bare-host reference curve.

"One key to our continuing advancement in . . . materials science problems is the availability of high-performance computers."

Various impurities affect the cohesive properties (indicated by the curve depths) and mechanical properties (as defined by the energy variation with Ni-Ni atom separation) in very different ways. Both Li and Al impurity atoms have a destabilizing (embrittling) effect on the nickel host clusters, while H and C bind strongly and have a stabilizing effect on the host.

An analysis of our calculation results enabled us to identify the atomic-level factors important in determining these effects of impurities on interfacial cohesion. In particular, the results from our study of boron and sulfur in nickel clusters provided the first reasonable explanation of why boron enhances cohesion in grain boundaries of superalloy nickel aluminide, whereas most impurities, such as sulfur, are embrittling species.

Superconducting oxides. The study of superconducting oxides represents another materials area where supercomputers will play an important role. Nancy Wright, Bill Butler, and I have initiated studies in the Metals and Ceramics Division to understand the interatomic forces underlying structural stability of the high-temperature superconducting ceramics. The complexity of these systems will require extensive computing resources for performing the calculations involved.

One key to our continuing advancement in applying electronic structure theory to more realistic models for complex materials science problems is the availability of high-performance computers. In a sense, the computer serves as the experimental tool of the theorist, allowing new concepts to be explored through calculations. Our analysis of electronic structure calculations is greatly aided by computer visualization of the results, such as the electron orbital densities shown in the figure on page 14. Future advances in this field will bring us nearer the ultimate goal of designing materials to have specific desirable qualities, based on an understanding of the atomic-level interactions involved.—*Gayle S. Painter, Metals and Ceramics Division*

Fusion Calculations on Cray Supercomputers

Many aspects of fusion energy research require large and complex computations. For example, the ORNL studies of the dynamics or motion of fluid plasmas magnetically confined in three-dimensional configurations (nonlinear magnetohydrodynamic, or MHD, studies) were made possible only when supercomputers became available to perform the necessary computations. The MHD model assumes that the plasma is an electrically conducting fluid, which can be confined inside a magnetic field because it tends to flow along field lines but not across them. The most common magnetic field configurations currently used in fusion research are toroidal (doughnut-shaped) fields that hold the plasma within a finite region, away from the fusion vessel walls.

Plasma instability problems. The sudden growth of instabilities in a plasma is a major problem in keeping it confined long enough for net fusion energy to be produced. Considering the plasma as a fluid, we can imagine that vortices develop; like wire loops moving in a magnetic field, these vortices induce currents in the fluid. In turn, these localized currents create perturbations in the confining magnetic field. The current loops in a magnetic field also exert forces on the fluid that may either reinforce the initial vortex (the unstable case) or damp it (stable case). In the unstable case, the magnetic field perturbations can be large enough to change the direction of the field lines, causing them to wander radially. They may even touch the vessel wall, resulting in a loss of plasma confinement.

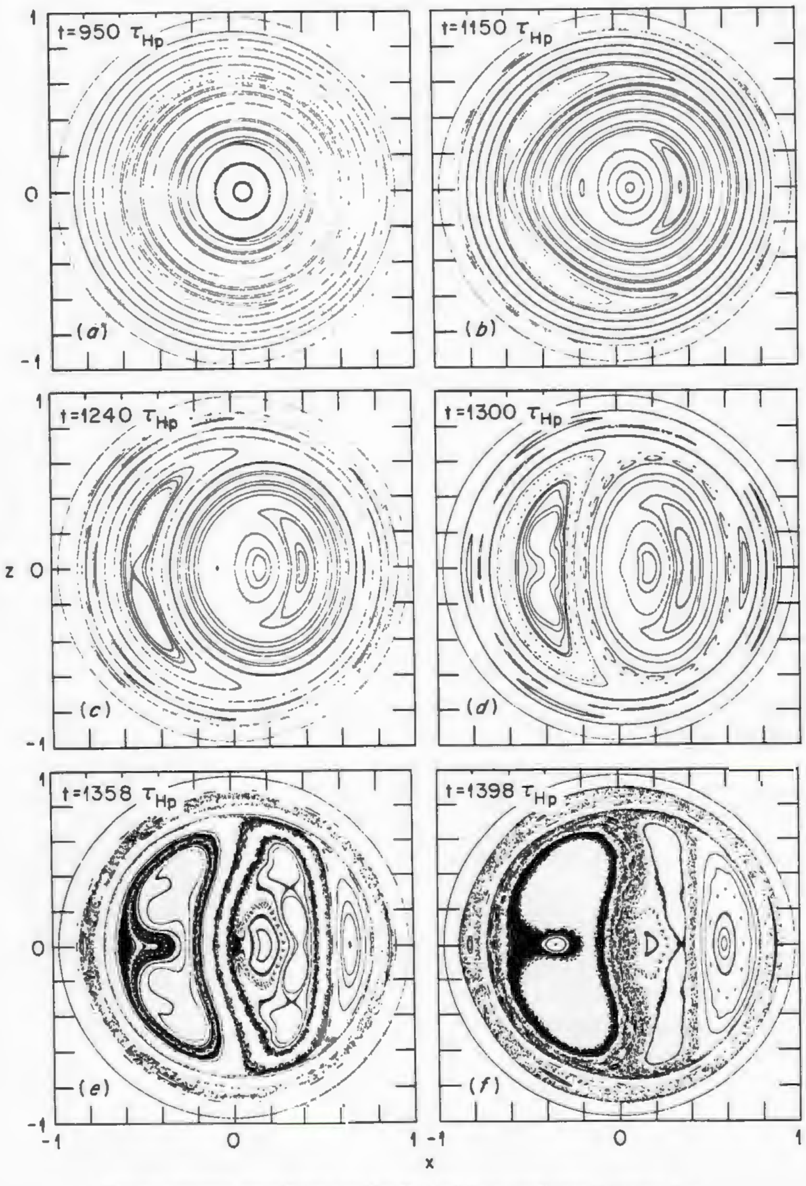
ORNL researchers are investigating these plasma instabilities and their consequences for plasma confinement in an effort to find ways to avoid them. These investigations will increase our understanding of the confinement properties of plasmas in existing fusion devices such as ORNL's Advanced Toroidal Facility and guide the design of more-advanced experimental devices.

From a mathematical point of view, the MHD model is defined by a system of seven partial differential equations in time and three spatial coordinates, with boundary conditions given on a torus. The intrinsic three-dimensionality of the problem demands large amounts of computer data storage. The problem is further complicated by the disparity in the time scales involved. The instabilities can develop within a microsecond. However, to assess their consequences for plasma confinement, we must follow their evolution for times on the order of 10 to 100 s. This determines the maximum time step for the calculation and implies that the number of time steps in the computation is on the order of 10^8.

The figure on page 18 shows a torus cross section at several times in the calculated evolution of a large-scale instability. Before the instability is triggered, all magnetic field lines lie on nested tori (shown as slightly shifted circles). As the instability grows, the magnetic topology changes and large magnetic "islands" develop (from field lines that wander radially in an organized fashion). Because of the nonlinear interactions between the large-scale modes of instability, chains of smaller islands are generated ($t = 1300$). When the magnetic islands overlap ($t = 1358$ to 1398), the magnetic lines wander radially in a chaotic fashion and confinement is lost in most of the plasma volume.

"Through the use of advanced numerical and computational techniques and the Cray-2 supercomputer, we can now solve problems of MHD turbulence that were previously impossible."

The California Crays. Because complex studies such as these are not possible without supercomputers,



Torus cross sections calculated for various times in the evolution of a fusion plasma instability.

the creation of the National Magnetic Fusion Energy Computer Center at Lawrence Livermore National Laboratory (LLNL) was critical to the development of this field. The Center provides two Cray-1 computers and a four-processor Cray-2 for fusion research and a two-processor Cray X-MP for energy research. ORNL's Fusion Energy Division normally uses the Cray-2 for the nonlinear MHD calculations. This supercomputer has a memory of 64 million words, which is shared by its four processors.

For 1988, the Department of Energy has allocated 1800 h of Cray-2 computing time to ORNL's Fusion Energy Division. The complexity of the calculations requires us to optimize our use of even this large allocation of time. Multitasking our calculations, or dividing them into simpler tasks that can be performed independently and in parallel on the four processors, is an important step in this optimization that leads to reduced costs for memory and throughput time.

Personnel in the Martin Marietta Energy Systems Computing and Telecommunications Division have worked closely with Fusion Energy Division theorists to develop a multidisciplinary approach to this nonlinear MHD research. Through the use of advanced numerical and computational techniques and the Cray-2 supercomputer, we can now solve problems of MHD turbulence that were previously impossible. For this work, we solve the equivalent of a half-million coupled nonlinear differential equations for 10,000 independent time steps. This level is still short of the computational demands expected for parameters of new fusion experiments with hotter plasmas. However, the information gained can be usefully compared with experimental measurements at the plasma edge. The results will substantially enhance our current understanding of the basic turbulence mechanisms and will make valuable contributions to the development of analytical fusion theory.—*Vickie Lynch, Energy Systems Computing and Telecommunications Division, and Ben A. Carreras, Fusion Energy Division*

Theoretical Atomic and Nuclear Physics

The advent of modern heavy-ion accelerators and supercomputers has revolutionized atomic and nuclear physics. A wide variety of new phenomena have already been discovered using these advanced tools. Scientists in ORNL's Physics Division can now study collisions between nuclei as massive as uranium at relative speeds very near the speed of light and distances ranging from about the size of atoms to a scale much smaller than the individual protons and neutrons that make up an atomic nucleus.

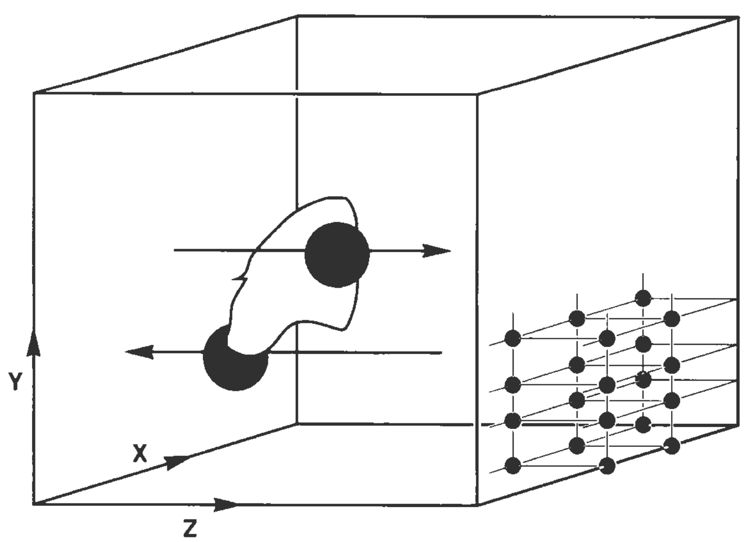
In studying the most energetic nuclear collisions, an interesting new feature has emerged: for short periods of time during the collision, the strengths of the electromagnetic forces (which hold the atom together) and the nuclear forces (which hold the nucleus together) become nearly equal. One of the new structures produced during this type of collision is a vacuum consisting of strongly coupled particle-antiparticle pairs. The new vacuum state decays, usually in $<10^{-19}$s, with the emission of the particle pairs. Experimentalists detecting the emission of these pairs are alerted to the fact that something unusual has occurred to disturb the normal vacuum. To interpret and verify what the experimentalist measures, it is essential to have a reliable means for computing the same phenomena using various theories.

The strong electric fields produced in these collisions can be as large as 10^{25} V/m, exceeding any other laboratory-produced electric field and comparable to the fields in the center of a neutron star. In contrast, the largest electrostatic fields that have been produced by conventional means were only $\sim10^{7}$ V/m, in ORNL's Holifield Heavy Ion Research Facility. The enormous nuclear-collision fields preclude the use of traditional analytical approaches for understanding the novel effects that appear. We found it necessary to completely reformulate the problem-solving method, to exploit the special advantages of supercomputer architectures. Our analysis method involves three steps:

- We first consider an approximation, based on a mean field picture, which reduces the complexity of the problem and results in a simpler, flowing-fluid description of the collision;
- We interpolate the fields, or fluid elements, using a linear combination of basis splines—mathematical devices introduced in the last century as a means for describing the contours of smooth objects such as the hulls of boats;
- We solve the mean field problem by evaluating the fields on a special space lattice. A diagram of the points on such a lattice is reminiscent of a crystalline solid.

To illustrate, the figure on this page represents a near-collision between uranium nuclei (solid circles) in a three-dimensional space lattice whose coordinate axes are shown in the lower left. The shaded region between the nuclei depicts the induced magnetic field.

Lattice field equations. In principle, the full quantum-mechanical, many-body equations of motion should yield an exact description of the



Representation of a colliding atomic or nuclear system in a space lattice.

"Our results lead us to believe that super-computers have an immense potential for nuclear and atomic physics applications."

nuclear collision, but the equations are not currently solvable. However, a simple model can provide us with a remarkably accurate view of the process. We treat the collision between the two heavy ions or nuclei as a fluid dynamicist treats the movement of complex bodies through a viscous fluid. Each nucleon or electron, as a first approximation, is considered to move independently in the field of the other particles. As each particle changes its position, the field it creates continuously changes. This is usually called a mean field picture of the collision, and the resulting motion of the nucleons or electrons is much like that of a classic magnetic field or fluid.

It is necessary to solve the mean field equations of motion without any other approximation. The wavefunctions of nucleons and electrons, and hence the mean fields, must be determined at each space point, x,y,z, and at each time, t, as the collision proceeds. The equations governing the motion of the mean fields are complicated nonlinear differential equations, which will not be discussed in this article, but we can imagine the colliding system placed in a box, as illustrated in the figure on page 19. Space inside the box is denoted by a mesh of points x_i, y_j, z_k. The size of this box depends on the problem under consideration: it would have to be tens of fermis (10^{-13} cm) across at the distance of closest approach of the colliding nuclei, and 10^5 times larger than this to describe the initial atomic states. The equations of motion governing the mean field can be represented by lattice field, or matrix, equations that can be solved in a straightforward manner with a variety of supercomputers.

Vector and matrix coprocessors. To solve our matrix equations, we have developed algorithms that exploit the respective advantages of the vector architecture of ORNL's Cray X-MP supercomputer and the matrix processing of the Floating Point array processor. These are the two principal supercomputers used by ORNL's Physics Division, and both machines can solve the lattice field equations of our studies with high efficiency.

The floating point FPS 164/Max array processor, which is accessible from the Physics Division VAX, is a pipeline machine with independent addition and multiplication processor units. The present configuration has 2.5 million words of fast memory and two matrix coprocessors, or Max boards. Each Max board consists of two addition and two multiplication processors. The basic machine cycle time yields addition or multiplication speeds of about 5.5 MFLOPS (Million FLOating Point instructions per Second) for each processor so that, as presently constituted, the system has a maximum cycle capacity of 55 MFLOPS. The specialized matrix multiplication is handled quite differently on the Max array processor system than on a vector pipeline machine such as the Cray.

For example, a test calculation was carried out on both the Cray X-MP and the FPS 164/Max, achieving 70 MFLOPS on the Cray and 40 MFLOPS on the Max. Although the Cray required only half as much time to complete our test calculation, we found the use of the Max array processor to be more cost effective because charges for Cray use at ORNL are greater than those for use of the array processor. In fact, we could not have completed this work without the availability of the low-cost supercomputing capacity of the FPS 164/Max. Our results lead us to believe that supercomputers have an immense potential for nuclear and atomic physics applications, because so many computations in these areas can be reduced to such simple matrix operations as we have described.—*Christopher Bottcher and Michael R. Strayer, Physics Division*

Parallel Computers for Efficient Problem Solving

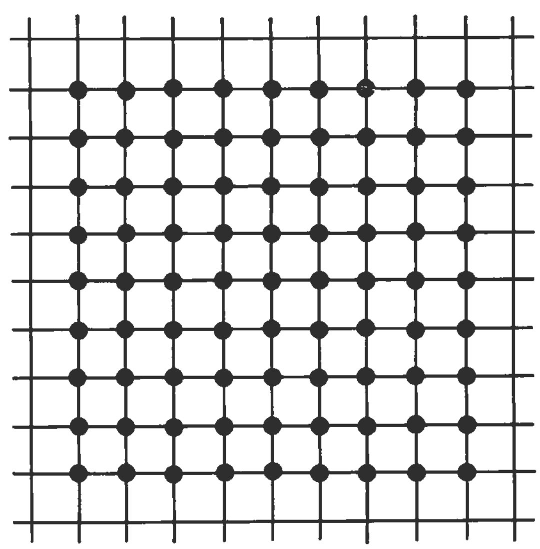
Computer users continually demand more computing power. Even on the current supercomputers, some relatively small problems can be intractable. For example, to accurately simulate the heat transfer in a 1-m^3 block using a simple computation method requires 4.8×10^{11} arithmetic operations per second of time simulated. For a computer to do the simulation in real time would require a sustained computation rate 1000 times greater than that achievable by a Cray X-MP.

To meet the need for greater processing speed, computer designs have emerged that make multiple processors available to the computer user, and almost all mainframe computers incorporate some sort of parallel processing. Existing parallel computers are generally one of two types: shared-memory multiprocessors and distributed-memory multiprocessors. The shared-memory type allows all processors equal access to memory, usually through a common communication channel, or "bus." As the number of processors sharing a bus increases, the maximum distance between a processor and the memory increases, and so does the potential for contention between processors for control of the bus. Both conditions degrade the communication speed. Thus bus architectures cannot efficiently employ a large number of processors, although commercially available computers of this type exist with up to 30 processors.

Distributed-memory multiprocessors are characterized by a network of communication channels, each of which connects a processor to other processors and memory units. Typically each processor has a local memory of limited size. When a processor needs data stored in a memory other than its own, the computer program must explicitly request transmission of those data. Extra programming effort is required for coordinated data movement. Because communication channels are not shared in distributed-memory architectures, they are more efficient than bus architectures in the use of processors and memory. But the lack of equal access to memory by all processors makes the use of distributed-memory computers more difficult and more limited.

Not all types of problems lend themselves to a parallel solution. However, our experience shows that a number of computationally expensive problems can be efficiently solved on parallel computers. For example, ORNL's Intel hypercube, a distributed-memory multiprocessor, and the Sequent Balance 8000, a shared-memory multiprocessor, have been used for the numerical approximation of problems in molecular dynamics, stress analysis, magnetohydrodynamics, contaminant transport, and electrostatics. All of these problems can be posed as partial differential equations (PDEs), and parallel computers seem to be particularly well-suited to their numerical approximation. In our work we have developed methods for solving several common types of problems, performing the exhaustive calculations on a distributed-memory multiprocessor.

Parallel solution of PDEs. Usually the solutions of partial differential equations are functions over some spatial domain—for example, the velocity of a fluid in a pipe or the electromagnetic potential on a plate. The solution may also vary with time. When solving such equations, it is sufficient to know the solution at some finite time point and locations within the spatial domain. For example, if the solution is defined on the unit square, then it may be enough to know the value of the solution at the points of intersection of the square with some uniform grid (see figure).



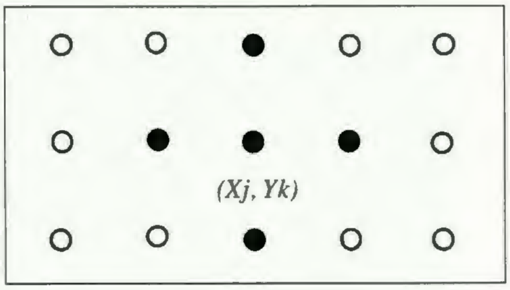
Example grid in unit square.

Partial differential equations express a relationship between the solution function and the problem data. A standard approach to numerically approximating the solution at the grid locations is to replace the PDE with an algebraic equation that relates the solution values at the grid points to the problem data. This algebraic relation is a *discretization* of the PDE. If some care is taken, the solution of the discrete problem approximates the corresponding solution of the partial differential equation. It is the discretized PDE that must be solved using parallel computation.

The efficiency of this computation is influenced by two factors: the computer's "load balance" and communication costs. If work is distributed unevenly, then most of the processors may be idle during much of the computation time—a waste of the computer's power. Even if the work is well-distributed, processors will be idle while they are waiting to receive the data they need to perform the next task. They are also effectively idle when they are too busy sending and receiving data to start the next computation task. These communication costs are strongly influenced by the relative positions of the processors within the network. A clever assignment of tasks to processors according to location can minimize the time spent forwarding messages to other processors as well as the time spent waiting for data to arrive.

"A clever assignment of tasks to processors according to location can minimize the time spent forwarding messages to other processors as well as the time spent waiting for data to arrive."

Explicit methods. Solving a PDE by an *explicit* method involves computing the solution value at a given location directly from data for nearby locations. For example, in a heat-transfer analysis, the temperature for time t, at location (Xj, Yk) in a grid, can be accurately approximated by using averaged data at time 0 from five nearby locations in the grid, if t is not too large (see the adjacent figure).



For this sample problem, the approximation of the solution at each location in the grid requires the same amount of computation, and it is best to compute the solution in parallel by

- partitioning the grid into equal-sized square blocks of locations and
- letting each processor calculate the solution values associated with one block.

Data for locations in the interior of a block are needed by only one processor, while data for locations on the boundary are required by more than one processor. Thus, dividing the computation according to this partition of the problem domain limits the sharing of data by the processors and makes the parallel computation efficient.

For a distributed-memory architecture, additional information is required. To specify the algorithm, we must

- assign the blocks of solution values that are near each other in the spatial domain to processors near each other in the computer and
- assign the data associated with a particular block of locations to a memory location near the processor that is calculating the associated solution values.

Because most of the data are needed in only one processor, they should be located as near as possible to that processor. The data that must be shared with other processors will require less computer time spent in transmission if all the processors needing this information are near its memory location. The optimal implementation of any explicit algorithm will depend both on the architecture of the multiprocessor being used and on the domain of the problem.

Implicit methods. Unfortunately, explicit algorithms are not always the best means to approximate the solution of the PDE. Generally, the approximation describes a relationship between a solution value, the nearby data values, and the nearby solution values. The discretization of the PDE is then represented by a system of coupled linear equations, also called a matrix equation. Thus the value of the solution at a given point is only *implicitly* defined for each time step. To calculate the solution values, we must use the parallel algorithms for solving simultaneous linear equations. This is currently an area of intense mathematical research and, for the most part, beyond the scope of this article. We will describe only some general approaches.

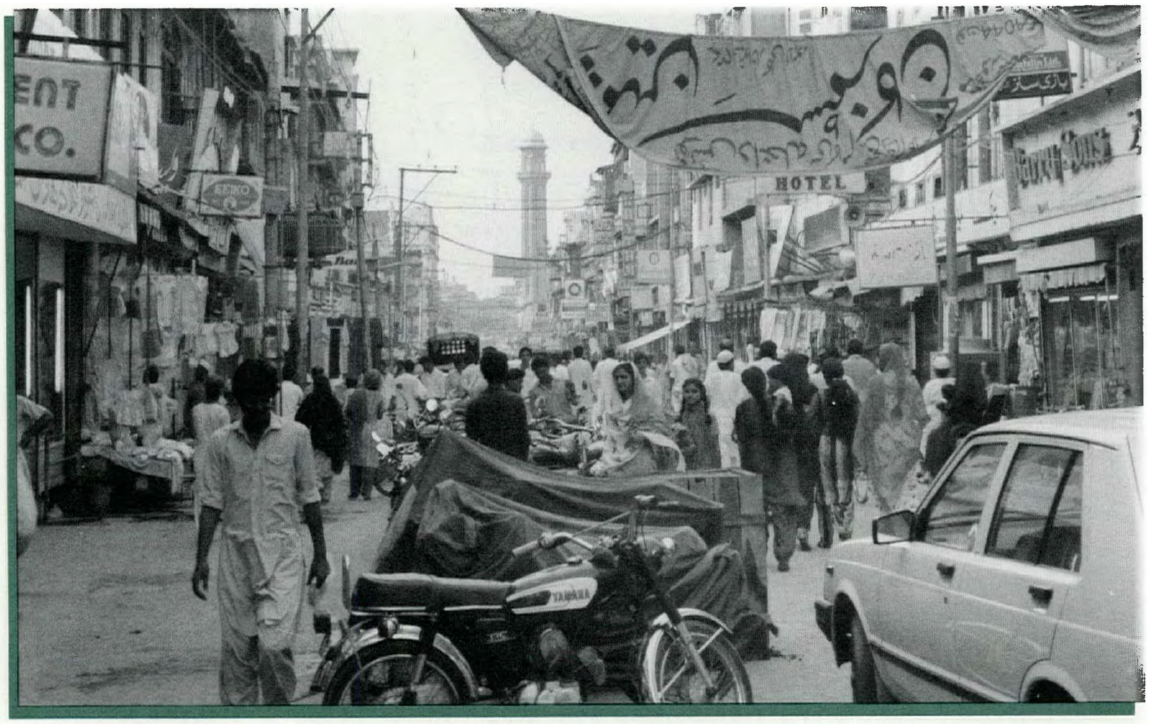
Techniques for solving matrix equations in parallel differ depending on whether the matrix has many nonzero entries (a "full" matrix), or only a few (a "sparse" matrix). The research of Mike Heath, Al Geist, and Chuck Romine of ORNL's Engineering Physics and Mathematics Division (EPMD) has led to excellent methods for the solution of matrix equations when the matrix is full, but the matrices for most PDEs are sparse, having perhaps only 10% nonzero entries.

There are two major approaches to solving sparse-matrix equations. The first, which calculates an exact solution, is similar to the algorithms for full matrices and is referred to as a direct method. Alan George and Esmond Ng, also of the EPMD, have been developing direct sparse-matrix algorithms for parallel computers.

The second major approach finds a solution to sparse-matrix equations by iteratively improving an estimate of the solution. Iterative methods are attractive for parallel processing, because each step of the iteration is relatively simple and can often be efficiently implemented on a multiprocessor. A particularly attractive method of this type, known as the preconditioned conjugate gradient method, has been implemented by a number of researchers on the ORNL hypercube. While iterative methods can work very well in parallel, they are not best for all problems. Typically, three-dimensional fluid dynamics problems are solved using iterative methods, while two-dimensional solid mechanics problems are solved using direct methods.

Conclusions. Neither the standard direct nor the standard iterative methods for solving PDEs were designed to be efficiently executed on multiprocessors. But our experiences using the ORNL parallel computers indicate that these multiprocessors are applicable to a wide range of energy-related research problems, and staff members of the Mathematical Sciences Section of EPMD are currently investigating new algorithms designed to exploit processing parallelism. Problems requiring the solution of PDEs seem particularly suited to the efficient utilization of parallel processors, and we have only briefly outlined some methods for utilizing parallelism in solving them. As the commercially available parallel computers increase in both number and speed of processors, they will increasingly be applied to the solution of computationally intensive problems.—*John B. Drake and Patrick H. Worley, Mathematical Sciences Section, Engineering Physics and Mathematics Division*

"Our experiences using the ORNL parallel computers indicate that these multiprocessors are applicable to a wide range of energy-related research problems"



Rising aspirations and population growth in developing countries such as Pakistan (shown here) add up to growing needs for energy services. The U.S. Agency for International Development, assisted by ORNL, is trying to help meet these needs.

Energy for Development: ORNL Returns to the Third World

By Thomas J. Wilbanks and Sherry B. Wright

The 1980s have been a quiet decade for energy research and development (R&D), as the energy crises of the 1970s have faded into the background. But lower prices for oil in world markets have not solved the energy problems of developing countries, where a shortage of reliable and affordable energy services has continued to slow the engine of social and economic development. At the same time, the growing appetites of these countries for commercial fuels have made them the fastest growing market in the world for energy technologies, and many observers believe that their energy decisions will have a profound effect on the world's total energy requirements (and the global environment) by the middle of the next century.

Since 1982, Oak Ridge National Laboratory has been involved in analysis and technical assistance to help developing countries meet their energy needs, as a part of the programs of the U. S. Agency for International Development (AID). In Asia, Africa, Latin America, and the Middle East, ORNL staff members from several divisions are working with their counterparts from the countries involved and with other colleagues to help solve current energy problems.

Of course, helping the developing world is not a new venture at ORNL. From 1959 through 1965, the Oak Ridge School of Reactor Technology trained 112 individuals from 27 countries—including Brazil, India, Indonesia, Pakistan, the Philippines, and Thailand—in nuclear reactor

ORNL subcontractor Jean-Roger Mercier and Energy Division's Robin Cantor record the weight, cost, and quality of a typical Malagasy family's charcoal purchase to meet a day's cooking needs. This kind of information is being tracked longitudinally by AID and the World Bank to reveal trends in actual household fuel costs throughout Antananarivo, Madagascar's capital and largest city.

hazards evaluation and operations supervision. In addition, ORNL staff members John Pinajian, Fritz McDuffie, Frank Plasil, and others lived and worked in developing countries as representatives of the former U.S. Atomic Energy Commission.

During this same period, ORNL was becoming a leader in examining the applications of "big science," such as the "Nuplex" concept, to development problems at a grand scale. As conceived by ORNL, a Nuplex would supply inexpensive power from a large generating facility—probably but not necessarily a nuclear plant—located on an arid seacoast in a developing region. A desalting facility would make fresh water from the seawater, pump this water inland to irrigate the desert, and provide electricity and thermal energy for the communities and agro-processing industries that would follow (see article in the *Review*, Summer 1967, pages 3–9). In the process, ORNL attracted world attention as a center of desalination expertise, stemming from the Laboratory's Molten Salt Reactor Program. By the early 1970s, ORNL was well-known in Asia and Latin America, and Laboratory leader Murray Rosenthal and others visited developing countries, such as Pakistan, to provide technical advice.

Because of the mushrooming demand for energy R&D and problem solving in the United States during the 1970s, the Laboratory's resources were needed at home, and ORNL's connections with developing countries decreased. In the 1980s, however, the situation changed as energy was shifted to the back burner as a domestic policy issue. ORNL needed innovative ways to keep its energy expertise fresh in order to be prepared to meet domestic needs certain to lie ahead. One response was to look for energy needs in other countries linked to U. S. government programs and the U. S. national interest.

AID, the U.S. government agency responsible for assisting developing countries, had developed significant energy programs during the 1970s. In 1982 a number of discussions among AID, the U.S. Department of Energy, and ORNL resulted in an interagency agreement with DOE to have ORNL conduct a one-year energy planning and assessment project in Liberia for AID.

Energy Planning for Liberia

Liberia is a small developing country on the west coast of Africa, about 10% smaller than the state of Tennessee, with a population of approximately two million people. In 1981, the gross domestic product (GDP) of the country was $841 million for the monetary economy and about $1 billion for the monetary and traditional economies combined (or roughly $500 per

"The most striking ORNL contribution . . . showed that Liberia should shut down its oil refinery rather than borrow money to upgrade it."

capita). This measure of development ranked Liberia a little below Bolivia, Zambia, and Indonesia but a little above Pakistan and the Sudan. During the late 1970s, the country's long-standing favorable trade balance had disappeared, as the bill for oil imports grew from $5.5 million in 1971 to $152 million in 1980 (in nominal dollars). The country was mired in a severe recession; real GDP was falling at the rate of 5% per year, and national indebtedness was rising rapidly.

It was natural to look to the energy sector for some of the solutions to Liberia's growing economic problems, but attempts in the late 1970s to identify initiatives in this sector had foundered because of a lack of reliable information about the country's energy system, its needs, and its options. At the request of the Liberian government, AID agreed to support a project to improve the base of information and to strengthen Liberian capabilities for energy planning. In turn, AID asked ORNL to conduct the project, in collaboration with Liberian colleagues and consultants from two universities and a private firm.

The initial project, a national energy assessment, was carried out over a one-year period in 1982 and 1983. At the time the project began, a highly factionalized energy policy-making system had led to a focus on three proposed actions: (1) large-scale development of hydroelectric power, which centered on the St. Paul Project, a proposed storage and generation facility (with an ultimate capacity of ~1000 MWe) at the confluence of two rivers upcountry; (2) renovating and upgrading Liberia's only oil refinery to increase its efficiency and shift its product slate toward lighter fractions (at an estimated cost of $50 million); and (3) domestic oil exploration and production, given the country's proximity to oil production offshore from the Ivory Coast. Working with Liberia's National Energy Committee (NEC), the U.S.–Liberian project team produced a summary assessment, 18 working papers, and a number of informal comments and advisories during that first year. The team was led by Bill Barron of ORNL's Energy Division and M.-H. Neufville, secretary of the NEC and director of what was then the Liberian Bureau of Hydrocarbons (now the Department of Energy) within the Ministry of Lands, Mines, and Energy. Seven ORNL staff members participated in the assessments that year.

By normal standards for such projects, the impact of that year's work was dramatic. Besides producing a mass of fresh data, which has been adopted by Liberian institutions and international lending institutions alike as a standard base for evaluating energy alternatives, the project changed the direction of energy policymaking in Liberia. The most striking ORNL contribution was a study, initially sketched out by Dick Barnes and later amplified by Garland Samuels and other Energy Division staff members, that showed that the country should shut down its oil refinery rather than borrow money to upgrade it.

An inefficient, simple, poorly maintained facility, the refinery was producing gasoline, diesel fuel, and other light petroleum products at a very high cost compared with world market prices. ORNL analyses showed that if, instead of refining oil within the country, Liberia imported oil products at world prices and sold them domestically at the higher prices to which domestic markets had become adjusted, the country would realize a revenue windfall of $15–20 million per year. This was equivalent to about a 2% increase in the GDP—a substantial payoff, indeed, from a $200,000 project! After this assessment was confirmed through an independent study by an international consulting firm, the refinery was shut down. As a result, Barron reported, the Liberian government was able to triple the tax on gasoline and diesel fuel while reducing prices at the pump by 10%.

Other contributions of the project may be equally important in the long run, even if they are less dramatic in the short run. For example, the project team showed that the proposal for the large St. Paul hydroelectric project was based on a demand forecast that ignored uncertainties about the country's rate of economic development during the next 20 years. A more appropriate strategy would be to add generating capacity in smaller increments, allowing it to be fine-tuned to the development actually experienced (e.g., first upgrading an existing hydroelectric facility).

As another example, the project team drew attention to Liberia's impressive wood resource, which could meet a sizeable share of the country's energy needs on a sustainable basis, especially in rural areas. Particularly interesting is the prospect of using wood gasification to power stationary internal combustion engines, which account for two-thirds of Liberia's oil consumption.

Other examples include the introduction, during an electric power shortage in December 1982, of a number of ideas about energy conservation and load management and the transformation of the NEC, which had previously been an ineffective body, into a major force for rational energy planning.

At the end of the first year, the government of Liberia and AID decided that further support was needed to help turn the project's information, ideas, and recommendations into a national energy strategy. Barron moved to Liberia for two years to serve as technical advisor to the NEC. ORNL staff provided support by conducting short-term analyses of still–unresolved issues, such as the economics of harvesting the wood resource and the potential for energy conservation in buildings. This period culminated with the issuance in June 1985 of *An Integrated National Energy Program for Liberia*, submitted by the NEC to the government of Liberia and adopted as the nation's energy strategy. In September of that year, just before Barron's return, he organized a retreat for high-level officials of the Liberian government, energy institutions in that country, major lenders, and others to discuss and publicize the strategy.

Soon afterward, a controversial election was held in Liberia and most development assistance from AID, the World Bank, and other lenders was placed on hold while the political situation was sorted out; thus, much of the strategy is yet to be realized. But it remains the road map being used by all parties interested in Liberia's energy future and the project itself was judged by AID to be one of the most successful on record. The refinery remains closed, the St. Paul project has been replaced by a successful rehabilitation of existing hydroelectric facilities, the possibility of wood-fueled facilities for power supply in rural areas is being actively explored, and the NEC is conducting energy planning and analysis on a continuing basis without external assistance.

ORNL's Role Expands

By 1984, AID's Office of Energy (see figure on page 29) was finding the entire program of which the Liberia project was a part—the energy planning and policy development (EPPD) portion of a larger program entitled Energy Policy Development and Conservation—difficult to manage. Without a staff arrangement for technical assistance, the program lacked coherence and was not producing the desired results.

AID decided that ORNL, which had performed impressively in Liberia, might be able to solve this problem. The Laboratory was world-famous as a diversified center of energy R&D, including energy policy analysis, and during the late 1970s, it had developed a strong reputation for program management (assisting busy federal program offices in connecting with the best available technical resources in the larger research community, based on the Laboratory's own technical strengths). With these qualities in mind, AID asked the Laboratory to lead and manage the EPPD project and, with the agreement of DOE, ORNL accepted this new challenge.

It seemed to ORNL that the first step should be to take a fresh look at energy conditions in developing countries in the 1980s. For example, by 1984, three years after EPPD program directions had been defined, oil prices had leveled and the dominant view within AID was that "the energy problem" had gone away, at least as a major priority for allocating scarce development resources. In addition, a major AID-sponsored conference in Reston, Virginia, in February and March 1983, held to take stock of the experience with national energy planning activities in developing countries, had concluded that, in many cases, national energy planning was not helping to meet energy needs. Quite simply, although the planning was sometimes being done reasonably well, it was seldom connected with actual decisions about major energy actions and investments.

"ORNL staff conducted short-term analyses of still-unresolved issues, such as the economics of harvesting the wood resource and the potential for energy conservation in buildings."

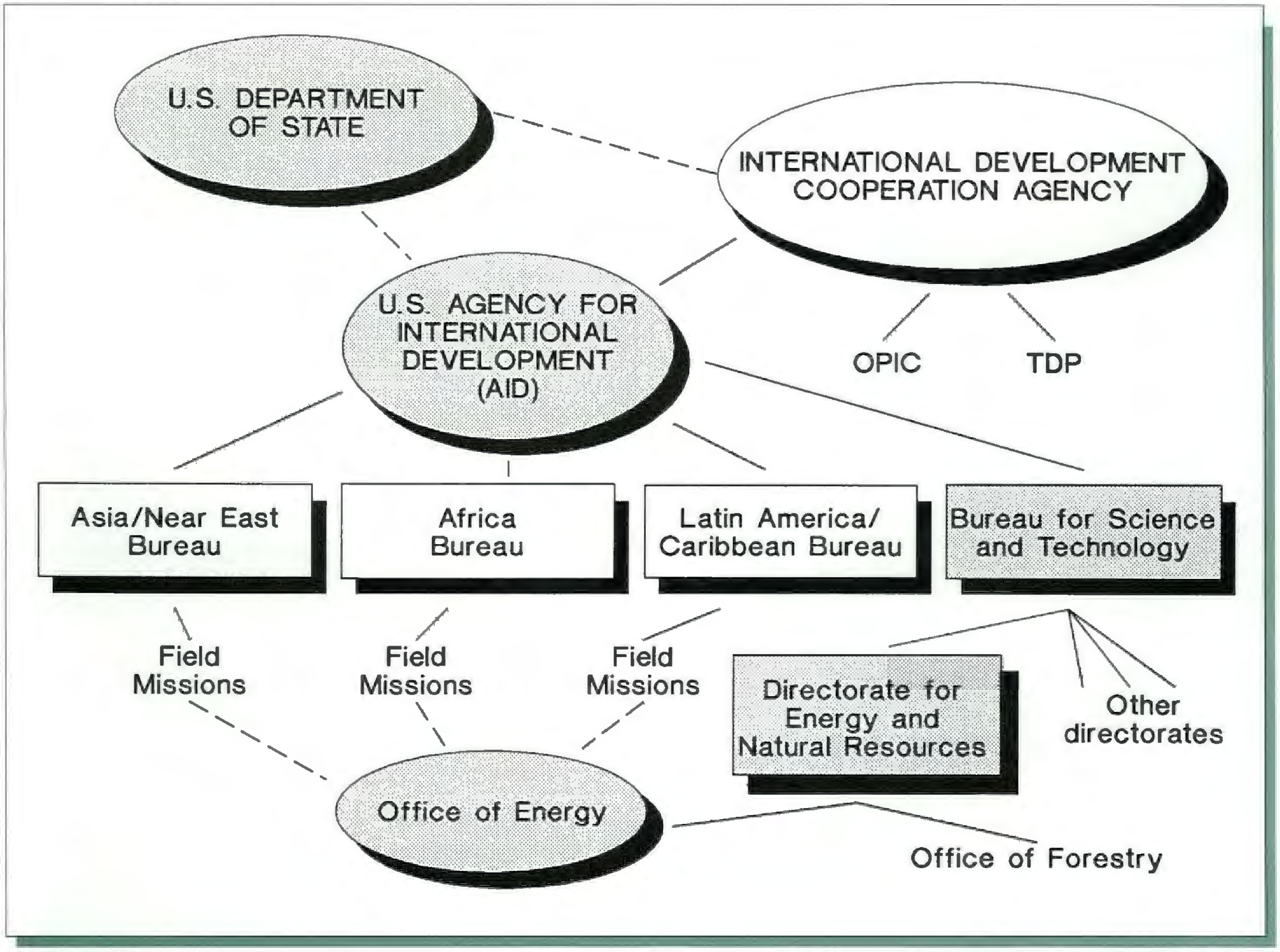
ORNL's Work for AID Is Global in Scope

	ASIA	AFRICA	MIDDLE EAST	LATIN AMERICAN CARIBBEAN
PROJECT ACTIVITIES TO DATE	PAKISTAN INDIA BANGLADESH PHILIPPINES INDONESIA*	LIBERIA ZAIRE MADAGASCAR SUDAN MALAWI KENYA	TUNISIA JORDAN MOROCCO*	HAITI COSTA RICA ECUADOR GUATEMALA CARIBBEAN* PERU*
WORKSHOP/ CONFERENCE PARTICIPATION	SRI LANKA NEPAL THAILAND MALAYSIA	BOTSWANA		BRAZIL CHILE
PROJECT ACTIVITIES UPCOMING	INDIA			
PROJECT ACTIVITIES UNDER DISCUSSION	PAKISTAN PHILIPPINES	NIGER SOMALIA SUDAN	EGYPT	BOLIVIA HONDURAS

*Through subcontractors

Out of a series of white papers by ORNL and several subcontractors, which were prepared as a part of the Office of Energy's first comprehensive program planning exercise, a different view took shape about the energy problem in developing countries in the1980s and of the challenges to AID and other development assistance agencies in their efforts to help with solutions. The studies targeted four major energy problems in most countries: capital requirements for power system expansion, needs for energy price reform, needs for adequate and affordable household fuels, and inadequate energy systems to support rural development. They also pointed out three general problems in the process by which energy needs of developing countries are addressed: insufficient attention to private-sector roles, a lack of attention to the process of implementing good ideas, and a failure to learn enough from experience.

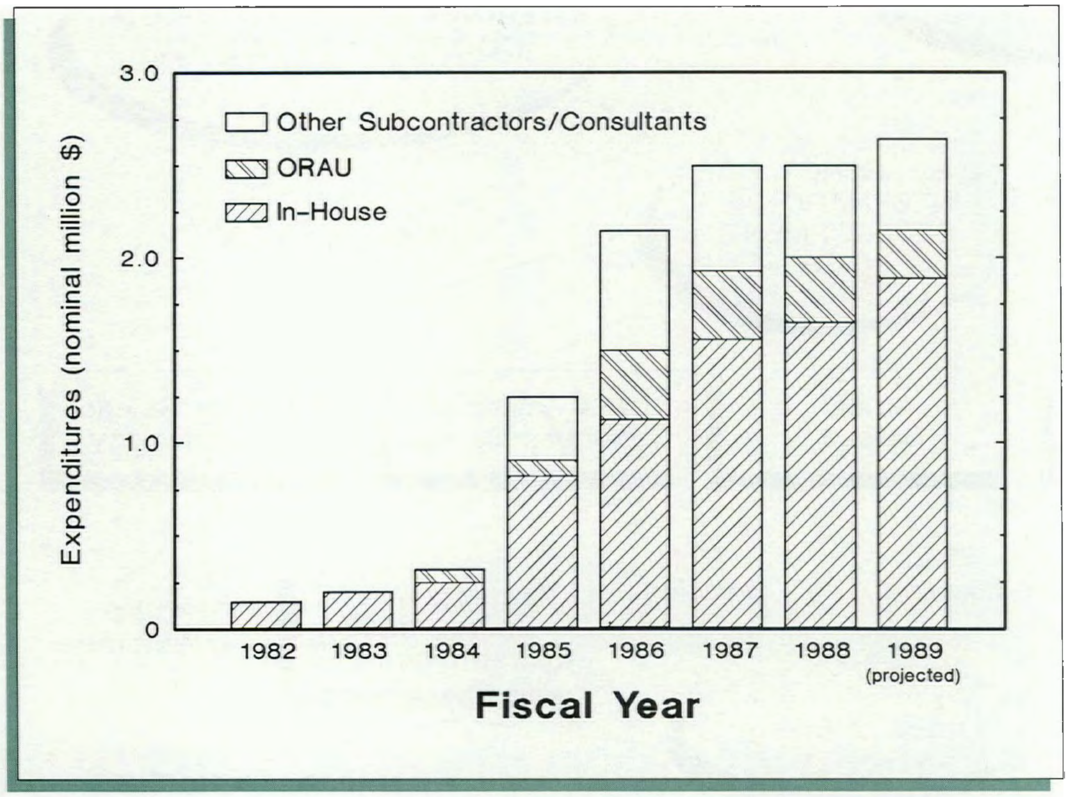
Another emerging problem that has significant ramifications for AID program planning was also identified. Increasingly, the development community is recognizing that the best development paths are sustainable ones. In other words, a strategy for development that exploits options that look attractive in the short run, but cannot be sustained over a longer term, can steer a country toward painful adjustments and changes, often just as economic growth is starting to take off. Clearly, such a trend should be anticipated and avoided if possible. In the energy sector, this concern has at least three manifestations: (1) the continuing reliance on imported oil; (2) wood fuel use associated with deforestation and ecological damage; and (3) the growing use of coal, especially in Asia, when management of the global environment may call for some constraints on fossil fuel emissions.



Organizational chart for AID.

Meanwhile, the 1986–1988 program plan of the Office of Energy called for an expansion of EPPD activities related explicitly to the new priorities; AID field missions were showing considerable interest in accessing ORNL's pool of technical resources through AID's Office of Energy. In addition, in 1985, the Laboratory was also asked to assume responsibility for a second Office of Energy program concerned with renewable energy applications and training (REAT). This combination of developments has resulted in substantial growth in ORNL-led AID projects. ORNL activities have reached $2.5 million per year in funding (see figure on page 30), with some of the recent growth reflecting support from AID field missions and regional bureaus. So far, the AID-supported work has involved 60 ORNL and Martin Marietta Energy Systems, Inc., staff members from the Energy, Environmental Sciences, Engineering Technology, Health and Safety Research, Fusion Energy, and Computing and Telecommunications divisions and the former Information Resources Organization, along with individuals from more than 90 subcontracted firms, universities, other national laboratories, and consulting practices. Project activities have taken team members to 26 developing countries, with activities upcoming in another and under discussion for six more (see table on page 28).

This rather sizeable and diverse activity is directed by Tom Wilbanks of ORNL's Energy Division, with substantial help from Al Ekkebus, Larry Hill, Ed Hillsman, Don Jones, Bob Perlack, Carl Petrich, John Reed, Bob Shelton, Dan Waddle, and Sherry Wright. Current directions and emphases, flowing directly from the analyses and planning conducted in 1984–1985, include power for development, household fuels, and institutional and policy reform.



The AID program at ORNL has grown rapidly.

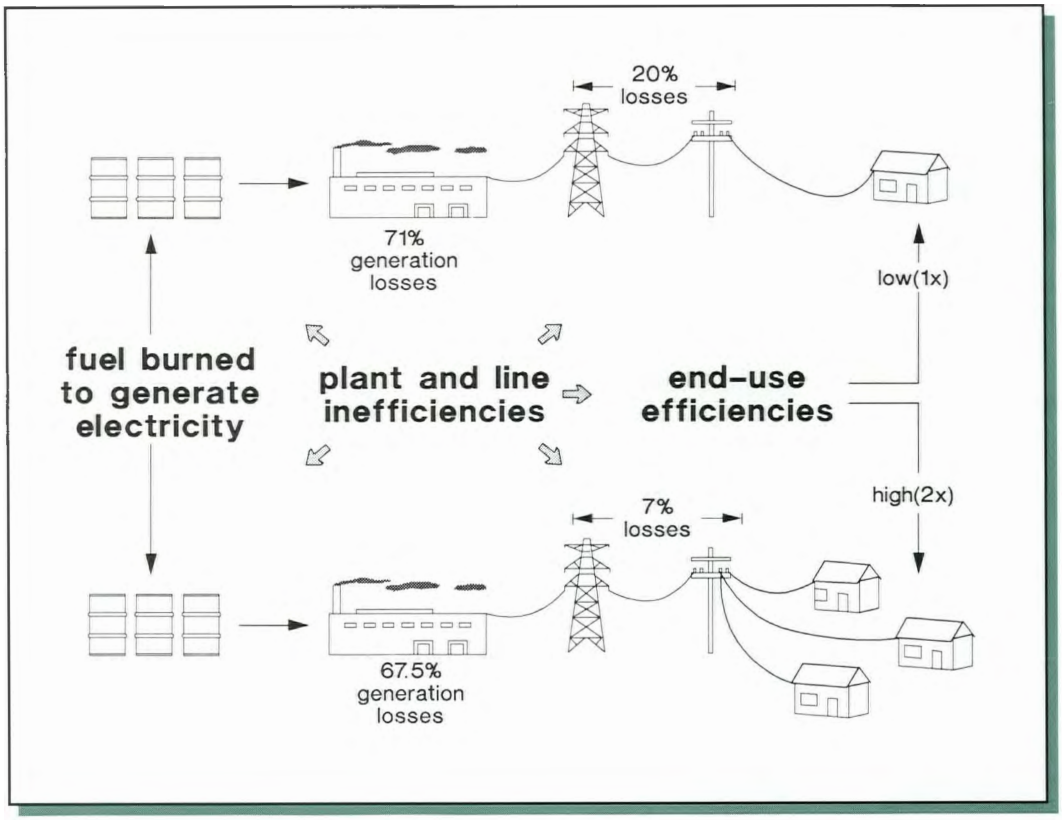
Power for Development

Throughout the developing world, electricity consumption is growing; annual growth rates in the range of 10 to 12% are common. According to the World Bank, this trend translates into a requirement for \$500 to \$900 billion in capital investment in the next 10 years for power system expansion in developing countries, or else the development process will be inhibited—a crisis indeed. If a solution is to be found for this power crisis, it lies in some combination of three strategies: (1) rationalizing energy prices to reduce demands resulting from inappropriately low prices, (2) increasing private sector roles in power sector financing, and (3) improving the efficiency of systems that provide electricity services to minimize the cost of increasing these services.

ORNL's power system planning program focuses on the third option: improving system efficiency through "least-cost" power system planning. For instance, in many cases the cheapest way to provide more electricity services (e.g., comfort, convenience, mobility, productivity increases) is not to build another power plant but to improve the efficiency of the power system: existing power plant operations, transmission and distribution networks, and end uses. During the late 1970s and early 1980s, many U.S. electric utilities became significant innovators in increasing efficiency. It seems certain that power system planners in developing countries can benefit from this experience. Power system efficiencies in developing countries are usually quite low (see figure on page 31), and adding new generating capacity—the approach assumed by the World Bank estimates—usually entails unnecessarily high capital costs for the services added. For example, a study conducted by Ed Hillsman of ORNL, David Jhirad of AID, and Pirooz Sharafi of Hagler, Bailly, and Company, Inc., indicates that an estimated capital requirement for power system expansion in India of more than \$50 billion in the next five years could be cut to \$30 billion or less by successful implementation of a least-cost approach to planning.

Putting such an approach to work in developing countries does not just depend on convincing the countries themselves of its merits, however. There is considerable evidence that the "least-cost" options are not always the most easily financeable options, and developing country decision makers are more likely to respond to signals from lenders than from analysts. Accordingly, the AID-ORNL program has also opened up a dialogue with the major development lenders, to pass on these perspectives.

Work at ORNL on the issues regarding power for development is also concerned with two other energy problems: power for rural areas and sustainable paths for energy system development. The current emphasis of activities related to rural power systems is on technological and institutional options for minigrids (i.e., medium-scale alternatives to extending the central grid, on the one hand, or self-generation, on the other). Bob Perlack of ORNL has helped to develop a strategy to pursue such options as: persuading a relatively large private-sector rural enterprise, for example a minerals extraction or agroprocessing plant, to generate enough power to meet needs of other users and sell it to a cooperative or other third party for distribution in a minigrid. Perlack and others have also analyzed the pros and cons of substituting a simple minigrid, connected to a small centralized power generator, for small decentralized equipment for water pumping. Advantages of the minigrid option include power for small rural industries (especially when requirements for water pumping are small) and for other village needs, as well as simpler operation and maintenance. Finally, David Eissenberg of ORNL's Engineering Technology Division has played a major role in preparing a basic guidebook on technologies for water lifting in developing countries.



Power system efficiencies in developing countries are usually quite low, placing heavy demands on energy and capital resources. For example, an efficient system (bottom) delivers 2.5 times more electricity services from a given amount of fuel than an inefficient system (top).

ORNL's program for AID includes three kinds of activities related to sustainable development. First, the Laboratory is helping to explore the role of coal and other solid fossil fuels in energy strategies for developing countries. ORNL organized the technical program for the first Pakistan National Coal Conference in 1986, at which Shelton, Wilbanks, and Eissenberg made presentations. R. Krishnan and others from the Engineering Technology Division are assisting an R&D institution in India in improving capabilities for evaluating experiments with fluidized-bed coal combustion. ORNL is leading AID's effort to determine the potential of coal as a wood-fuel substitute in developing countries. Additionally, ORNL is joining with Bechtel and Pyropower to assess the feasibility of using oil shale to generate electric power in Jordan.

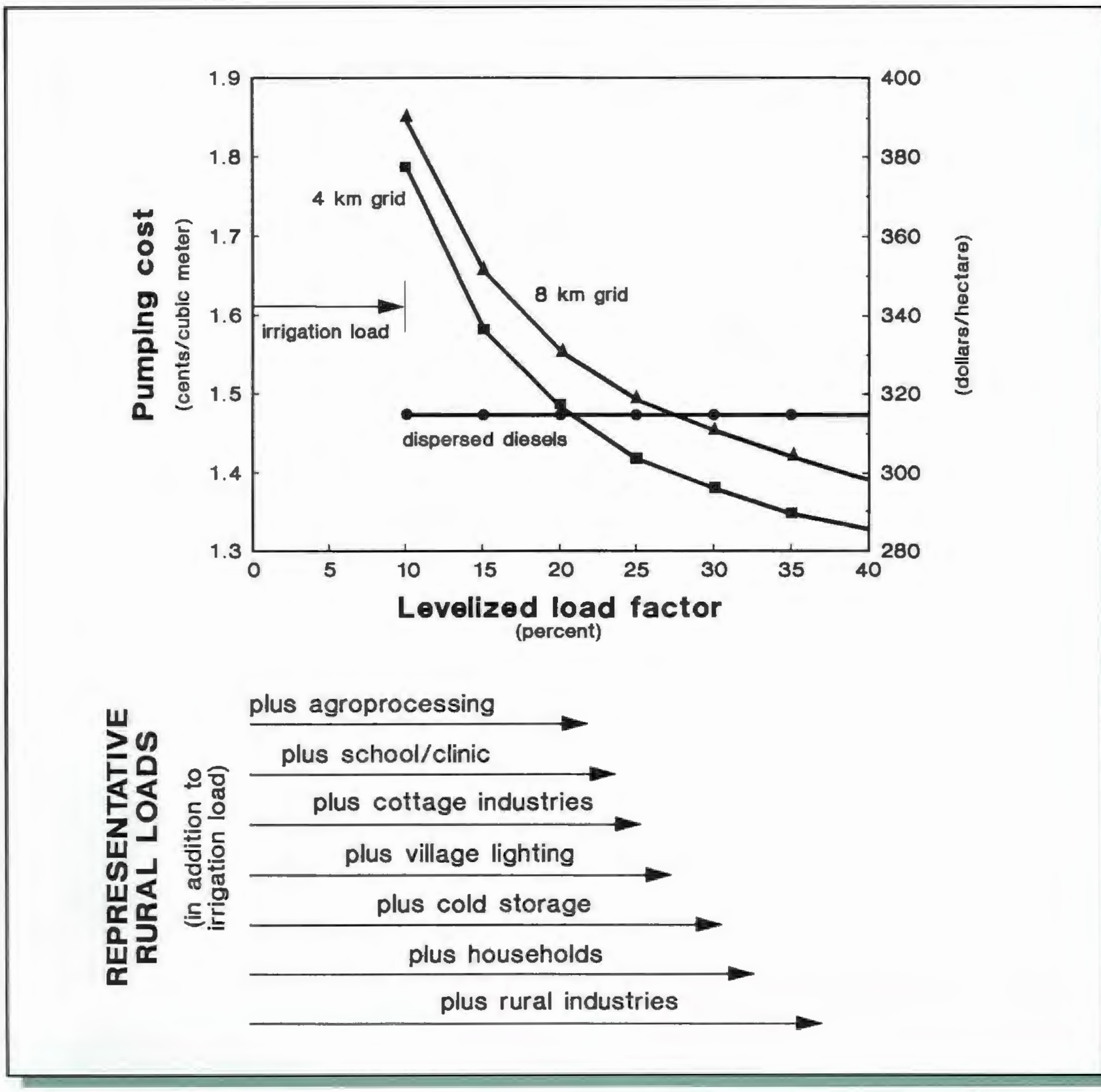
Second, the Laboratory—in association with Oak Ridge Associated Universities' Institute for Energy Analysis—has taken stock of more than a dozen years' experience in renewable energy applications in developing countries to focus AID programs more effectively on projects and technologies that have high probabilities of success. Under the leadership of Dan Waddle, ORNL is helping to initiate new projects in several countries.

ORNL and ORAU-IEA have assessed experiences with a variety of renewable energy technologies in Third World countries over the past 12 years. Here a photovoltaic system (designed by the National Aeronautics and Space Administration and Lewis Research Center) provides a West African village with power to supply drinking water, lighting, and grain milling. (Photo courtesy of VITA.)

Third, ORNL has helped to develop a new program component for EPPD that is intended to increase attention to environmental management in energy project planning in developing countries.

Household Fuels for Wood-Scarce Areas

The basic options for better meeting the household energy needs of people in wood-scarce areas of developing countries, besides encouraging more tree cultivation, are (1) finding alternatives to wood as sources of energy, (2) finding alternative sources of wood energy, and (3) improving the efficiency with which wood is produced and used as an energy source. Since 1984, ORNL investigations have focused on the potential of substituting clean-burning coal briquettes for wood charcoal in wood-scarce areas with a coal resource. Seventeen AID-assisted countries fit this description, and coal briquetting is a familiar, well-established technology (usually involving pyrolysis, except where the source coal is anthracite). In 1985, ORNL developed a generic approach for evaluating the potential of individual countries for coal-briquette–substitution. This approach was first applied in Haiti, the most deforested country in the Western hemisphere (and the poorest). The prototype feasibility study, led by Glenn Stevenson, uncovered a market in the Port-au-Prince area for the output of a 50,000-tonne/year coal briquetting plant. But it also concluded that briquettes made from the best-known deposit of Haitian lignite would not compete successfully with wood charcoal at current charcoal prices. Briquettes made from coal of higher energy value, however, whether from imports or other deposits in Haiti, might be competitive even with inexpensive charcoal.

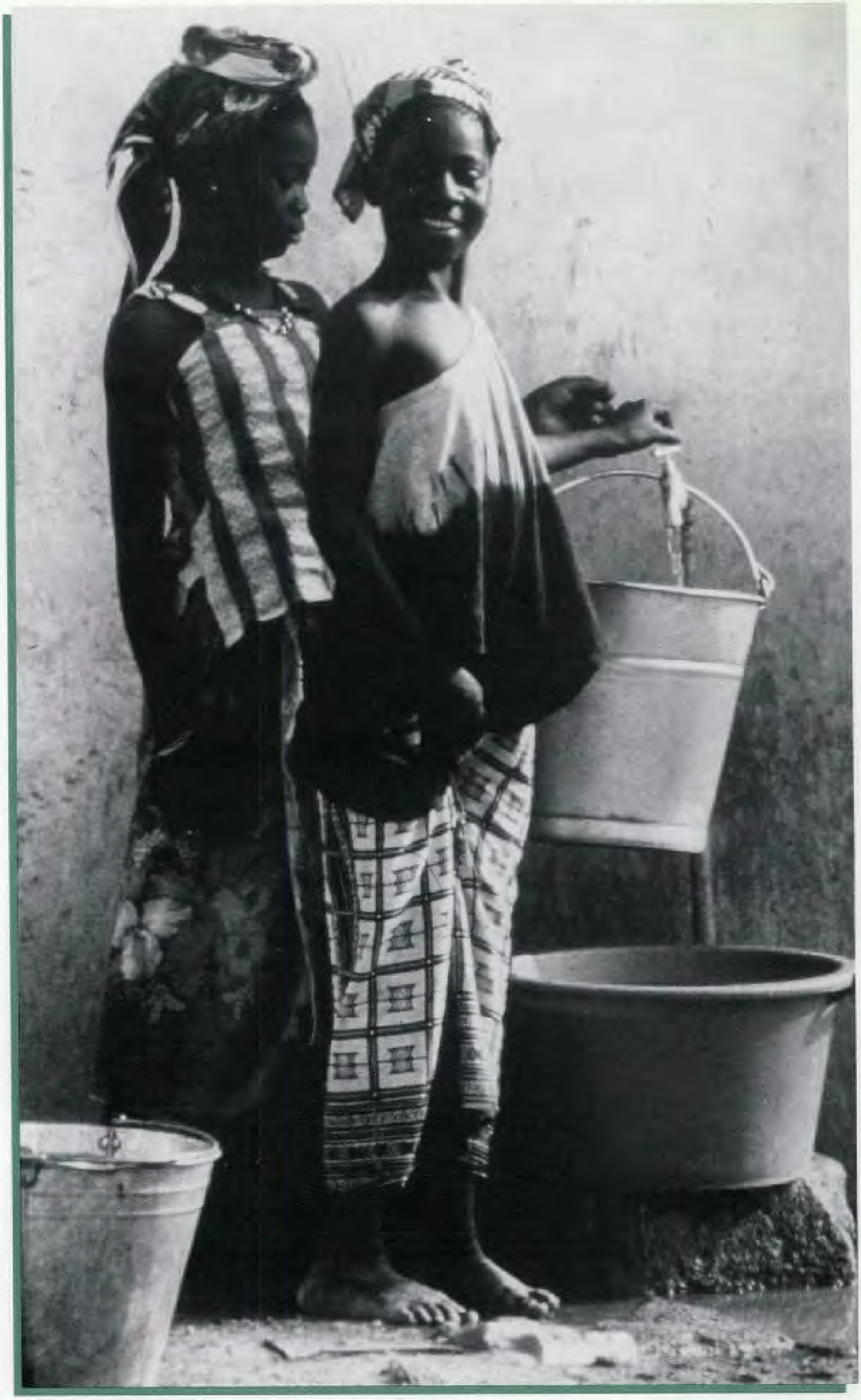


ORNL's Energy Division analyzed the costs and benefits to a typical rural village in Senegal if it were to meet its needs for irrigation water pumping through a centralized power generation system coupled to a "minigrid" rather than continuing to use small independent diesel pump sets. If village amenities and small local industries develop to use off-peak power from a central facility, overall pumping costs decline until the unit cost of power is lower than the current level.

Discussions of further tests of this idea are under way with private-sector entrepreneurs.

ORNL also led a recently completed effort to evaluate markets for coal briquettes in Pakistan. The assessment indicated that, with some care in selecting high-energy source coals and with high-density urban markets, coal briquetting is an attractive Pakistani business proposition. A briquette production operation, however, would need to penetrate firewood and/or kerosene markets to some degree (in addition to the relatively small charcoal markets) to justify building a 50,000-tonne/year plant.

Increasingly, ORNL's household fuels program has been expanding to cover other options as well, including briquettes from agricultural residues and hybrids from coal and residues. Moreover, 1985 assessments of household fuel options in Zaire and Madagascar, conducted in collaboration with the World Bank, prompted a more detailed examination of the possibility of producing charcoal from alternative sources of wood—that is, from source areas or species that could be used without exacerbating deforestation. In early 1986, ORNL's Carl Petrich and Robin Cantor, together with three consultants, assessed the potential of converting smallwood from a large pine plantation in Madagascar to charcoal to slow down deforestation in the capital city area. The research effort included a pioneering (in developing countries) use of "focus groups" to evaluate the market acceptance of pinewood charcoal. The



A nearby windmill pumps drinking water to this central storage tank, which supplies a village in Mali (photo courtesy of VITA).

team concluded that, although pinewood carbonization for the general urban charcoal market faced a number of obstacles, the potential was significant. The World Bank and the government of Madagascar are currently negotiating a major loan to go forward with such a project.

In 1988, ORNL has been evaluating options for improving the efficiency of household fuel production and use to reduce wood requirements. A remarkably successful effort to produce and sell more-efficient cookstoves in Kenya is being examined to identify lessons that can be transferred to other countries, and markets for improved cookstoves in urban areas in Central America are also being assessed.

Institutional and Policy Reform

Because energy pricing problems, insufficient private-sector roles, and problems implementing good ideas are major impediments to meeting energy needs, institutional and policy reforms are important in most developing countries. In this connection, the Laboratory's research and technical assistance for AID are focused on energy price reform, problems in the implementation of good ideas, and technology transfer.

Most of the professional attention to energy price reform in developing countries to date has been devoted to estimating the appropriate price, generally related to the marginal cost of producing the energy. Frequently, however, this process has actually been counterproductive, because the estimated "rational" price is so much higher than the current price; consequently, price reform often seems to local decision makers to be politically and economically risky. ORNL's work has been directed instead toward developing approaches to energy price reform that can be implemented realistically. A recent study by

Local private entrepreneurs in Kenya have found that manufacturing and selling more energy-efficient cookstoves can be a good business opportunity.

Charcoal is the cooking fuel for most families in Haiti, and charcoal consumption is associated with severe deforestation. ORNL has assessed the potential for manufacturing and marketing a clean-burning coal briquette in Haiti as a substitute for wood charcoal. (Photo courtesy of Mike Benge, USAID.)

Larry Hill, for example, proposed a generic strategy that combines gradual price increases with

- improvements in the efficiency of energy supply institutions (to reduce the marginal cost of producing energy and distribute the burdens of price reform to suppliers as well as consumers),
- improvements in the efficiency of energy use (so that the price of energy services will rise less rapidly than the price of energy), and
- changes in institutional structures associated with energy pricing (so that more appropriate price levels will be self-sustaining).

As this indicates, a general problem in developing countries is *implementing* good ideas once they are identified. In fact, literally hundreds of good ideas have been proposed in recent years (e.g., energy facility investments offering payback periods of 18 months or less) but not acted on, while less appropriate actions have been taken. The problem seems especially acute where the right choices involve innovation, because new options are difficult to evaluate and, if they involve financial and institutional changes, they are harder to put into action. Clearly, ORNL's activities related to power for development and energy price reform are focused on this problem.

In addition, ORNL has been contributing to the development of a major new AID project in India, the Project to Accelerate the Commercialization of Energy Research (PACER). A five-year effort budgeted at more than $20 million, the goal of this project is to develop better connections between indigenous Indian energy R&D institutions and

Buses are important public transportation in most developing countries. Analyses by ORNL and others have shown that oil fuel consumption can be reduced by transportation system efficiency improvements.

the country's electric power system. The hope is that such institution-building will speed the process of communicating and evaluating new technology options for improving electricity services. ORNL will serve as an important source of U.S. technical assistance. In addition, ORNL is assisting AID's Office of Energy in taking a more comprehensive look at the implementation problem.

Besides representing a significant attempt to break new ground with implementation, the PACER project is also an experiment in technology transfer. In other project activities, ORNL is encouraging technology transfer by seeking private-sector participation in coal briquette production in Haiti and Pakistan, improving the state-of-the-art for market acceptance studies in developing countries, assisting AID with information dissemination, and providing insights about the special challenges faced by U.S. energy technology producers in the competition for markets in developing countries.

Other Activities

As long as this list may seem to be, it still neglects a host of other recent ORNL–AID activities. For example, the work of David Greene (Energy Division) and others on the potential for improving the energy efficiency of transportation systems in developing countries, based on field investigations in Tunisia and Costa Rica, is considered the best available reference work on this subject. In one major contribution, Greene, ORNL's Frank Southworth, and colleagues from Hagler, Bailly, and Company, Inc., conducted experiments in Costa Rica that established for the first time that driver training and improving maintenance practices can pay off in significant reductions in fuel use by bus and taxi fleets (see table on page 38).

	% FUEL SAVINGS BY CONSERVATION OPTION				
	DRIVER TRAINING	DRIVER INCENTIVES (BUSES)	PROPER MAINTENANCE	RADIAL TIRES	TOTAL**
BUS FLEET	4.2*	1.2	6.5*	-1.8	11.5%
TAXI FLEET	15.1*	-	1.8	0.2	16.8%

*Statistically significant results
**Totals include other conservation options that are not listed here

Driver training and improved maintenance of bus and taxi fleets in developing countries can yield significant fuel savings, according to analyses by ORNL and Hagler, Bailly, and Company, Inc.

In other AID activities, ORNL

- conducts policy analyses for AID,
- assists with energy project design and evaluation (including recent project evaluation efforts in Bangladesh, the Philippines, Ecuador, and the Sudan),
- conducts an energy policy research program for AID's Office of Energy (which issues requests for proposals and awards contracts for small research projects to provide information and maintain a research base for AID programs), and
- provides a variety of technical information and decision support assistance to AID, ranging from technical information assistance from Al Ekkebus and the Administrative Services organization to technical assistance from Sherry Wright and others with office automation and decision support systems, including the development of new decision support tools for the Office of Energy.

Outlook

Given all the uncertainties, forecasting the future of any energy program is risky. But the prospects for further ORNL contributions to meeting energy and other needs in developing countries are bright. As we look ahead in our program development, we see particular opportunities in

- power system development—connecting power system planning with technology advances ranging from generation to end-use,
- exploring the potential of coal and natural gas as transition fuels from oil to renewable energy sources, which depends both on technology R&D and environmental assessment; and
- identifying and helping to fill technology gaps for the longer term (e.g., the clear need for better, cheaper, cleaner technologies to meet relatively large energy requirements in developing countries in the next 25 to 50 years).

We also see opportunities for the Laboratory to contribute in other fields of science and technology. The best prospects seem to be in environmental management, a rapidly growing area of concern in the developing world, and in uses of microcomputers and modern decision support systems in developing countries (e.g., electric utilities could use microcomputers to reduce delays and inefficiencies in billing). Other possibilities include water resource issues, especially in Africa, and transportation system management, especially in the increasingly clogged urban areas of developing countries.

Our hope is that, in addition to helping ORNL stay in the energy business during the 1980s, this kind of direction for the Laboratory will add to our impact in solving real problems of real people. For most of the ORNL staff members who have been a part of the program so far, the greatest satisfaction has come from knowing that they could directly and personally make a difference in improving the lives of others.

More generally, of course, the world faces a half-century in which two great transformations

This mule-driven kerosene "tanker," tethered to a power pole in Pakistan, illustrates the energy changes taking place in developing countries.

must occur at the same time—an economic transformation in developing countries and a transformation in energy systems away from such a heavy reliance on petroleum and natural gas. Achieving both of these transformations concurrently is one of the great challenges to science and technology in our time. This challenge is tied directly to the well-being of a majority of the world population and, thus, to such larger issues as world peace. ORNL has traditionally looked for challenges such as this—big, rich, complex, multidisciplinary, focused on energy and the environment, rooted in science and technology, long-lasting rather than transitory, and of undeniable importance to society. Because of the Laboratory's interests and activities in developing countries since the late 1950s, and especially since 1982, ORNL has the opportunity to play a major role in meeting this challenge.

(The authors would like to acknowledge the research assistance for this article provided by Steve Olive, now affiliated with the University of Hawaii.)

Biographical Sketches

Thomas J. Wilbanks (center) is an ORNL Corporate Fellow and senior planner for ORNL's Energy Division. He holds a Ph.D. degree in economic geography from Syracuse University, is the author or coauthor of five books or monographs and more than 50 journal articles and professional papers, and has served on a variety of national and international panels and committees related to energy policy and technology assessments.

Sherry B. Wright is a technical associate in the Energy Division and serves as the general manager of ORNL project work for the Agency for International Development (AID). She holds a B.S. degree in business education from Cumberland College.

Carl Petrich, who provided substantial assistance to the authors in assembling illustrations for this article, is a research staff member in the Energy Division, a key member of the AID project team, and a specialist in graphic design and communication. He has an M.S. degree in resource planning and landscape architecture from the University of Michigan.

A Prisoner's Puzzle

A prisoner is given an opportunity to participate in a random-selection experiment, the outcome of which may set him free. He is given two identical urns and 10 green balls and 10 red balls. He is asked to distribute the 20 balls into both urns. When the prisoner has finished, one of the urns will be chosen at random, and the prisoner will be asked to pick a ball at random from this urn. If the ball is green, he will be set free. The question is: How can the prisoner best apportion the balls in the two urns?

It turns out that the prisoner's best strategy is to put one green ball in one urn and the remaining 19 balls in the other urn. With that distribution, the probability that he will be set free after the experiment is nearly 75%.

100th Power of Natural Numbers

Take the natural number 7, raise it to the 100th power, and note that it ends in 1. Similarly, raise 2 to the 100th power and note that it ends in 6. It can be shown that when any natural number is raised to the 100th power, the results end with either digits 0, 1, 5, or 6. If 5 is raised to the 100th power, the final two digits are 25. In fact, when any natural number is raised to the 100th power, the last two digits can be only 00, 01, 25, or 76. Even more interesting, the final three digits of the 100th power of any natural number will be either 000, 001, 625, or 376.

Designer Steels for Advanced Energy Applications

By Carolyn Krause

Ron Klueh (left), Phil Maziasz, and Bob Swindeman discuss the behavior of designer steels after creep testing in the Multi-Frame Skutt Creep Testing Facility behind them. Creep behavior of small specimens (like the one held by Swindeman) is used to predict the lifetime behavior of machine components (like the tubes in the foreground) in energy production facilities.

A quiet revolution in the design of new stainless steels and other iron-based alloys for use in advanced, high-temperature energy systems is under way at Oak Ridge National Laboratory. Since 1984, ORNL researchers in the Metals and Ceramics (M&C) Division have designed several outstanding new alloys:

- A modified 14% chromium, 16% nickel stainless steel, which has excellent resistance to radiation damage—swelling and severe embrittlement caused by prolonged irradiation at elevated temperatures—and creep—the long-term tendency to stretch at high temperatures under an applied stress. This material, which has up to 1000 times the creep resistance of type 316 and other commercial stainless steels at 700°C, could be used in both advanced coal power plants and nuclear reactors.

- A modified alloy that consists of 20% chromium, 30% nickel, and less than 50% iron by weight (hence, the designation alloy rather than steel). Resistant to corrosion as well as creep, this alloy may prove to be particularly useful for superheater and reheater boiler tubes in advanced steam cycles for coal-fired power generating systems and other high-temperature uses.

- A modified 12% chromium, 20% manganese steel that, compared with conventional steels, is expected to be both resistant to radiation damage and to have a much greater and more rapid decay of radioactivity induced by long-term exposure to intense neutron irradiation in a fusion reactor. Fusion reactor components made of this "low-activation" material would pose less of a radioactive disposal problem at the end of their useful lives.

The developers of these alloys are metallurgists Phil Maziasz, Ron Klueh, and Bob Swindeman of the M&C Division. Together they have expertise in advanced electron microscopic analysis along with an understanding of the mechanical behavior and fabrication processing of iron-based steels and alloys.

Their alloy design is based on knowledge gained from intensive years spent studying creep and other effects of neutron irradiation and thermal exposure on alloys. In particular, they have made use of new information about irradiated alloys gained from analytical electron microscopy (AEM), which can provide structural and compositional information at the 2- to 10-nm scale. The new alloys are a direct spin-off of ORNL alloys already designed and developed to improve resistance to radiation-induced void swelling and helium embrittlement in fusion energy applications.

Maziasz calls these new materials "designer steels" or "gourmet alloys" because their properties are predetermined by adding unique combinations of key trace elements and because knowledge of material behavior is essential for deriving the right alloy "recipe." Understanding the complexities of alloy behavior during use is the key to designing steels. Just as a gourmet cook inventing a new dish must know the critical ingredients and understand their possible interactions during cooking, the metallurgist designing a new alloy must know the likely contribution of each ingredient in specific proportion to the alloy recipe during use as well as the synergistic effects of combined ingredients. Will interactions with other constituents improve the alloy enough to achieve a desired characteristic? Or will they degrade the alloy's desirable properties? If a little is good, would a lot more be better—or worse?

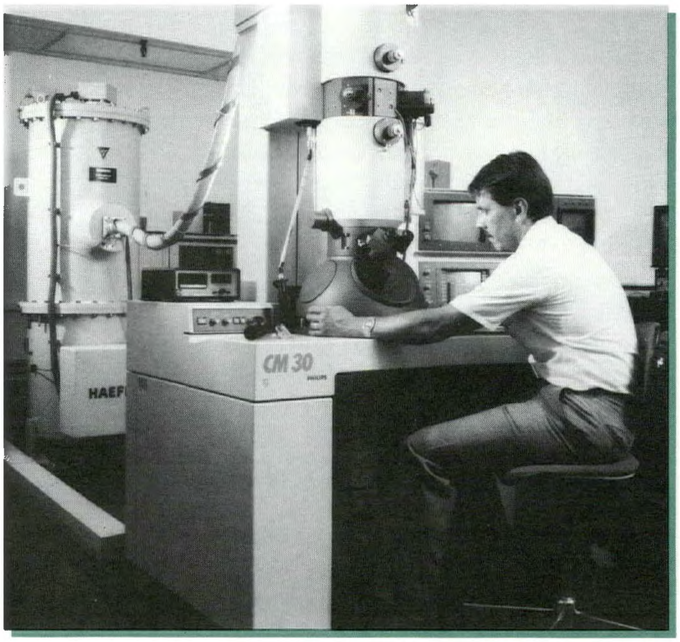
ORNL metallurgists have shown that minor changes in the composition of alloys can change their microstructure enough to produce desired properties, just as adding a touch of thyme and a pinch of garlic can improve an ordinary tomato sauce enough to please a discriminating gourmet. "Small changes make a big difference," Maziasz says. "For years, M&C researchers have added small amounts of titanium to steel to produce fine metal carbide precipitates that improve radiation or creep resistance. In recent years, Arthur Rowcliffe and Eal Lee have observed that adding small amounts of phosphorus to steel improves its radiation resistance. Adding small amounts of boron has been known for years to improve creep resistance in steels and has been found at ORNL to improve the ductility of nickel aluminides.

"However, the secret of our success has been the realization that combinations of these elements are more effective than any single addition by itself. The alloys developed at ORNL are not produced by a mysterious black art or random guesswork. Minor additions are deliberately and carefully controlled to preserve or add good properties. Decisions about what and how much to add are based on the special insights gained from studies of the effects of long-term radiation on steels using AEM. This information has suggested ways to design alloys to meet special needs by altering their microstructures." (See sidebar on page 48.)

Gourmet Alloys

In 1976, Jim Stiegler, now director of the M&C Division, started a group to demonstrate the concept that a material's microstructure is linked to its properties, suggesting that manipulation of the microstructure could achieve desired properties. In the past 12 years, several groups in the division have shown that these ideas are correct.

In 1983, ORNL's Magnetic Fusion Energy Materials Program, headed by Everett Bloom of the M&C Division, encouraged Maziasz to try to design a steel for fusion reactors that has better radiation resistance than the titanium-modified steels that had been developed at ORNL in 1977–1978. Design engineers want to build fusion reactor "first walls" from a steel that resists



Maziasz peers at an irradiated steel specimen in a Philips CM30 analytical electron microscope, one of the key instruments for understanding how alloys of specific compositions change during irradiation.

Ed Bolling performs cyclic fatigue testing of an advanced austenitic steel specimen heated by inductive eddy currents.

damage by the 14-MeV neutrons produced by fusion reactions of hydrogen isotopes in plasmas.

Maziasz' recipe for a modified stainless steel has proved doubly successful: the new alloy exhibited both better radiation resistance and excellent high-temperature thermal creep-rupture strength. Radiation resistance is resistance to swelling and embrittlement—caused by point defects produced by displaced atoms and by helium produced by transmutation—during intense, prolonged neutron irradiation. Creep-rupture strength involves a combination of (1) resistance to strain (stretching) accumulation during long, high-temperature exposures when stresses below the tensile yield stress (often quite small) are applied and (2) resistance to embrittlement and premature fracture.

In 1984, Tom Roche of the M&C Division made the first small heats for reactor irradiation experiments and limited tensile testing. Irradiation of small disks in ORNL's High Flux Isotope Reactor for the Fusion Materials Program showed very good swelling resistance, as measured by a new remote precision densitometer designed specifically for such measurements on small, highly radioactive specimens by Lloyd Turner and Roy Buhl.

What is the recipe for this steel? Says Maziasz, "If you had 100 grams of this steel, it would contain 64.4 grams of iron (Fe), 14 grams of chromium (Cr), 16 grams of nickel (Ni), 2.5 grams of molybdenum (Mo), 2 grams of manganese (Mn), 0.5 gram of vanadium (V), 0.05 gram of phosphorus (P), 0.01 gram of boron (B), 0.3 gram of titanium (Ti), 0.1 gram of niobium (Nb), and 0.1 gram of carbon (C)." In technical shorthand, the alloys are called new Fe-14Cr-16Ni-2.5Mo-2Mn steels modified with carefully controlled additions of V, P, B, Ti, Nb, and C.

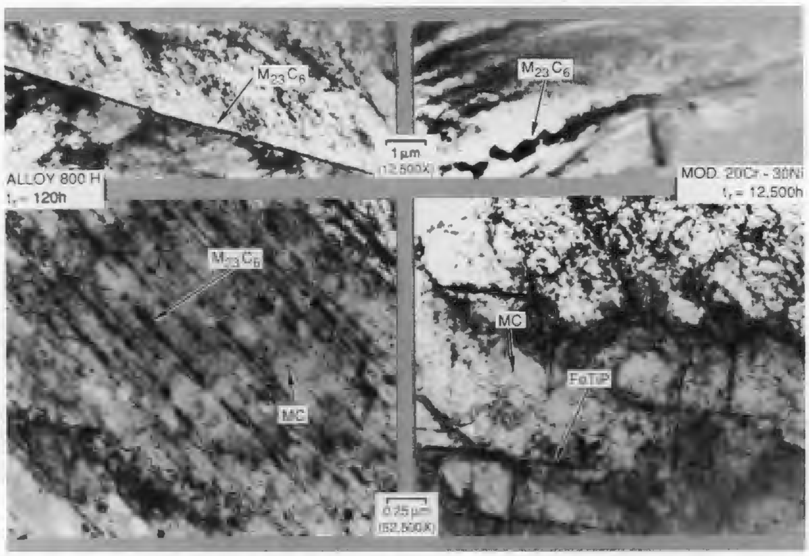
This new modified 14Cr-16Ni steel could also be used for fast-breeder reactor core and structure applications. In addition, high-temperature tensile testing (done by Noble Rouse of the M&C Division) and microstructural analysis of unirradi-

Maziasz shows one of the weights used to "stretch" a steel specimen inside the machine during a creep test. Hanging weights at left indicate that a creep test is in progress.

ated specimens of these same experimental steels showed good strength and precipitate structures, suggesting that these steels might also resist straining during longer-term creep testing and at lower stress levels. This behavior inspired thoughts of a spin-off of these steels from fusion and breeder applications to some new high-temperature, nonnuclear application.

On June 15, 1984, Ron Bradley, then manager of ORNL's Fossil Energy Materials Program, attended an M&C Division staff meeting during which Maziasz presented a talk on advanced austenitic steels for irradiation resistance in steam-cycle materials. He suspected that the radiation-resistant steel that Maziasz had developed was also creep resistant. Bradley expressed interest in this material because of its potential use in advanced steam-cycle, power generating systems that burn pulverized coal. A number of countries, including the United States, are interested in building such systems, which, compared with conventional fossil power plants, use hotter steam to produce electricity more efficiently. An advanced steam-cycle fossil power plant has not been built in the United States since the Eddystone Unit 1 went into operation for the Philadelphia Power and Electric Company in 1960, because materials then available could not withstand the high temperatures and stresses of long-term operation.

From mid-1982 to mid-1984, the Fossil Energy Materials Program assessed the materials needs of advanced steam cycles. To build a highly efficient, reliable steam-cycle plant, the ORNL researchers concluded, it is critical that the superheater and reheater tubes in the boiler be made of a material that can withstand the damaging effects of fire (on one side) and steam at 650°C (on the other). Plant operation and lifetime depend on various criteria, one of which is the ability of these materials to resist excessive creep or cracking. Alloys such as CR30A (trademark of Nippon-Kokan Steel Corporation, Japan) and alloy 617 could be used for this purpose, but they are expensive because of their high chromium and nickel content (alloy 617 also contains cobalt and molybdenum, which, along with chromium, are strategically important for defense and industry and subject to supply interruptions because of political instabilities). Consequently, DOE funded an effort to develop an alloy that is "lean" (lower in chromium, nickel, cobalt, and molybdenum), less dependent on foreign supplies, less expensive than superalloys, and better in its high-temperature creep resistance than the reference copper-molybdenum (17-14CuMo) alloy used in Eddystone Unit 1.



Microstructures of mill-annealed materials, creep tested at 700°C and 170 MPa. The photos on the right compare the microstructure of conventional alloy 800H with that of the new, modified, 800H alloy (20Cr-30Ni) developed at ORNL. The marked differences in precipitate microstructures are directly responsible for the property differences.

In the summer of 1984, the Fossil Energy Materials Program and M&C Division staff developed a proposal for alloy development for superheaters for advanced steam cycles. Thus, Maziasz began collaborating with Swindeman and Gene Goodwin of the M&C Materials Joining Group for Welding Studies to test his alloy to determine if it could have fossil energy applications. Because only small heats of material had been made at ORNL for reactor testing, larger heats were procured from commercial vendors—Combustion Engineering in Chattanooga in 1986 and AMAX in Ann Arbor, Michigan, in 1987—for the Fossil Energy Materials Program studies. In the first creep tests run by Bob Swindeman and Ed Bolling, the new steel exhibited excellent high-temperature creep resistance on the basis of its designed microstructure.

In September 1987, at the International Conference on Advances in Material Technology for Fossil Power Plants in Chicago, Maziasz and Swindeman reported that their modified 14Cr-16Ni stainless steel had twice the rupture strength of type 316 stainless steel, 50% more strength than alloy 800H, and a measurable increase in strength over that of the reference 17-14CuMo alloy. The creep strengths of these ORNL steels could meet that required for an advanced superheater alloy at 700°C and approach the superalloy creep strength of alloy 617. While a stainless steel such as type 316 can withstand stresses of about 40 MPa at 700°C for 100,000 h without rupture, ORNL's lean steel can withstand up to 100 MPa at 700°C for the same period.

However, it was anticipated that the new lean steel would be suitable for advanced steam-cycle plants only if it could be protected by claddings or coatings to improve its corrosion resistance. So Swindeman and Maziasz decided to pursue a parallel effort to modify corrosion-resistant alloy 800H to improve its creep resistance, which is only marginally better than that of type 316 stainless steel. Maziasz and Swindeman readjusted the proportions of minor alloying element additions while changing the Cr-Ni content of 14Cr-16Ni stainless steels to that of alloy 800H, which has 20% Cr and 30% Ni to provide corrosion resistance. The original alloy 800H has a composition somewhat between that of a superalloy (titanium and aluminum are added to provide strength) and that of a carbide-strengthened steel. They also readjusted the base composition (by adding molybdenum and eliminating aluminum) to make the alloy act more like a steel having fine carbides and phosphides for strength. Based on findings from his welding studies, Goodwin suggested that phosphorus additions be limited to improve the alloy's weldability. The result was a 20Cr-30Ni-2.5Mo-2Mn alloy, modified with various minor element additions, several heats of which were also produced commercially by AMAX in 1986.

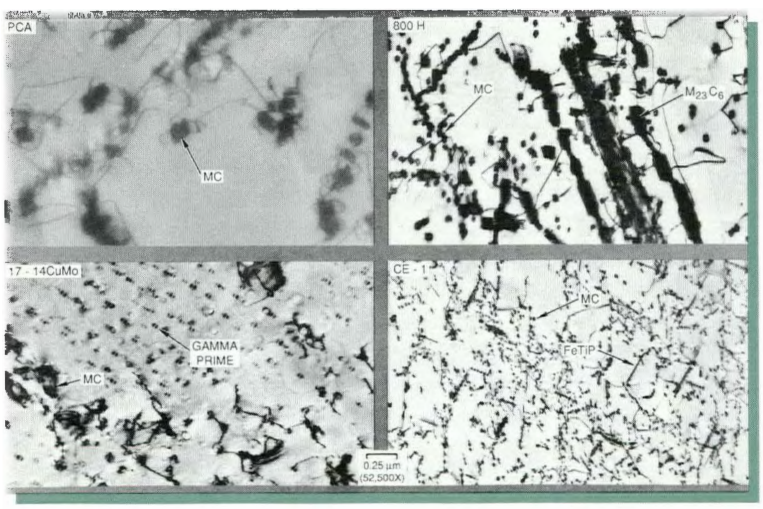
The new modified 20Cr-30Ni alloy is 100 times more rupture-resistant than alloy 800H at 700°C and 170 MPa and is comparable to the modified lean stainless steels. In addition, this corrosion-resistant alloy is also tougher and more resistant to cracking along grain boundaries during creep than alloy 800H. In short, this new designer alloy is well suited for either advanced steam-cycle or fludized-bed combustion fossil power plants because it is highly resistant to both creep and corrosion.

From the standpoint of DOE's fusion materials program, Maziasz's 14Cr-16Ni steel scored high marks for radiation resistance. Unfortunately, a changing set of design and safety requirements made this alloy unsuitable for commercial fusion devices because of possible disposal problems. It contains elements such as nickel, niobium, and molybdenum that, when subjected to prolonged neutron irradiation, are transmuted to highly radioactive isotopes having long half-lives. The material could be too radioactive to be easily and safely buried once its useful life has expired.

Applying the principles for *a priori* design of alloys, Maziasz and Klueh attempted to design a low-activation steel that is as strong and resistant to radiation damage as the modified 14Cr-16Ni-2.5Mo-2Mn stainless steel. The initial overall strategy for designing low-activation steels had been developed by Klueh and Bloom several years before.

To reduce neutron-induced radioactivity, Klueh and Maziasz eliminated nickel, niobium, and molybdenum from their steel and increased the manganese content. Manganese is a good substitute for nickel because it, too, stabilizes the austenitic alloy and because its neutron-induced radioactivity decays more rapidly than that of nickel. The resulting Fe-12Cr-20Mn-0.25C base alloy, with minor alloying modifications to produce fine precipitates, is a low-activation steel that has good strength and should have good radiation resistance. Calculations of radioactivity induced by fusion reactor exposure indicate that this new steel would be 1000 times less radioactive 50 years after exposure to intense neutron radiation than a typical conventional steel (e.g., type 316 stainless steel). Besides its apparent applicability to future fusion components, the new Fe-Cr-Mn steel also has good strength at high-temperature strength and may soon find other nonnuclear applications.

Maziasz says that these alloy successes show the value of interdisciplinary programs at national laboratories. "Development of these specialized alloys resulted from the combination of our expertise and the needs of ORNL's fusion and fossil programs. This cross-fertilization, made easy by ORNL's organizational structure, produced rapid breakthroughs in the design of novel materials."



Solution-annealed steels aged for 166 h at 800°C. Note the large differences in precipitate microstructures among the various alloys. ORNL's new steels have a unique combination of phases that are more finely distributed than precipitates in the other alloys.

Maziasz, Klueh, and Swindeman are achieving their goal of designing dramatically improved steels and alloys for advanced energy applications. These alloy designers have shown that correctly "spicing up" a material's microstructure can produce gourmet alloys having the properties to meet special needs. ornl

A Matter of Precipitates

> ***"If the right composition is selected, precipitates formed in the alloy during use will beneficially alter the microstructure."***

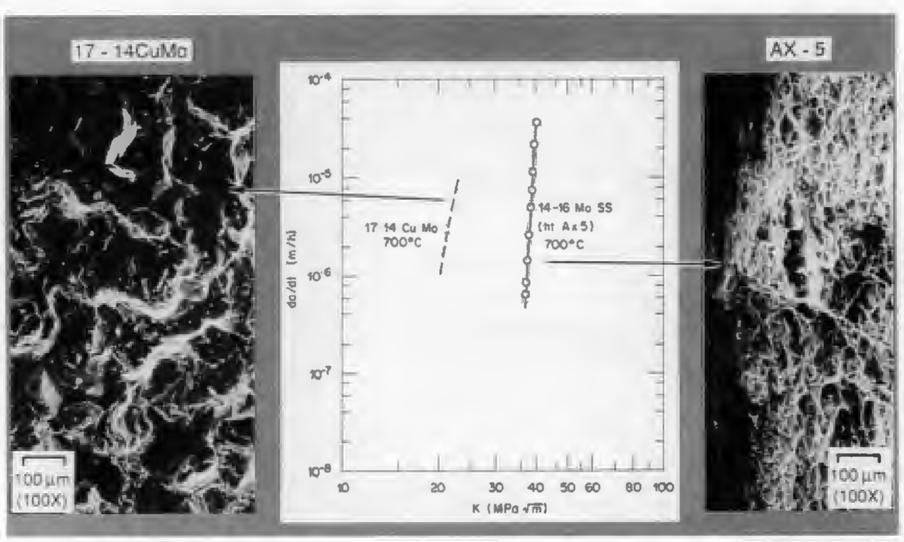
During prolonged exposure of metals and alloys to neutron radiation, atoms are displaced, creating vacant atom sites and interstitial defects (displaced atoms in the interstices between normal lattice atoms). These point defects can agglomerate into voids (holes) and dislocations that cause the material to swell and become brittle.

"The best way to stop this process, which is activated by prolonged radiation, high temperatures, and applied stresses, is to pin the dislocations with precipitates—that is, to induce the formation of particles that trap these extended defects in the crystal structure and keep them from moving throughout the material," says Phil Maziasz of the M&C Division. "But, it is easier said than done. Precipitation in irradiated materials is hard to study and characterize, harder to understand, and even harder to control."

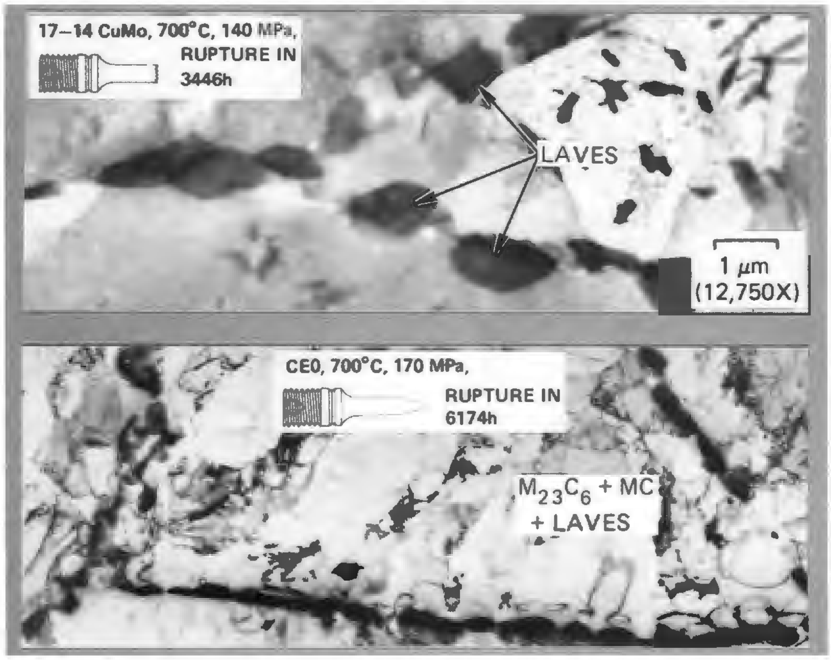
Precipitation is an elevated-temperature reaction between alloying elements—initially in solid solution, which then becomes supersaturated—that forms particles of new crystal phases from the original homogeneous parent material. These precipitate phase particles, whose structure and composition differ from those of the alloy matrix, may stimulate, inhibit, or block other changes in the microstructure, thus affecting properties.

Precipitate effects are directly responsible for improvements in mechanical properties such as creep resistance. If the right composition is selected, precipitates formed in the alloy during use will beneficially alter the microstructure, producing a "tailored precipitate microstructure."

What is a microstructure? A metal or alloy has grains of near-perfect crystal in various orientations. The submicroscopic structure includes grains (crystallites) of different sizes, grain boundaries (interfaces between grains), precipitates, and dislocations. These microstructural elements can change considerably under the influence of elevated temperature and/or exposure to radiation.



Fractography by scanning electron microscopy and creep-crack growth rate data from alloy specimens tested at 700°C. The new steels developed at ORNL (AX-5) are very resistant to cracking. The 17-14CuMo alloy cracks more easily because it fractures in a brittle manner along grain boundaries.



Laves precipitation along grain boundaries in the 17-14CuMo alloy causes brittle failure along grain boundaries, which shortens the creep-rupture life at 700°C (see upper photograph). By contrast, carbide precipitation along grain boundaries in the new ORNL steels contributes to a dramatically different, ductile failure mode that lengthens the rupture life (see lower photograph).

ORNL metallurgists have spent many years identifying the precipitates formed in steels that have been irradiated for a long time in reactors and understanding their effects on steel properties. In 1965, Arthur Rowcliffe, now in the M&C Division but then a doctoral student at Manchester University in England, discovered the existence of chrome phosphide precipitates in steel and suspected that they could improve the creep resistance of austenitic stainless steels. Ironically, almost 20 years later Maziasz, working at ORNL on his doctoral thesis and on improving the precipitate stability of titanium-modified austenitic stainless steels, uncovered evidence, together with Rowcliffe, that new iron-titanium phosphides also play an important role in the creep resistance of steels modified with titanium and phosphorus. Subsequent transmission electron microscopy work by Maziasz and others showed that certain fine precipitate phases, such as FeTiP, are much more effective at pinning dislocations than other phases.

"My AEM studies of irradiated and unirradiated steels," says Maziasz, "also verified that some precipitates are rich in certain elements that cause desired effects and block undesired effects in the surrounding microstructure. I also learned the importance of fine tuning the alloy composition to achieve formation of the desired precipitate phases while eliminating the unwanted ones."

Maziasz cites phosphorus as an example. "If you add too much phosphorus, the steel is hard to weld. But if you add a little phosphorus and supplement it with a little vanadium, it can greatly strengthen the steel."

During the lifetime of a steel, bad precipitate phases can form. These can be brittle intermetallic phases that are detrimental to desired properties; for example, "Laves phases" can cause severe grain-boundary embrittlement. The trick is to alter the steel composition so that irradiation or creep aging will produce other precipitates, which then prevent formation of these bad phases. For example, additions of carbon and boron stabilize the formation of carbides and retard the formation of the harmful intermetallic phases in irradiated steels.

These findings have been made possible by a highly sophisticated AEM facility, which allows use of such techniques as scanning transmission electron microscopy, electron energy-loss spectroscopy, convergent-beam electron diffraction, and the most useful of all for development of these designer steels, X-ray energy-dispersive spectroscopy for compositional microanalysis.

"Our AEM studies," Maziasz says, "provide a fountainhead of new ideas about how to alter the microstructure to obtain desired properties." ornl

New DNA Stain Aids Cell Studies

By Luci Bell

"A recently completed interdisciplinary project at ORNL allowed chemists to work in collaboration with biologists to enhance their means of unraveling the details of fundamental cell structures and processes."

During the past century, scientists have learned much about the mysterious processes and microscopic structures found inside living cells. Although most cells are naturally somewhat homogeneous and nearly transparent in appearance, biologists have been able to study the minute, but complex, internal cell mechanisms by developing structure-specific dyes that will cling to and highlight the particular cell components they wish to investigate. In the mid-19th century, researchers first began using several natural and synthetic dyes, or staining agents, to prepare cell samples for microscopic examinations that revealed the intricate basic structures of cells. Since that time, the knowledge and instrumentation used in biological studies have become much more sophisticated, but the cytochemical staining agents and techniques have not kept pace with this development.

In this century, transmission electron microscopy (TEM) has become an important investigative tool for distinguishing among fundamental cell structures such as chromosomes, composed of deoxyribonucleic acid (DNA)—the material that reproduces cell characteristics generation after generation. TEM produces images of cell components based on their electron density differences and, since most living cells are of relatively uniform density, the "stain" used for TEM imaging must adhere to some cell structures in preference to others (i.e., be structure-specific) and increase the density of the targeted structures enough to make them appear darker than other parts of the cell (i.e., produce significant contrast). Compounds of heavy metals, such as uranium or osmium, are routinely used to prepare general (i.e., nonspecific) contrasting reagents for TEM work, but reagents with high specificity are generally either unavailable or extremely difficult to prepare and use.

A Collaborative Effort

In a recently completed interdisciplinary project at ORNL, chemists worked in collaboration with biologists to enhance their means of unraveling the details of fundamental cell structures and processes. Using "seed money" from ORNL's Exploratory Studies Program, the scientists were able to develop and test a new DNA-specific staining agent that significantly improves the use of electron microscopy as a technique for understanding fundamental cell processes and the complexities of cellular genetic materials.

The collaboration began when Ada L. Olins and Donald E. Olins, researchers in ORNL's Biology Division and professors in the University of Tennessee–Oak Ridge Graduate School of Biomedical Sciences, needed a reliable DNA-specific stain for their cytochemical studies. The Olinses are using a new method of electron microscope tomography, which they recently developed in collaboration with Henri A. Levy (now retired) of ORNL's Chemistry Division and computer specialists in Martin Marietta Energy Systems' Computing and Telecommunications Division. Their major goal is to determine the three-dimensional path of DNA in active and quiescent chromosomal structures. An effective, reliable, DNA-specific staining agent was considered essential for this work.

Ada Olins and Bruce Moyer use an electron microscope to view cell structures stained by a new DNA-specific agent.

The only known DNA-specific stain was an unstable, hard-to-produce, osmium-ammine complex (a chemical of uncertain composition, but which has been determined to contain both osmium atoms and ammonia molecules in some combination). This osmium complex, called the Gautier stain, was first prepared and studied by the Swiss biologist, A. Gautier. The Olinses' request for a batch of the stain seemed simple enough, so Bruce Moyer of ORNL's Chemistry Division readily agreed to prepare it, following Gautier's published procedure. As Gautier's publication warned, however, the stain proved to be difficult to make and use and not reproducibly specific for DNA. Moyer's interest and previous experience investigating the chemistry of heavy-metal compounds, and the obvious need for a better, more reliable, staining agent for DNA, subsequently led Moyer and Ada Olins to file a joint application for seed money to synthesize and chemically characterize an improved DNA-specific cytochemical stain.

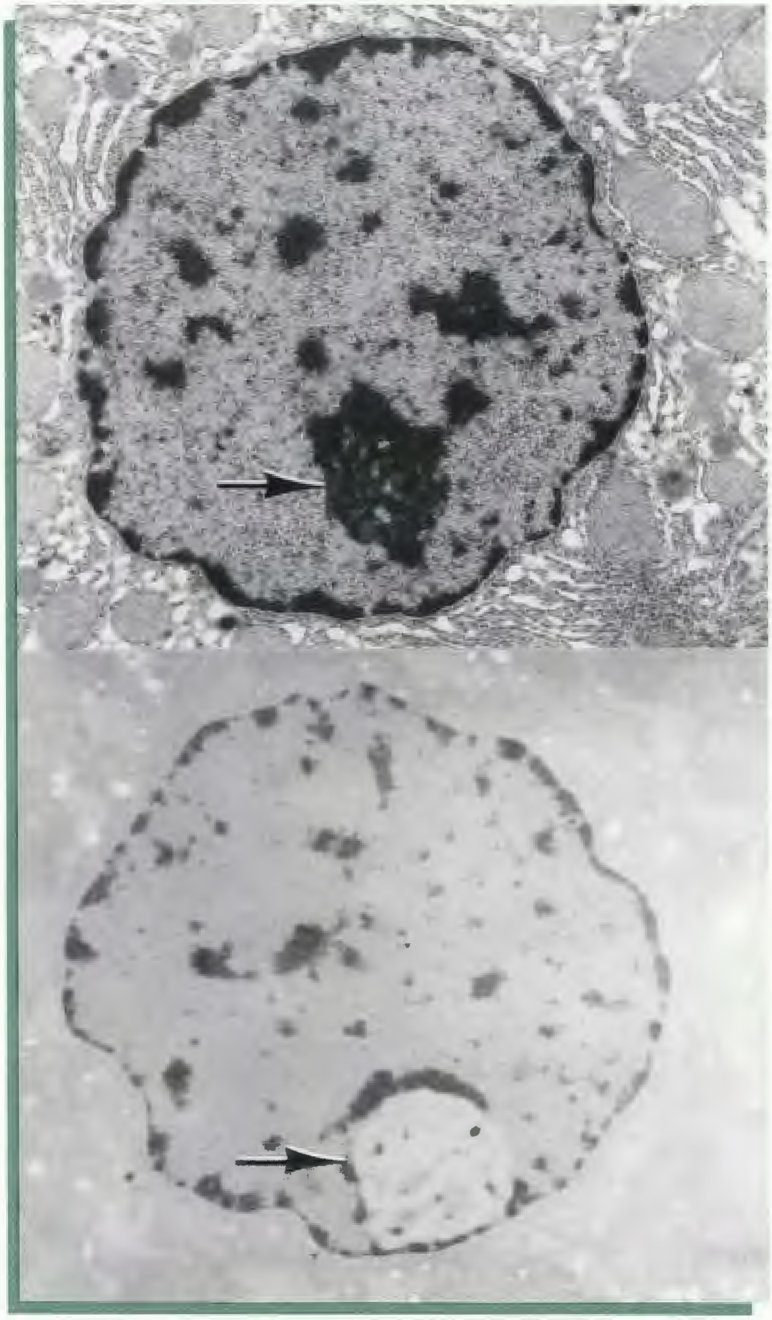
Beginning with a thorough literature search, Moyer prepared a chart identifying several promising osmium-based compounds having potential DNA-staining capabilities. With the funding received, he was able to enlist the services of an Oak Ridge Associated Universities Postgraduate Research Associate, Sook-Hui Kim, to begin preparing, purifying, and characterizing these compounds. David Allison, electron microscopist in the Biology Division, agreed to test the compounds for actual staining performance.

A Superior Stain

In one of those occasional serendipitous occurrences in scientific investigations, one of Kim's first preparations proved superior to Gautier's stain in several ways:

- Sample preparation is greatly simplified, requiring only a few hours, rather than the usual 4 to 10 days;
- Staining results are consistent, reproducible, and DNA-specific;
- The ORNL stain is completely soluble in water (unlike Gautier's stain) and leaves less visible precipitate on the specimen (see electron micrographs on page 52);
- The new stain has a longer shelf life, making it more suitable for research use; and
- Greater imaging contrast is provided by the new compound, even when tenfold lower concentrations than usual are used.

The contrast between cells stained with a conventional agent and cells stained with the new ORNL osmium-ammine preparation is illustrated in the electron micrographs of rat liver cells shown on page 52. The top cell, which was prepared with a conventional heavy-metal agent, strongly stained most cellular structures, showing little specificity. In the bottom cell, treated with the newly developed osmium-ammine complex,



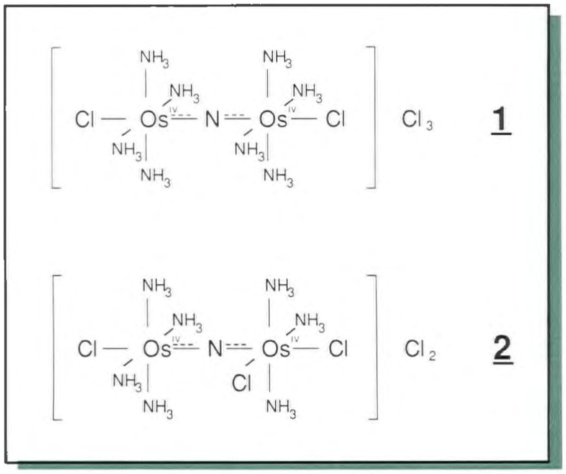
Electron micrographs of rat liver cells (bar length = 1 μm) stained with conventional agent (top cell) and new ORNL agent (bottom cell).

only the DNA-containing structures are strongly stained, enabling cytologists to differentiate these from other cell inclusions. The large arrows point toward the nucleolus of each cell. Almost total staining occurs with the conventional agent (top), but the ORNL agent (bottom) stains only the DNA-containing chromatin structures in the nucleolus.

After a half-dozen subsequent chemical syntheses of other osmium compounds by Kim gave products inferior to this successful mixture, the project participants shifted their focus to separating and purifying the active staining ingredient of the new reagent and optimizing procedures for its preparation and use.

Efforts to chemically characterize the new stain resulted in the separation of three components, and there may be others. Two of these components were purified and identified by both their spectral and chemical properties as nitrido-bridged osmium dimers (see figure on page 53). Although the exact arrangement of the atoms in these compounds remains to be determined, the key structural feature is thought to be a "backbone" consisting of two osmium atoms linked by a nitrido ligand (N^{3-}, essentially a fully dissociated ammonia molecule). The diagrams shown here illustrate the hypothetical structure of these dimers. Dimer 1 has a structural formula that has been known for nearly 35 years, but dimer 2 is a new osmium compound. When dissolved in water, both dimers initially behave as salts, in that the chloride ions shown outside the brackets dissociate immediately. Over a period of days, however, the chloride ions shown bonded directly to the osmium atoms also dissociate and are replaced by water molecules, in a process called aquation. Each of the osmium complexes in the new set thus formed has its own individual properties, which have been only partially explored.

Ironically, though dimer 1 was exactly the compound sought by Kim and Moyer when they planned the synthesis of the new stain, Allison's testing of the purified compound showed that it exhibited no staining ability. Purified dimer 2, as well as the aquated derivatives of both dimers, also failed to stain DNA. Unfortunately, funding for the work expired before the active staining component (or combination of components) could be determined. But, the project achieved its goal of developing a more reliable cytochemical stain and has contributed valuable information about the inorganic chemistry of osmium compounds.



Possible structures of the nitrido-bridged osmium dimers.

Visualizing Cell Structures

The Olinses are eager to continue their work using the new DNA-specific stain and their electron microscope tomography method to create a sophisticated three-dimensional reconstruction of the assymetric DNA-containing cellular structures. Ada Olins was recently honored for her research contributions toward visualizing the structure of chromatin, a complex of DNA and proteins that makes up the chromosomes and controls the expression of genes. For this work, she was named one of six 1988 winners of the University of Tennessee Chancellor's Awards for Research and Creative Achievement. Ada Olins has also been an Eleanor Roosevelt International Cancer Fellow, and Donald Olins has been an American Cancer Society Scholar. Both Olinses worked, in 1987, as visiting scientists at the Pasteur Institute in France and at the Max Planck Institute for Biophysical Chemistry in the Federal Republic of Germany.

Although a patent disclosure has been filed for the newly developed staining agent, Moyer sees little immediate economic incentive for commercial production of the new stain. However, both Moyer and the Olinses believe it will be a valuable aid to the basic biological research that is resolving the chromosomal structures within living cells.

Cell biologists have an equally fundamental need for an improved ribonucleic acid–specific (RNA-specific) stain. If funding can be obtained, future research will be directed toward the development of such a stain through the collaborative testing of various osmium complexes and toward continuing the challenging chemical characterization work. ornl

RE: Awards and Appointments

O. B. Morgan

John Sheffield

Sheldon Datz

Alvin W. Trivelpiece, executive officer of the American Association for the Advancement of Science and former director of the Office of Energy Research of the Department of Energy, has been named director of Oak Ridge National Laboratory and vice president of Martin Marietta Energy Systems, Inc.

Raymond S. Wiltshire, former ORNL executive director, has been named vice-president for Computer-Aided Productivity of Martin Marietta Corporation. On September 1, 1988, he assumed his new position at corporate headquarters in Bethesda, Maryland. Replacing him as ORNL executive director is **O. B. Morgan,** formerly director of ORNL's Fusion Energy Division. **John Sheffield**, former associate director of the Fusion Energy Division, has been named its director.

Martin Marietta Energy Systems, Inc., has conferred its highest honor, the rank of senior corporate fellow, on **Sheldon Datz.** Only three other Energy Systems employees hold this distinction.

Dale D. Huff has been named head of the new Environmental Engineering and Hydrology Section in ORNL's Environmental Sciences Division.

Tuan Vo-Dinh has been named to the editorial board of *Applied Spectroscopy.*

John F. Cooke has been elected a fellow of the American Physical Society.

Louis K. Mansur has been appointed to the editorial boards of *Advanced Materials and Processes*, *Journal of Nuclear Materials*, and *Journal of Materials Engineering*.

R. J. Norby has been appointed to the editorial review board of the journal *Tree Physiology.*

Linda Cain served as president of the 39th International Science and Engineering Fair in Knoxville, the largest such fair ever held.

Glenn W. Suter II has received the annual Scientific Achievement Award of ORNL's Environmental Sciences Division.

R. Julian Preston has been named a member of the Toxicology Study Section of the National Institutes of Health.

Diana Popp has been invited to write an article on "Lymphocytic Subsets and Abnormalities in Retrovirally Infected Mice" for publication by CRC Press in *Critical Reviews in Immunology.*

ORNL women employees who received 1988 awards from the East Tennessee Chapter of the Association for Women in Science (AWIS-ETC) are **Elizabeth Peelle**, Distinguished Leader and Advocate Award; **Kimiko Bowman**, Distinguished Achievements in Science Award; **Ellen D. Smith** and **Lynn L. Wright**, Outstanding AWIS-ETC Service Award.

Ray C. Hudson has been named ORNL Standards Coordinator.

Walter P. Eatherly has been elected chairman of the ASTM Committee C-5 on Manufactured Carbon and Graphite Products, a standards-writing committee.

Robert Hightower and **W. Wilson Pitt, Jr.**, have been named fellows of the American Institute of Chemical Engineers.

Chester R. Richmond has been elected to the Board of Directors of the National Council on Radiation Protection and Measurements.

M. B. Adams has been elected to the Executive Steering Committee of the Air Pollution Workshop, an annual international meeting of scientists and policy managers interested in air quality issues.

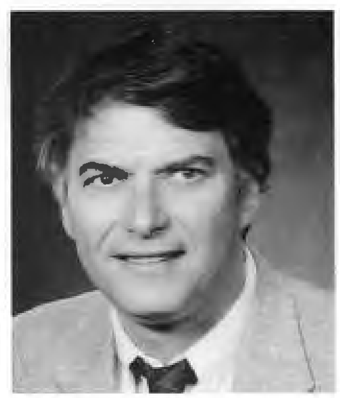
Martin Marietta Energy Systems, Inc., honored its employees on May 20, 1988, at the fourth annual dinner and awards presentation program at the Hyatt Regency Hotel in Knoxville. More than 130 ORNL employees or Energy Systems employees working on ORNL projects received awards. The engineer of the year was **Ray L. Johnson**; the inventor of the year was **Terry Tiegs**; the author of the year was **Mark Rasolt**; and the manager of the year was **Paul Haubenreich**, who is now secretary of the International Thermonuclear Experimental Reactor Council of the International Atomic Energy Agency in Vienna, Austria. They are among the five Energy Systems employees who each received Martin Marietta Corporation's highest award, the silver Thomas Jefferson Cup.

Fourteen ORNL employees received the Inventor Award, which recognizes innovative employee contributions to the activities of Energy Systems. The winners were **Charles W. Forsberg**, for the invention of the Process Inherent Ultimate Safety Boiling Water Reactor, a power reactor in which the safety systems contain no electronics or moving parts; **John B. Hayter** and **Herbert A. Mook, Jr.**, for innovative design and development of improved neutron optical devices; **Scott Hunter** and **Loucas G. Christophorou**, for development of gas mixtures that possess temperature-enhanced glow discharge characteristics for use in repetitive pulsed-power closing switches; **Mark A. Janney**, for numerous innovative contributions to the synthesis and processing of ceramic powders; **Harold D. Kimrey, Jr.**, and **Terry L. White**, for the development of a microwave furnace and insulation concept for processing ceramics; **Vinod K. Sikka**, for unusual creativity in devising new and improved procedures in materials processing, for development of new materials, and for innovative welding techniques; **David P. Stinton**, for numerous contributions to the development of advanced materials through the application of chemical vapor deposition techniques; **Terry N. Tiegs**, for innovative approaches to the development of ceramic composites for high-temperature applications; **Graydon L. Yoder, Jr.**, **Jack E. Smith**, and **David G. Thomas**, for invention of a multilayer shield to protect orbiting spacecraft against hypervelocity impact by micrometeorites, space debris, and orbiting particles.

Thirty-eight Energy Systems employees working on ORNL projects received Technical Achievement Awards, which recognize excellence of employee contributions of a scientific or engineering nature to the activities of Energy Systems. The winners were **Kimiko O. Bowman**, for a lifelong contribution to the theory of statistics with emphasis on properties of small sample estimators and computational statistics; **Everett E. Bloom**, for sustained leadership in the development of structural materials for fusion power systems; **David O. Campbell**, for his expertise, which has merited worldwide recognition, and his many significant contributions to chemical aspects of nuclear fuel reprocessing, separations chemistry, reactor chemistry, and nuclear waste management; **Richard D. Cheverton**, **John G. Merkle**, and **Randy K. Nanstad**, for outstanding leadership in the development and application of advanced fracture-mechanics methods to evaluate pressure vessel embrittlement problems and to provide a sound technical basis for projecting the vessel's remaining useful life; **David K. Christen**, for continued excellence in experimental investigations that have led to a better understanding of regular and high-temperature superconductors, which constitute a technologically important class of materials; **James M. Corum**, for outstanding leadership and contributions to international collaborative efforts to develop a structural design methodology for advanced high-temperature reactors; **Cabell B. Finch** and **Lynn A. Boatner**, for the solution of technical problems and contributions to the development of the first promethium laser; **Michael R. Guerin**, for pioneering the development and application of modern organic analytical chemistry within the health and environmental programs of the Department of Energy and many other agencies and institutions; **Richard G. Haire** and **John K. Gibson**, for the first measurement of the cohesive energy of fermium, element 100, thus establishing the divalent nature of the bonding in fermium metal; **Steven P. Hirshman**, for long-term contributions to creation of a theoretical basis for analyzing fluid equilibrium and collisional particle and heat transport in complex three-dimensional magnetic

Ray L. Johnson

Terry Tiegs



Mark Rasolt

Kimiko Bowman

Richard Cheverton

David Christen

systems; **Wayne A. Houlberg**, for his long-term contributions in development and validation of methods for time-dependent modeling of toroidal fusion plasma devices; **Ray L. Johnson, R. D. Benson, M. J. Cole, B. E. Nelson, J. A. White, K. K. Chipley, D. J. Taylor, G. H. Henkel, M. J. Saltmarsh,** and **J. L. Yarber**, for leadership in completion of the intricate final assembly of the Advanced Toroidal Facility within the required tolerances and within budget; **Kenneth Liu**, for the development of a high-temperature mechanical properties test system that allows the determination of tensile properties of brittle ceramic materials; **Richard Lorenz**, for significant technical achievements, from 1961 through 1987, associated with determination of fission-product source terms from nuclear reactor accidents; **Samuel B. McLaughlin, Jr.**, for outstanding research contributions to understanding the physiological responses of forests to air pollution stress; **Robert E. Mesmer**, for sustained scientific contributions and leadership in basic research with high temperatures and pressures, in aqueous chemistry, and in geochemistry; **Michael K. Miller**, for the design and development of ORNL's atom probe and for its application to important questions in materials science; **Liane B. Russell** for a brilliant research career in mammalian genetics, reproductive and developmental biology, and radiation biology; **Harold G. Smith**, for enhancing the understanding of the martensitic phase transformation in lithium metal through neutron-scattering experiments; **Cullie J. Sparks, Jr.**, for development of ORNL's Synchrotron X-Ray Facility at the National Synchrotron Light Source and for leadership in the application of synchrotron X-ray radiation in materials research; **Dennis J. Strickler**, for his pioneering contributions to defining the poloidal magnetics design of elongated divertor plasmas in the Compact Ignition Tokamak in collaboration with Princeton Plasma Physics Laboratory scientists; **David G. Thomas, Jack E. Smith,** and **Graydon Yoder, Jr.**, for the conception and demonstration of a kinetic energy/laser shield for space platforms with effectiveness equal to that of conventional concepts but with only 10% the weight; and **Man H. Yoo**, for his outstanding contribution to the fundamental understanding of micro-mechanisms responsible for thermal strengthening and embrittlement of structural metals and alloys, including ordered intermetallic compounds.

Sixty-five ORNL employees received a Publication Award, which recognizes superior employee performance in the authorship of a paper, technical article, or book that represents a significant advance in the author's professional field. The winners were **C. Bottcher** and **M. R. Strayer**, *Relativistic Theory of Fermions and Classical Fields on a Collocation Lattice*; **J. D. Budai, J. Z. Tischler, A. Habenschuss, G. E. Ice,** and **V. Elser**, *X-Ray Diffraction Study of Phason Strain Field in Oriented Icosahedral Aluminum-Manganese*; **T. A. Carlson, P. Gerard, M. O. Krause, F. A. Grimm,** and **B. P. Pullen**, *Photoelectron Dynamics of the Valence Shells of Benzene as a Function of Photon Energy*; **L. G. Christophorou, S. R. Hunter, L. A. Pinnaduwage, J. G. Carter, A. A. Christodoulides,** and **S. M. Spyrou**, *Optically Enhanced Electron Attachment*; **S. A. David, J. M. Vitek,** and **T. L. Hebble**, *Effect of Rapid Solidification on Stainless Steel Weld Metal Microstructures and Its Implications on the Schaeffler Diagram*; **D. C. Gregory, L. J. Wang, F. W. Meyer,** and **K. Rinn**, *Electron-Impact Ionization of Iron Ions: Fe^{11+}, Fe^{13+}, and Fe^{15+}*; **J. A. Horton** and **M. K. Miller**, *Atom Probe Analysis of Grain Boundaries in Rapidly Solidified Ni_3Al*; **C. H. Johnson, D. J. Horen,** and **C. Mahaux**, *Unified Description of the Neutron-^{208}Pb Mean Field Between -20 and +165 MeV from the Dispersion Relation Constraint*; **F. W. Larimer, E. H. Lee, R. J. Mural, T. S. Soper,** and **F. C. Hartman**, *Intersubunit Location of the Active Site of Ribulose-*

Bisphosphate Carboxylase/ Oxygenase as Determined by In Vivo Hybridization of Site-Directed Mutants; **S. H. Liu**, *Electronic Polaron Effects in Heavy-Electron Materials*; **D. H. Lowndes, S. J. Pennycook, G. E. Jellison, Jr., S. P. Withrow**, and **D. N. Mashburn**, *Solidification of Highly Undercooled Liquid Silicon Produced by Pulsed Laser Melting of Ion-Implanted Amorphous Silicon: Time-Resolved and Micro-structural Studies*; **P. K. Mioduszewski, R. C. Isler, J. E. Simpkins, P. H. Edmonds, E. A. Lazarus, C. H. Ma**, and **M. Murakami**, *Improvement of Plasma Performance with Chromium Gettering in ISX-B*; **G. S. Painter** and **F. W. Averill**, *Effects of Segregation on Grain-Boundary Cohesion: A Density-Functional Cluster Model of Boron and Sulfur in Nickel*; **M. Rasolt**, *Superconductivity in High Magnetic Fields*; **R. D. Spence** and **A. L. Wright**, *The Importance of Fission Production/Aerosol Interactions in Reactor Accident Calculations*; **D. A. Spong, D. J. Sigmar, K. T. Tsang, J. J. Ramos, D. E. Hastings**, and **W. A. Cooper**, *Effects of Alpha Populations on Tokamak Ballooning Stability*; **T. Vo-Dinh, B. J. Tromberg, G. D. Griffin, K. R. Ambrose, M. J. Sepaniak**, and **E. M. Gardenhire**, *Antibody-Based Fiberoptics Biosensor for the Carcinogen Benzo*(a)*pyrene*.

Fourteen ORNL employees (or Energy Systems employees involved in ORNL projects) received an Operational Performance Award, which recognizes outstanding exemplary performance in management, business, personnel, manufacturing, and other similar functions. The winners were **Sheila T. Brooks**, for outstanding contributions in Performance Improvement Projects, special assignments at ORNL, and long-time exemplary performance as a senior secretary; **Paul N. Haubenreich**, for his personal commitment and outstanding contributions to the international Large Coil Task for the development of fusion superconducting magnets; **Lester J. King**, for leadership and coordination of extensive efforts to provide safety documentation and technical requirements for successful startup of the TURF Californium Facility; **Sterling A. Meacham, E. Craig Bradley, Bruce M. Winchell**, and **Donald W. Jared**, for planning, developing strategies for, and leading the effort to commercialize the Advanced Servo-manipulator; **Morris H. Slabbekorn, Kenneth S. Davis**, and **R. Bruce Johnston**, for development and sustained improvement in Graphic Arts capabilities that have resulted in a state-of-the-art operation and consistently high placement in national competition with private companies and governmental agencies; **Donald R. Stallions**, for three consecutive years of innovative leadership and strong management skills that led his Safeguards and Security Department and ORNL to achieve "superior" ratings from DOE on the Nuclear Materials Control and Accountability function; **Victor J. Tennery**, for leadership in expanding high-temperature materials research at ORNL, especially in development of the new High-Temperature Materials Laboratory and in managing research in the High-Temperature Materials Section of the Metals and Ceramics Division; **Christine S. Travaglini**, for sustained outstanding performance in the development and administration of the Laboratory's capital equipment, budgets, overhead, material, and cost projections; and **Frederick W. Young, Jr.**, for outstanding sustained management and program coordination in the solid state sciences.

Felicia M. Foust received a Community Service Award, which recognizes outstanding and noteworthy performance by Energy Systems employees engaged in voluntary, uncompensated activities (social, civic, or governmental) that provide significant benefit to the community. She was honored for 30 years of dedicated involvement in volunteer work with the elderly and with schools, athletic programs, and other youth activities.

Vic Tennery

Christine Travaglini

Fred Young

CHAOS: Making a New Science

by James Gleick, Viking Press, New York, 1987, 352 pages.

Reviewed by N. B. "Woody" Gove, Data Systems Research and Development, Martin Marietta Energy Systems, Inc.

"The most ardent chaos advocates believe that 20th-century science will be remembered for just three things: relativity, quantum mechanics, and chaos."

Is there order in chaos? Can a system that exhibits chaotic, apparently unpredictable behavior actually be following a simple set of rules? Classical science has traditionally been concerned with describing systematic, orderly behavior—such as the rotation of planets about the sun or the tidy linear relationships of Euclidian geometry. When confronted with disorder in the natural world, such as the turbulence of ocean or wind currents, fluctuations of wildlife populations, or oscillations of the heart, classical physicists and mathematicians have generally been ignorant or, in some cases, annoyed. But in the1970s, a few scientists around the world became interested, even concerned, about the inability of science to address such problems. Working in many separate fields, they began to think seriously about *disorder*, and to wonder whether there might be some universal principles connecting the various types of irregularity found in nature. Gleick's book pulls together the thinking of these "out-of-step" scientists who began looking at the natural world from a new perspective, seeking to find some universal order within its many forms of "chaos."

Mitchell Feigenbaum, a Los Alamos physicist who thought about the turbulence in cloud formations and lightning paths—watching them from airplane windows until his scientific travel privileges were suspended on grounds of overuse—was one of the early investigators of chaotic phenomena. Almost simultaneously, a mathematician in Berkeley, California, a population biologist at Princeton University, a geometer working for IBM, and a French mathematician studying liquid turbulence were also beginning to investigate the complex behaviors that can result from relatively simple model systems. They began searching for some organizing principles or periodicity, using new techniques and the newly available computing power to analyze their apparently random data sets. New terms, such as "dynamical systems," "fractals," and "strange attractors" began appearing in scientific literature. Now, nearly two decades later, this fast-growing movement has come to be known under the shorthand name of "chaos," although traditional scientists sometimes find other terms, such as "studies of nonlinear phenomena" or "fractal geometry" more acceptable. The terms previously mentioned are increasingly used to describe various manifestations of this new science, which has been called a science of process rather than state.

Gleick points out that, in its descriptions of the global nature of systems, chaos science has cut across the lines of scientific disciplines and reversed the trend toward specialization that characterized science in the 1970s. In fields such as particle physics and molecular biology, scientists at that time seemed to be learning more and more about less and less. The emphasis was on analyzing the smallest details of systems: quarks, chromosomes, or neurons. Chaos scientists are looking at the whole, seeking order and universal behaviors within nature's randomness and complexities. The most ardent chaos advocates believe that 20th-century science will be remembered for just three things: relativity, quantum mechanics, and chaos.

Many systems, both physical and mathematical, can be shown to have a very sensitive dependence on initial conditions. Even simple recipes for generating numbers can lead to surprisingly complicated patterns. Physicist Edward Lorenz, working with one of the earliest computers at the Massachusetts Institute of Technology, discovered how a very small perturbation can cause an ultimately huge change when he hurriedly entered some rounded-off numbers in a simple computerized weather-forecasting program. The original program, stored in the computer's memory, had numbers with six decimal places; on a hurried day Lorenz reentered the numbers, rounded to the first three digits, assuming that such a small change (one part in ten thousand) would cause a correspondingly small change in the weather pattern predicted by the computer. To his surprise, the pattern that emerged was grossly different from anything the program had previously predicted. Intuitively, Lorenz realized that this effect was enormously unexpected and important. Ultimately, it meant that long-range weather forecasting is impossible, because the many small perturbations occurring constantly in the real atmosphere can have enormously magnified and unpredictable effects. He later described this phenomenon, which he called the Butterfly Effect, in a paper (presented in 1979 at an American Association for the Advancement of Science conference) entitled: "Predictability: Does the Flap of a Butterfly's Wings in Brazil Set Off a Tornado in Texas?"

Lorenz applied his new way of thinking to develop some simple-looking equations describing a hydrodynamic process called convection. He asked the question, "How can we calculate how quickly a hot cup of coffee will cool?" If cream is added, the swirls produced by convection can be complicated, and Lorenz realized that traditional physics provided no means to calculate the patterns of these convection currents or predict their cooling effects. Even though the set of convection equations Lorenz developed appear simple, they contain nonlinear terms and, as Lorenz explained, "You think there must be a way to get around them. But you just can't." He pointed out that it is very difficult to predict the temperature of the coffee one minute in advance, although it is easy to predict it for one hour ahead, because it will eventually reach room temperature.

Lorenz and other mathematicians and physicists went on to develop other systems in which our intuition—and classical science—can be proved wrong. Consider the behavior of such diverse "systems" as waterwheels, population models, investment curves, and static occurrences on a telephone line—all of these could be expected to reach some steady state under certain conditions. But Lorenz and others found that they do not; instead, they show a strange sort of regularity within irregularity—always changing in a nonlinear, unpredictable fashion, yet always remaining within certain bounds and showing unusual islands of periodic stability within the chaotic whole.

Gleick describes, in a very readable way, the new wave of research approaches that some (including former ORNL Director Alvin Weinberg) regard as a "revolution" or "paradigm shift" in science comparable to that of relativity or quantum mechanics. The book also traces the history of chaos studies and the people who left or "stretched" their previous scientific experience and disciplines to study chaos.

Some looked for patterns in chaotic systems and others found chaos, or nonlinear, unpredictable behavior, within systems previously believed to be quite orderly and predictable, even going so far as to proclaim that "the regularity Galileo saw is only an approximation." At low amplitudes of any dynamic system, any extremely small nonlinearity can be—and often has been—attributed to error and, for practical purposes appears to have no discernible effects, but "It is there and it is measurable," and its effects are real, say the chaos investigators.

Robert May, an Australian physicist turned biologist, studied a simple equation used for population studies, $x(\text{next}) = rx(1-x)$. He showed that, for certain values of r, the population would oscillate between two points. At higher values, a phenomenon now called "period-doubling" or "bifurcation" occurs, with population values reaching four times those expected, then eight, and eventually chaos. According to Weinberg, this type of behavior was seen earlier by E. Fermi and S. Ulam in a nonlinear oscillator model. (At first, I thought Gleick had missed this item, but it's actually mentioned in the notes at the back of the book.) James Yorke, a University of Maryland mathematician, proved that, if an oscillation involving three variables occurs in any one-dimensional system, then chaotic behavior will also occur. From his paper, "Period Three Implies Chaos," an emerging field of science took its name.

In the 1970s, Benoit Mandelbrot, an IBM mathematician, realized that Euclidian measurements could not capture the essence of irregular shapes. He puzzled over problems such as how to describe the dimensions of a ball of twine. With his access to what Gleick describes as the "high-speed idiocy" of IBM's considerable computing resources, Mandelbrot developed a new geometrical concept called fractals, characterized by "scale symmetry." If a rough surface is magnified, it may show both smooth and rough areas, and the "degree of roughness" usually depends on the degree of magnification. A fractal surface,

*"After reading **Chaos**, you will never look at the world in quite the same way again."*

"Some of the new computer and mathematics methods described in this book are also currently being used at ORNL."

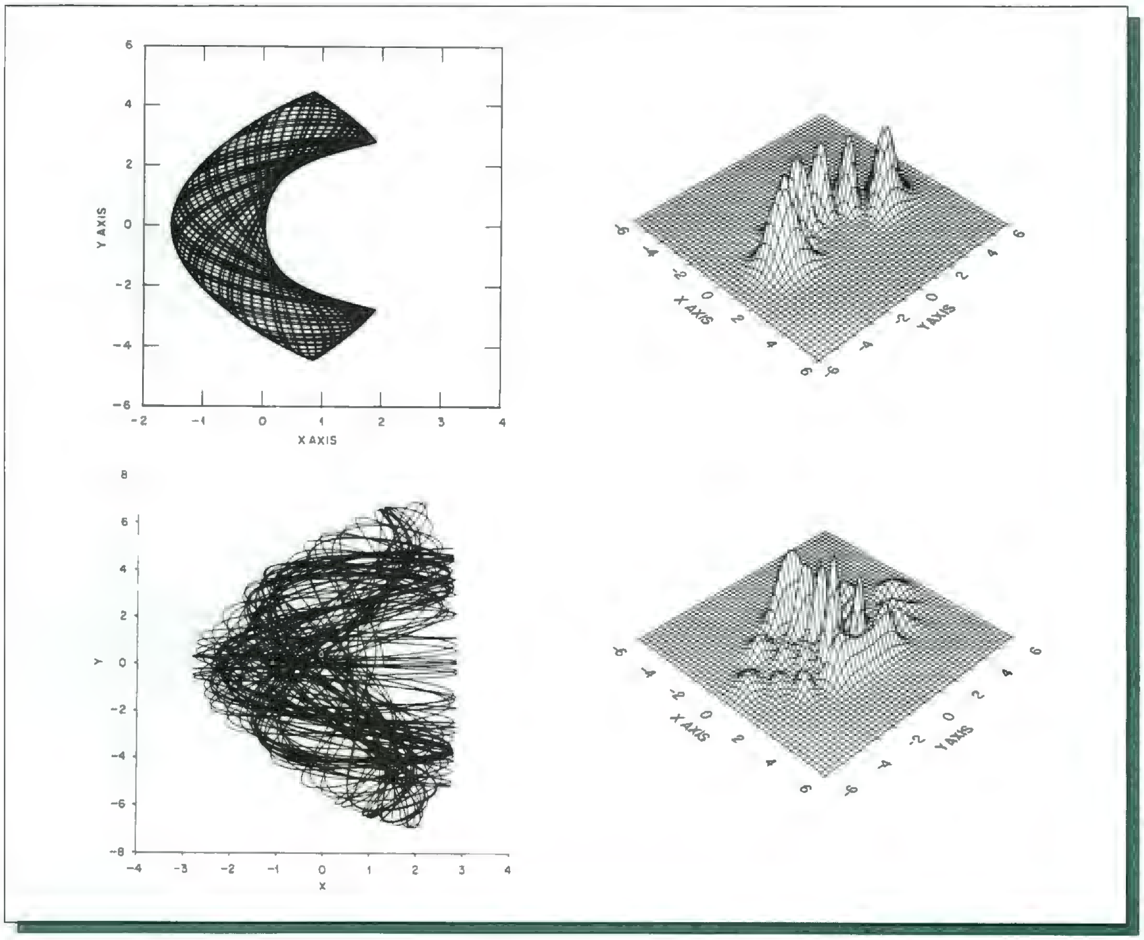
however, exhibits the same degree of roughness or irregularity pattern at any scale of magnification. Clouds, feathers, cauliflowers, and volcanic plumes are examples of the fractal surfaces found in nature. Our human mind cannot visualize the whole of such infinite self-embedding complexities, but mindless computers can create them by performing endless iterations of a mathematician's imagined form. Such a surface could even (theoretically) be infinite in area yet enclose a finite volume, and several mathematicians since Mandelbrot have delighted in finding or devising such fractal figures, once they knew what to look for. Fractal geometry has been applied to many natural systems and problems that exhibit some degree of scale symmetry, such as earthquake and income distribution, tree shapes, the human circulatory system, neural networks, snowflakes, and galaxies. Christopher Scholz, a Columbia University professor specializing in the form and structure of the earth, considers fractal geometry indispensable to his work, calling it "a single model that allows us to cope with the range of changing dimensions of the earth."

In 1971, David Ruelle, a Belgian mathematical physicist, and Floris Takens, a Dutch mathematician, published a paper, "On the Nature of Turbulence," which introduced the term "strange attractors" to describe the patterns of nonrepeating oscillation around two or more points in phase space, leading to an appearance of chaos. The term caught on, and strange attractors soon became the subject of several conferences. (A good description of strange attractors is given by Douglas Hofstadter in the November 1981 issue of *Scientific American*.) The strange attractors concept has been used in studies of phenomena ranging from galactic orbits to dripping faucets; Gleick says they are everywhere in nature, if we know how to look for them.

Scientists have found the universal property they sought in chaos. In 1977 two physicists, Joseph Ford and Guilio Casata, organized the first chaos conference in Como, Italy. ORNL chemist Don Noid attended this conference. Then a postdoctoral researcher at the University of Illinois, he presented a paper on polyatomic dissociation by infrared heating that included the figures on the opposing page. The contrast between quasiperiodic and chaotic motion for a classical two-node coupled oscillator model is illustrated in (1a) and (1b). For both trajectories, the Hamiltonian is the same and is very similar to that for the famous Henon-Heiles model, well-known to physicists. In chemical application, it shows the effect of coupling between two vibrational modes of a polyatomic molecule. Figures (2a) and (2b) represent the corresponding quantum-mechanical probability densities for these two trajectories (see Noid's discussion of chaos science in "Using a Supercomputer for Theoretical Chemistry," on page 10 of this issue).

Chaos researchers have shared the same hardships most revolutionaries have—lack of funding, a scarcity of advisors, and difficulty in having their work accepted (and published), because frequently it does not fit the boundaries of any traditional discipline or match the goals of a funding source. Chaos research remains controversial, but it has gained respectability and proven its usefulness in many areas. For example, Ilya Prigogine, a Nobel laureate chemist and author of a 1984 book, *Order Out of Chaos: Man's New Dialogue with Nature*, organized a 1985 conference on chaos in economics, and a NATO conference on fractal and nonfractal patterns in physics was held in 1986. Los Alamos National Laboratory recently established a Center for Nonlinear Studies, and Oak Ridge National Laboratory started a Center for Nonlinear Phenomena that is now operated by the University of Tennessee. The U.S. Defense Advanced Research Projects Agency (DARPA) is funding a Georgia Institute of Technology project on "rule-based" algorithms for fractals, with wide-ranging applications—missile target recognition, pine forestry, submarine design, the study of human faces, flight simulation, and cinematic special effects (a discussion of the latter appears on page 28 of the February 1988 issue of *Scientific American*). Chaos theory has also appeared in the local press, in an economics article published by the *Knoxville News-Sentinel* on February 14, 1988.

Some of the new computer and mathematics methods described in this book are also currently being used at ORNL. For example, Sam Liu, Ted



These figures, some of the first examples of quantum-mechanical representation of a chaotic system, were presented by Don Noid at the first chaos science conference at Como, Italy, in 1977.

Kaplan, and Len Grey used fractals in studying the interface between a metal and an electrolyte. Mark Rasolt is investigating the turbulence caused by large optical excitations in semiconductors. Don Noid does research on chaotic behavior in polymers.

The reader may wonder how many of the "new" results of chaos theory are really new. It is probably impossible to trace the intellectual heritage completely, but Gleick does describe earlier related works and adds 20 pages of notes on sources. Ideas on unpredictability and sensitivity to initial conditions are traced as far back as Poincaré. Fractals are related to a 60-year-old class of shapes called Julia sets (after French mathematician Gaston Julia), and two earlier mathematical creations of infinite complexity, called "Cantor dust" and the "Koch snowflake," are also described.

"After reading *Chaos*, you will never look at the world in quite the same way again," states the book jacket. This assertion may well be true. Certainly Gleick presents a fascinating wealth of material on a wide range of chaos problems in natural systems (several pages on cardiac models, for example) and on the scientists pioneering in this field. Because Gleick, a *New York Times* reporter, is writing for the public, he avoids technical terms and equations and does not attempt mathematical or physical precision in his discussions. Extensive references are given for technical readers who want to investigate further.

Gleick conveys a sense of excitement in the promise or hope that a new scientific era is beginning and that everyday phenomena may be, if not predictable, at least better understood. He suggests that the new science may revitalize and reunite other disciplines, conjuring up a picture of young renegades overthrowing the established order to set up a new utopia. Even if his expectations are overdrawn and chaos research causes only a little chaos in science, this book is important—and fascinating—reading. ornl

Trivelpiece Is ORNL's New Director

Oak Ridge National Laboratory will have a new director on January 1, 1989. On September 30, 1988, former ORNL director Herman Postma announced the appointment of Alvin W. Trivelpiece as ORNL director. Trivelpiece will also be a vice president of Martin Marietta Energy Systems, Inc., and will report to Postma, Energy Systems senior vice president.

In his formal announcement to the Laboratory's research and supervisory staff, Postma said, "Dr. Trivelpiece brings extensive academic, industrial, governmental, scientific, and administrative experience to this job, with a sound record of scientific and engineering accomplishments."

Trivelpiece, executive officer of the American Association for the Advancement of Science, is perhaps best known at ORNL for his work as director of the Office of Energy Research in the Department of Energy from 1981 to 1987 and, from 1973 to 1975, as assistant research director for the U. S. Atomic Energy Commission's Division of Controlled Thermonuclear Research.

Both a Fulbright and a Guggenheim scholar, he has a doctorate in electrical engineering from the California Institute of Technology and has taught electrical engineering at the University of California at Berkeley and physics at the University of Maryland. His industrial experience includes executive positions with Science Applications, Inc., and Maxwell Laboratories, Inc.

In his informal remarks to the staff, Postma praised the "thorough and very professional" work of the ORNL Search Committee, headed by ORNL Associate Director Murray Rosenthal, in securing a Laboratory director with such outstanding background and experience. More than 147 candidates were nominated or applied for the directorship.

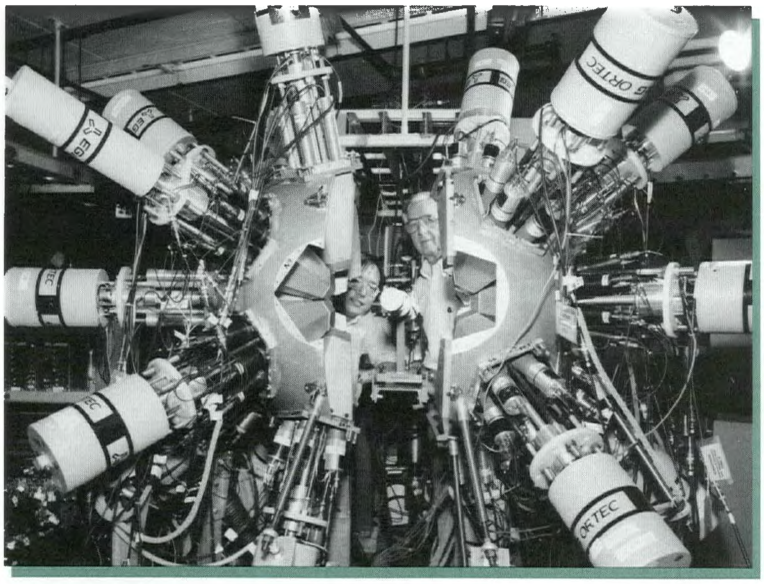
Acting Director Alex Zucker was commended by Postma for his effective leadership since early February in what Postma termed some "very difficult times for scientific management." Zucker will continue to serve as director during the transition period through the rest of this year.

Postma pointed out that Trivelpiece is the first ORNL director appointed from outside the Laboratory and the first to be selected by an internal search committee. He is, however, the second plasma physicist (Postma being the first) and the second Alvin (Alvin Weinberg being the first) to be named director.

Trivelpiece is also a journeyman electrician in good standing, a certified flight instructor, and an avid marathoner. He speaks fluent Dutch (as Postma does) and rides a unicycle (a feat Postma has tried and pronounced impossible). Postma quoted Trivelpiece as saying that he feels he has moved "too far from where science is done" and expects to enjoy being "back where important things in science happen."

Two HHIRF Devices Begin Operation

Two new devices have recently come on line at the Holifield Heavy Ion Research Facility (HHIRF). The Close-Packed Array, which packs 21 Compton-suppressed germanium gamma-ray detectors around a central core is the result of a



ORNL researchers Noah Johnson (right) and I. Y. Lee, architects of the Compton-Suppression-Spectrometer system, watch as the Close-Packed Array is fitted around the reaction chamber.

nearly $2 million collaborative effort involving scientists from ORNL, the University of Tennessee, and Vanderbilt University. The special detector elements (see photo above) were developed in cooperation with EG&G ORTEC.

One of the interesting uses of this device at the HHIRF will be the search for super-deformed nuclei—heavy nuclear systems that, at high angular rotation, assume a very elongated shape. Jim Ball, director of ORNL's Physics Division, says these have been identified in only a few cases, but some theorists believe they may occur more commonly than now thought and that hyper-deformed nuclei may be found with this powerful new detector array.

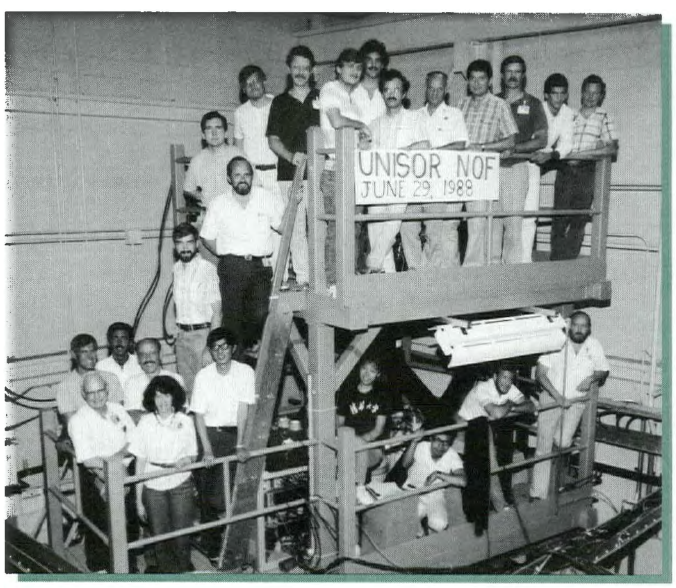
Holifield's second new addition is the Nuclear Orientation Facility, recently added to the UNISOR Isotope Separator there. Ball says the NOF is the most powerful instrument of its type in the world. With this advanced instrument, scientists are able to determine all angular distribution coefficients of the gamma-ray decay from targeted molecules. The unique device for the study of nuclear structure is operated by ORNL as a national user facility and is funded by Oak Ridge Associated Universities.

This first NOF experiment involved a total of 20 researchers, including 3 international research associates, 3 UNISOR staff members, and 6 faculty members along with 8 graduate students from 8 universities. In the experiment, the NOF magnetically oriented mercury-191 nuclei, which decayed by positron emission to excited-state forms of gold-191. The results provided information about energy levels in the mercury-191 nucleus. The NOF is unique in the United States in its ability to characterize nuclear decay modes and test nuclear theories.

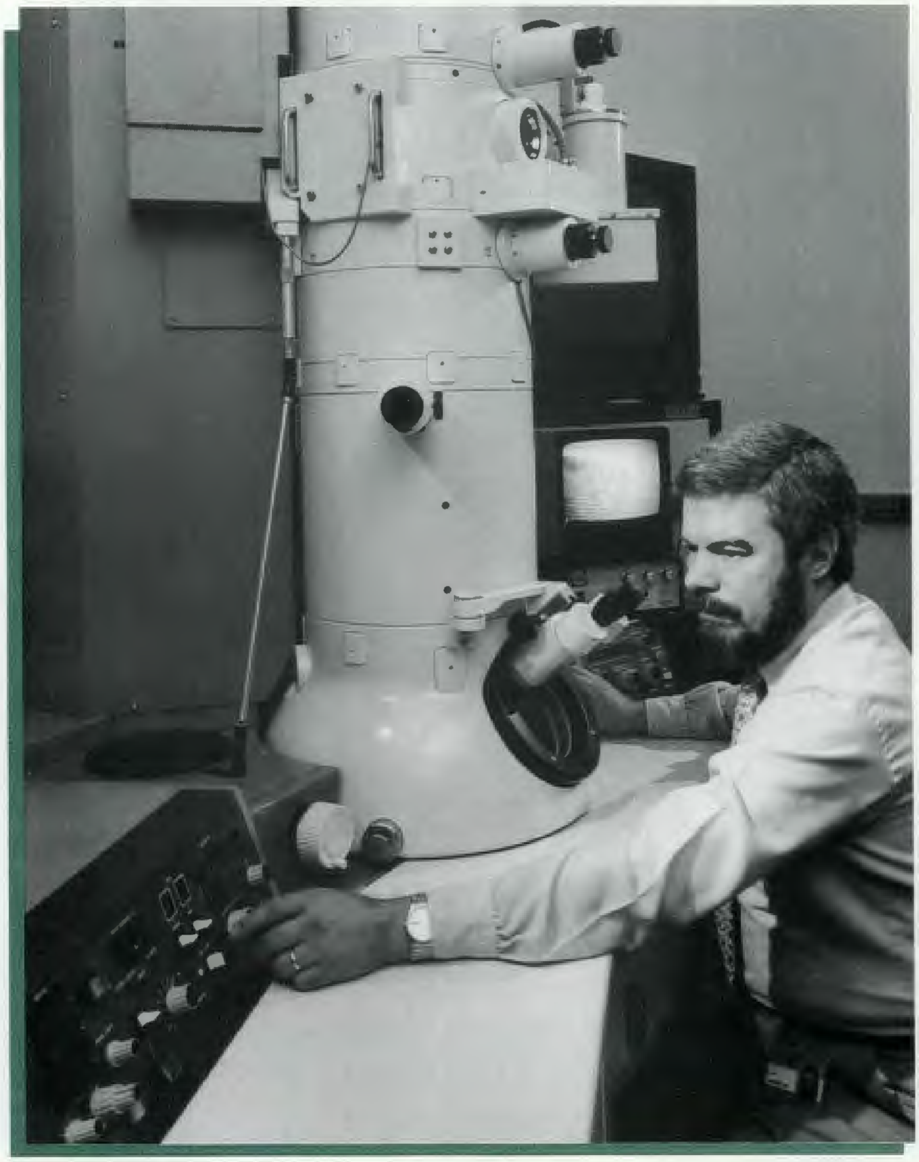
Tritium Pellet Injector Works

Refueling fusion plasmas with pellets of frozen deuterium, a heavy hydrogen isotope, has been demonstrated by ORNL in the 1980s at several tokamaks. ORNL injectors have accelerated deuterium pellets into the plasmas of the Tokamak Fusion Test Reactor at Princeton Plasma Physics Laboratory and the Joint European Tokamak at Culham Laboratory in England.

Now, ORNL has demonstrated for the first time that pellets of another frozen heavy hydrogen isotope—tritium—can be made and accelerated. This milestone brings the fusion community closer to the achievement of deuterium-tritium plasmas, which are more likely than deuterium plasmas to be used first in commercial fusion power devices because they require less



UNISOR staff, along with faculty and graduate students from eight universities who participated in the first successful on-line experiment, are shown at HHIRF's new Nuclear Orientation Facility.



Larry Allard uses the JEOL 4000EX transmission electron microscope to characterize high-temperature superconducting materials. This ultrahigh-resolution microscope was recently installed in ORNL's High Temperature Materials Laboratory.

demanding conditions. Deuterium is readily available from seawater, and tritium can be bred by neutron bombardment of a lithium blanket in a fusion reactor.

In May 1988, the Tritium Proof-of-Principle (TPOP) Pellet Injector, which ORNL designed and built, formed and accelerated pellets of frozen tritium at the Tritium System Test Assembly at Los Alamos National Laboratory. The TPOP device injected pellets (4 mm long and 4 mm in diameter) into the plasma at veloci ties up to 1200 m/s.

Developers were P. W. Fisher, of the Chemical Technology Division, and members of the Plasma Technology Group of the Fusion Energy Division.

DOE Superconductivity Pilot Center at ORNL

One of three DOE Superconductivity Pilot Centers has been established at ORNL. The centers will collaborate with industries in advancing the technology of high-temperature superconductivity.

The other two pilot centers are located at Los Alamos National Laboratory and Argonne National Laboratory. All three DOE laboratories have been active in high-temperature superconductivity research.

"The pilot centers are a key element in the Superconductivity Initiative announced by President Reagan last year," Secretary of Energy John S. Herrington said. They are designed to speed up the contracting and project approval process and the transfer of patent rights and other intellectual property from the national laboratories to industry.

The director of the ORNL pilot center is Anthony C. Schaffhauser. David Christen is scientific coordinator and Louise Dunlap is manager of the industry partnership program at the center. So far a number of private companies, including AT&T Bell and IBM, have expressed interest in using ORNL's facilities to characterize high-temperature superconducting materials. ornl

Hood River Conservation Project Attracts Participants, Saves Energy

A recently completed project in the Pacific Northwest involving work by ORNL researchers suggests that energy conservation is an important "source" of electricity.

The Hood River Conservation Project (HRCP) in Oregon has shown that home energy conservation measures—when applied systematically and thoroughly—can be a legitimate, reliable source of power for public and private utilities. "Conservation can be a cost-effective energy source," says Eric Hirst of ORNL, "because it often costs less to save electricity than it does to produce it. Thus, it helps eliminate the need to build expensive generating plants."

The five-year, $21-million HRCP "turned out to be a remarkably popular residential weatherization program, thanks to extensive word-of-mouth communication among Hood River residents and the project's offer of free weatherization," says Hirst.

"About 90% of the 3500 eligible households received free energy audits and installation of water heater wraps, ceiling insulation, storm windows, caulking, door weatherstripping, duct insulation, and other measures to reduce consumption of electricity for water heating and space heating. This participation rate is far higher than that usually achieved in conservation programs," Hirst points out.

Most of the nonparticipants were owners of single-family homes and earned higher-than-average incomes. The unusually large response to the program yielded a rich harvest of information on the tangible benefits of conservation to a utility.

The project had another important component besides weatherization: research and data collection and analysis. Data collected on the HRCP from 1982 through 1986 were analyzed by the Decision Systems Research Section in ORNL's Energy Division.

The results showed that an overwhelming majority of utility customers are willing to participate in an energy-saving program, that cooperation can be achieved between groups and institutions that may otherwise be at odds, and that, adjusting for climate, the Hood River community had the lowest space-heating consumption ever recorded following a retrofit program. The results have been used by the Bonneville Power Administration and the Northwest Power Planning Council to design and plan future conservation programs.

The HRCP spent about $4400 per household on weatherization measures. As a result of these measures, the weatherized homes each reduced electricity use by about 15% of the amount consumed before weatherization (an average saving of 2600 kWh per year). The savings would have been greater if the region had less unemployment and if many of the residents had not been accustomed to burning wood for space heating and taking other measures to keep electric bills down in response to the dramatic price rises of the 1970s.

The success of the project was partly the result of cooperation among environmentalists, government officials, and utility managers. It was proposed by a private environmental protection group, the Natural Resources Defense Council; funded by a federal agency, the Bonneville Power Administration; and operated by a private utility, the Pacific Power and Light Company in cooperation with the Hood River Electric Cooperative.

"The questions behind the project were 'Is conservation a true energy resource?' and 'Can utilities rely on it?' From what we have learned from the Hood River project, the answers are 'yes,' " said Hirst, who headed the evaluation of the project for the Decision Systems Research Section. Much of the analysis was done by group leader Marilyn Brown and Rick Goeltz.

"The results showed that an overwhelming majority of utility customers are willing to participate in an energy-saving program."

Contractors install storm windows on a Hood River house.

"Conservation measures in the home can keep consumers just as warm in winter and just as cool in summer as can a coal-fired power plant," said Goeltz. "The difference is that building a new plant could drive up electricity rates to cover the capital investment and interest costs. Our analysis shows that conservation can be a reliable, valid source of energy because it reduces the need for power."

The extensive use of conservation as an energy resource is less costly in the long run, says Brown. "The utility can buy conservation in small amounts, see what works and what doesn't, and expand or reduce the program as needed. On the other hand, ordering a new nuclear power plant is a major, difficult-to-reverse commitment requiring $2 billion, 10 years of construction and testing, and special measures to satisfy the public and government regulators."

The research and analysis provided by the Decision Systems Research Section and others began a year before the program started in 1983 and continued more than a year after conservation measures were installed in 1985. According to Hirst, this work was vital to the program's goal of determining the appropriate role of utilities in securing conservation resources to aid in regional energy planning.

"ORNL was asked to evaluate the HRCP," explained Hirst, "because we have a good reputation for analyzing energy-use data, because we were viewed as unbiased as a result of our track record in conducting similar evaluations for the Department of Energy and Bonneville, and because we are located outside the Pacific Northwest region."

How Acid Rain Can Cause Decline in Tree Growth

The decline in tree growth in the Great Smoky Mountains National Park may be a result of the greater availability of aluminum to the trees because of the effects of acid rain and air pollution on soils, according to an ORNL researcher.

Tree-ring evidence showing that aluminum levels are higher in trees whose outside rings have decreased in size was presented May 12, 1988, by Ernie Bondietti of ORNL's Environmental Sciences Division at the 14th Annual Scientific Research Meeting of the National Park Service at the Smokies park headquarters.

"The trees are the silent monitors of changing levels of industrial air pollution," says Bondietti. "Since the 1940s, many Appalachian trees, from the red spruces of New Hampshire to the shortleaf pines of Tennessee, have experienced declines in radial tree growth and increases in aluminum levels. The effect is particularly noticeable for the past 25 years, when regional fossil fuel combustion emissions from industry have increased as much as 200%."

Research by Fred Baes and Samuel McLaughlin of ORNL's Environmental Sciences Division has shown that aluminum concentrations in tree-ring tissue have risen since the 1940s. The ORNL researchers have also observed that the tissues of trees showing decreasing ring growth have a higher level of aluminum than calcium.

"Our findings," says Bondietti, "support the results of U.S. Forest Service research indicating that aluminum in the soil inhibits the uptake of calcium by trees. This reduction in calcium uptake may inhibit tree growth."

Acid rain is formed when sulfur oxides and nitric oxides, produced from fossil-fuel combustion, react with atmospheric moisture to form acids (sulfates and nitrates). Since 1984, ORNL researchers, including Dale Johnson, have been examining the idea that acid precipitation makes aluminum, iron, and other metals in soil more available to trees and other vegetation.

In most soils, positively charged ions of aluminum are attached to negatively charged soil particles. When negatively charged sulfate and nitrate ions are introduced to the soil through acid precipitation, some of the aluminum is stripped away from the soil particles and brought into the acid solution. The solution can carry the previously soil-bound aluminum into streams or make it available for absorption by tree roots.

"Tree-ring evidence shows that aluminum levels are higher in trees whose outside rings have decreased in size . . ."

Bondietti says that the evidence suggests that decreasing industrial emissions of sulfates and nitrates should lessen the release of aluminum from soil and foster increased tree growth.

The aluminum studies build on research done by Baes and McLaughlin in 1984, when they sampled numerous trees in East Tennessee and North Carolina. They deciphered the metallic element content of tree-ring tissues by a technique called inductively coupled plasma optical emission spectroscopy.

They found that annual growth rings from shortleaf pine trees in the southeastern portions of the Smokies showed both suppressed growth and increased iron content between 1863 and 1912. During this period, large sulfur dioxide releases from the copper smelting 56 miles upwind at Copperhill, Tennessee, caused extensive mortality of trees within about an 11-mile radius of the smelter. ornl

ORNL Alloy Licensed to Supplier of Aircraft Fasteners

"Energy Systems recently granted Valley-Todeco the exclusive rights to supply aircraft fasteners made of nickel aluminide to the private sector."

A high-temperature, nickel aluminide alloy developed at ORNL has been licensed to one of the aircraft industry's leading suppliers of bolts and other fasteners.

Energy Systems recently granted Valley-Todeco the exclusive rights to supply aircraft fasteners made of nickel aluminide to the private sector. Valley-Todeco, located in Sylmar, California, is a division of The Lamson & Sessions Company.

Nickel aluminide, which becomes stronger at higher temperatures, is six times as strong as stainless steel at 1100°F (600°C). Unlike many materials commonly used in the aerospace industry, it is not subject to stress-corrosion cracking.

Valley-Todeco President Patrick Dansby said his company anticipates that nickel aluminide will permit the development of new, high-performance fasteners for the high-temperature operating environment of tomorrow's fuel-efficient engines. "Manufacturing and testing programs to determine the engine capabilities of new high-strength, high-temperature materials have been started, and Valley-Todeco is working closely in this endeavor with a major manufacturer of metal alloys," Dansby added.

Energy Systems negotiated the license with Valley-Todeco following a waiver of patent rights from DOE. Licensing royalties, under a DOE-approved formula, will be used to support other technology transfer activities. Four previous licenses have granted the right to manufacture and market nickel aluminide and to use the alloy in large diesel engines, heating elements, cutting devices, and tools and dies.

Other potential applications of nickel aluminide include high-performance jet engines, gas turbines, advanced heat engines, and heat exchangers in nuclear and coal-fired steam plants.

Metallamics To Manufacture Nickel Aluminide Products

Energy Systems has announced a licensing agreement with a new Michigan company that will use the high-strength, high-temperature nickel aluminide alloy developed by ORNL for its products.

The company, Metallamics, Inc., of Traverse City, Michigan, has acquired nonexclusive rights to the heat- and corrosion-resistant alloy for the fabrication of industrial parts that must withstand extremely high temperatures.

Normally a brittle material, nickel aluminide has been made ductile through a patented ORNL process. The alloy is described as "intermetallic" because it shares some characteristics of both nickel and aluminum. Nickel aluminide has the unusual characteristic of increasing in strength at higher temperatures. At 1100°F (600°C), it is six times as strong as stainless steel.

Robert McDonald, Metallamics president, says his firm intends to use a proprietary powder metallurgical process for specialty applications of the nickel aluminide, such as tool and dies, cutting devices, and structural and working components.

Licensed Ionization Source Is Key Component of Explosives Sensor

A California company has agreed to make a multimillion-dollar investment over a several-year period to design and produce a commercial version of an ORNL device that can "sniff out" minute traces of the telltale vapors from chemicals such as concealed explosives. Licensing efforts were led by Jon E. Soderstrom, technology applications director for Energy Systems.

The Finnigan Corporation, based in San Jose, California, has been granted a license for an Atmospheric Sampling Glow Discharge Ionization Source which, when coupled with a mass spectrometer, can instantly detect low-level atmospheric chemicals. Finnigan is a worldwide producer of a broad range of mass spectrometers, which are analytical devices used to identify and quantify elements and isotopes in samples.

The proposed device will detect and identify explosives at levels lower than one part per billion in less than a second by chemically identifying organic nitrogen-oxygen compounds that are the basis of explosives such as TNT, plastiques, and nitroglycerine.

The key to this increased sensitivity is the novel ion source developed by Gary Glish and Scott McLuckey of ORNL's Analytical Chemistry Division. This source is a simple and durable instrument, capable of high-sensitivity, trouble-free operation for prolonged periods.

"We see this device as having application in many fields, not only explosives detection," Michael Story, a Finnigan co-founder, said. "It is suited for many low-level remote sensing applications, such as hazardous wastes and industrial work-site monitoring, plant fugitive emissions monitoring, personnel or security screening, and even military applications." ornl

"We see this device as having application in many fields, not only explosives detection."

OAK RIDGE NATIONAL LABORATORY *REVIEW*
P.O. Box 2008, Oak Ridge, Tennessee 37831-6144

U.S. Postage
PAID
BULK RATE
Oak Ridge, Tenn.
Permit No. 3

NEXT ISSUE

New ways of managing wastes and correcting the results of past waste-disposal practices will be treated.