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Energy&Technology

The State of the Laboratory 1

Defense Systems 4

Laser Research 24

Magnetic Fusion Energy and Beam Research 42

Energy and Earth Sciences 50

Biomedical and Environmental Science 60

Engineering 68

Physics 76

Chemistry and Materials Science 86

Computations 94

Laboratory Administration 100

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The State of the Laboratory

"I am confident that the Livermore Laboratory will be a crucial part of our ability to meet the challenges of the new decade and the new century."

The mission of the Lawrence Livermore National Laboratory is to provide a national resource of scientific and engineering research and development capabilities with special focus on national security. The Laboratory has a living mission: throughout our history, the federal government has, from time to time, broadened the LLNL mission to address new, important national needs. In addition to nuclear deterrence, our mission includes strategic defense, energy, the environment, biomedicine, education, and the economy.

As we enter the last decade of the 20th century and look forward to the 21st, the University of California (UC) Lawrence Livermore and Los Alamos National Laboratories are the world's premier large-scale applied science laboratories, each with 8000 extraordinarily talented UC employees, multibillion-dollar plant and facilities at the frontiers of science and technology, and billion-dollar annual budgets.

In the short lifetimes of these laboratories, they have had a key role in meeting the challenge of peace—in achieving an unprecedented 40-year period without major war after half a century scarred by two World Wars. The laboratories also have had a key role in successfully meeting the challenge of freedom articulated by President Kennedy in 1960 at the height of the Cold War: "In the long history of the world, only a few generations have been granted the role of defending freedom in its hour of maximum danger."

Speaking to the Laboratory during his visit here last February, President Bush cited LLNL's "truly remarkable ... technical prowess" and thanked the Laboratory for its "role in preserving the peace and keeping the world stable and America secure." He emphasized that the "strength of the U.S. nuclear deterrent developed through the efforts of our national labs ... has helped to guard the peace and freedom so precious to all of us ... The world's movement toward democracy and freedom is a direct result of our ability to stand firm in the face of threats to stability and peace."

The world today is far different than it was 38 years ago when the Laboratory was founded. Every

decade of our history has been a decade of change. During the past two years, the pace of change has accelerated. Powerful geopolitical, economic, and technological forces are revolutionizing the world. The Laboratory has an outstanding record of responding to new national needs that appear in periods of change and uncertainty. We live by Edward Teller's vision that "the future is uncertain, and because it is uncertain we can change it." Now the nation and the world face major challenges in broad areas where the Laboratory has major strengths: defense, energy, environment, economy, and education. These strengths include the science and technologies of nuclear weapons, high-power lasers, fusion, large-scale computational modeling, and biology and the environment.

Through our stewardship of the nuclear deterrent, we have the opportunity to contribute to achieving another 40 years without major war and to help freedom and democracy spread throughout the world. Through the development of verification technologies, we are making possible arms-control agreements that will lead to a more stable world. President Bush cited this continuing public service: "Our national labs will be as crucial as ever as we adapt both the size and shape of our nuclear deterrent ... But to protect the American people, we will settle for nothing less than the highest confidence in survivability, effectiveness, and safety of our remaining forces."

Through our leadership in developing new strategic defense technologies, we have an opportunity to provide safeguards against attacks by ballistic missiles armed with weapons of mass destruction. Through the development of nonnuclear technologies, we are making possible a world less dependent on nuclear weapons. Of strategic defense technologies, including LLNL's Brilliant Pebbles, the President said: "Beyond their contributions to deterrence, they underlie effective arms control by diminishing the advantages of cheating, and they can also defend us against accidental launch or attack from the many other countries regrettably acquiring ballistic missile capabilities. In the 1990s, strategic defense make much more sense than ever before."

The Laboratory has equally exciting opportunities to make major contributions in nondefense areas including the "four E's"—energy, environment, economy, and education. In the 21st century, liquid fossil fuels will be exhausted. Possibly disastrous global greenhouse-induced climate change will be driven by carbon dioxide released from the burning of fossil fuels. Economic competitiveness is essential to this nation's future, as are educated citizens and an educated workforce. Looking to the future, President Bush said "the scientific expertise of the laboratories like Livermore will also serve the national interest in other areas, like economic capabilities, education, energy, space exploration, waste cleanup, and sound environmental practices. These will be enormously important challenges in the future ... The Livermore Laboratory will be a crucial part of our ability to meet the challenges of the new decade and the new century."

The projected budget for the 1990 fiscal year is $1059.6 million, slightly more than last year's $1055.6 million. In round numbers, $336 million is earmarked for defense work (including nuclear weapons work, verification and arms control, and other DOE defense projects), $227 million for laser research (including inertial confinement fusion and laser isotope separation), $25 million for magnetic fusion energy, $14 million for biomedical and environmental research, $23 million for energy research, and $35 million for the National Energy Research Supercomputer Center. The nuclear weapons program suffered a 12% decrease in purchasing power in the 1990 fiscal year. With an annual inflation of 4 to 5% together with the various environmental restoration and ES&H programs that must be funded out of operating expenses (more than $17 million), the LLNL's overall finances are very tight indeed. This year, the Laboratory sponsored an early retirement program and more than 300 employees took advantage of it.

This has been a very productive year for the Laboratory. Among the highlights are, for Defense Systems, completion of Phase-3 testing of the W89 warhead for the SRAM II missile. The warhead is now ready for preproduction engineering. This is a very timely accomplishment as the W89 will replace the current SRAM warhead, which has recently been offloaded from alert aircraft. The Physics Department "O" Group developed a design for space-based defensive interceptors, called Brilliant Pebbles, that has been adopted as the baseline design by the Strategic Defense Initiative Organization.

The Laser Programs continued to make excellent progress toward the goal of demonstrating the technology to support building a large-scale uranium enrichment plant in this decade. This technology has the technical and commercial potential to dominate a multibillion-dollar-per-year market. Breakthroughs in inertial confinement fusion research in both target design

and laser technology will make possible the achievement of ignition with an upgrade of the Nova laser to the 1- to 2-MJ scale. This year, we achieved near-ideal implosions by using temporally shaped laser pulses to increase the performance of the targets; the combination of density, confinement time, and temperature reached in these implosions set a new record and is within an order of magnitude of that required for ignition. Another achievement was the demonstration of x-ray lasing at 4.48 nm, the optimal wavelength for imaging biological specimens.

The Magnetic Fusion Energy Program demonstrated the use of a free-electron laser—the ETA II—for microwave heating of a tokamak plasma.

In Energy and Earth Sciences, artificial neural network algorithms were applied to discriminate and classify seismic events as earthquakes or underground explosions.

In our Biomedical research, we successfully cloned the human gene responsible for the repair of DNA damage caused by ultraviolet light and, as part of the human genome project, we devised a technique to rapidly develop probe molecules needed to map human chromosomes. Also, in recognition of the Laboratory's excellence in genetics and related biomedical research, the Department of Energy announced, on July 11, 1990, the establishment of LLNL as a Center for Human Genome Research. There are only two other such DOE centers in the country, one at the Los Alamos National Laboratory and the other at the Lawrence Berkeley Laboratory. The mission of these centers is to participate in an international effort to construct a physical map of the genetic material—DNA—in all 24 human chromosomes.

Engineering demonstrated important advances in methods for nondestructive evaluation of materials, including wide-bandwidth acoustic probing and computerized tomography.

In Physics, we used data from the SN 1987A supernova event to verify our detailed theoretical models of supernova explosions. The Electron Beam Ion Trap has sparked a revolution in atomic physics by making virtually all ionic states of all elements in the periodic table experimentally accessible. In addition, experimental programs conducted in collaboration with Lawrence Berkeley Laboratory and Argonne National Laboratory have produced evidence of the existence of shape isomers.

Chemistry and Materials Science developed an extremely lightweight silica aerogel foam that has a density only four times that of air and yet is strong enough to support 1600 times its weight. Potential applications for this material range from refrigerator insulation to capturing micro-meteorites in space.

In Computations, a new technique for solving very-large-scale systems of previously inaccessible nonlinear equations was devised, and new software for archival computer storage was recently licensed to a private industry.

On an institutional level, the problems facing the Laboratory—tight budgets, environmental issues, safety and security, the need to ensure a drug-free workplace—mirror those of any community today.

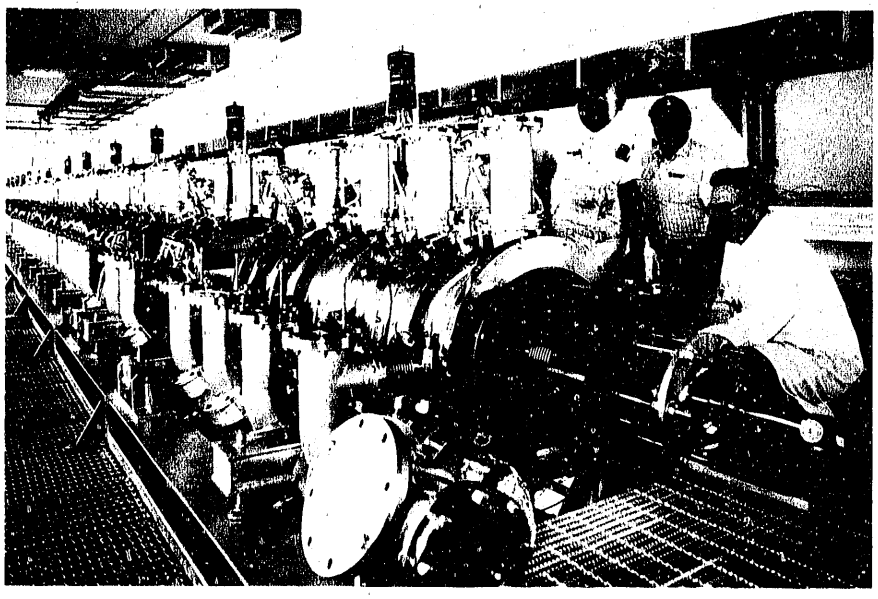
We are giving top priority to environmental protection, safety, and health (ES&H). We are adapting existing methods and devising innovative new techniques to address and remediate environmental problems at LLNL, many of them the product of previous activities at the site before the Laboratory was established. An ES&H Council was formed this year to oversee the Laboratory's ES&H activities. We are also transferring LLNL-developed ES&H technologies to other facilities.

In spite of constrained financial circumstances, we were able to make a number of major improvements to Laboratory facilities. The upgrades of Building 111 and the Tritium Facility are nearing completion, the new Medical Facility opened, and the first phase of our Safeguards and Security Enhancement is almost finished. In addition, ground was broken for the Nuclear Directed Energy Research Center and the Nuclear Test Technology Center, and a revitalization of Site 300 facilities is planned.

LLNL employees are our principal strength—exceptionally talented and deeply committed to their work. This human resource is crucial to the Laboratory's ability to meet the challenges of the future. As President Bush said, "these will be enormously important challenges ... challenges that your skill, your talents, those flashes of insight matched with long hours of labor will help us meet squarely and well."

John H. Nuckolls
Director

Defense Systems



This 4-MeV linear accelerator (the FXR), together with other diagnostic equipment in Bunker 801 at Site 300, provides the most capable facility in the U.S. for performing the hydrodiagnostic experiments that are essential for our nuclear weapon design and development activities.

The rapid and unexpected changes that have taken place in this past year, especially in Eastern Europe and the Soviet Union, underscore the uncertainty of the world we live in. This uncertainty complicates the already difficult job of long-range planning for the LLNL's Nuclear Weapons Program. Over the past several years, funding from the Department of Energy for Weapons, Research, Development, and Testing (WRD&T) has declined. These reduced budgets have resulted in the loss of full-time employees for the Weapons Program; staffing has decreased roughly 20% over the last three years.

Amid this increased uncertainty and in spite of reduced resources, we must attempt to anticipate the likely directions that U.S. weapons requirements will take so that we can plan accordingly. For example, given recent arms-control agreements as well as the ongoing negotiations, it is clear that the U.S. will have to depend on a nuclear deterrent composed of fewer warheads as well as fewer weapon systems that are nuclear-capable. Also, future reduced budgets for the Department of Defense will probably translate into less funding for new or modified weapon systems, which, in turn, will probably mean fewer programs to design and develop new nuclear warheads. In addition, the Secretary of Energy recently outlined a ten-point initiative to make the DOE nuclear weapons complex, including the Laboratory, as environmentally and safety responsive as possible; this initiative is to be funded from our already limited resources.

LLNL's Weapons Program must also deal with several imperatives. The first arises from legislation passed by Congress tasking the DOE and the weapons-development laboratories to develop a responsive Nuclear Test Ban Readiness Program. Should an agreement be negotiated between the U.S. and the Soviet Union that either limits or halts nuclear testing, the laboratories must have a program in place so that an adequate U.S. nuclear deterrent can be maintained with reduced or no testing.

A second imperative facing the Weapons Program is a shortage of plutonium and tritium resulting from the shutdown of the production reactors at Savannah River. These reactors have not operated for two years. Thus, with time, a shortage of

tritium (which decays radioactively by approximately 5% per year) will develop.

A third imperative arises from environmental, safety, and health (ES&H) considerations. As mentioned above, the Secretary of Energy requires that all DOE facilities operate within all established ES&H guidelines. The Weapons Program will be fully responsive to the ES&H requirements; however, meeting these requirements places a further demand on our already severely declining resources. To meet the ES&H requirements, we must reduce support to such important projects as nuclear test ban readiness, special nuclear material research, and advanced weapon-concepts research.

A Laboratory-imposed imperative is our initiative to place increased emphasis on advanced safety and security features in the design of modern nuclear weapons. This often entails considerable effort in the design and engineering of new warheads and requires extensive calculational modeling as well as nonnuclear and nuclear testing.

Taken together, these imperatives give us direction for the future of the Weapons Program. Certainly, weapon effectiveness and weapon survivability represent areas of great importance. As the number of weapons in the U.S. stockpile is reduced, the qualitative improvements to enhance a weapon's effectiveness or its ability to survive an offensive strike become much more critical. Insofar as land-based systems are concerned, improvements in systems survivability often involve mobility, and, with mobility, issues involving weapon safety and security take on new dimensions. The rail-mobile Peacekeeper (MX), which involves placing MX missiles on railroad cars, and the Small ICBM, which would be deployed on truck-mounted launchers, must be able to survive worst-case scenario accidents and remain absolutely safe. We have made great strides in recent years in improving the inherent safety of nuclear warheads. We believe, however, that there are further qualitative safety and security improvements that we can make, and we intend to pursue them vigorously in the coming years.

It is also true that as the size of the U.S. nuclear force is reduced, the impact of technological surprise will increase. To guard against this possibility and to provide weapon options for sustained stockpile weapon effectiveness, a portion of the Laboratory's weapons efforts is focused on the examination and evaluation of advanced technologies. If we are to cover sufficiently all of the WRD&T areas that we believe will be necessary in the future, our efforts in this area must increase.

Computational physics is and has always been an essential ingredient in weapon development. Numerical simulation and modeling allow us to explore more design options and in more detail than would be possible if we had to rely solely on expensive nonnuclear and nuclear testing. Recently, we developed the capability to use, on a fairly routine basis, three-dimensional calculations in the design and assessment of our warheads. This capability is critical for safety assessments of developmental and stockpile systems. The scale and complexity of these calculations is immense and is straining the capacity of our already-large computer resources; an increase in computing capability by a factor of a hundred or a thousand is needed if we are to be able to adequately perform these new three-dimensional calculations to the level required for projected program activities. This increased computing capability is even more essential in the face of future limits or bans on nuclear testing.

As noted above, possible future additional nuclear testing restrictions may be imposed, perhaps in the form of reduced yield thresholds or quotas on the number of tests that can be conducted. We are quite confident that we understand what must be done to explore the types of WRD&T activities that could take place under such test limitations. However, the resources that we have been able to apply to such exploratory programs have not been sufficient to enable us to assess these programs in a reasonable time scale.

Underlying all of these important activities is a basic element of concern that we refer to as "nuclear competence." The Livermore and Los Alamos laboratories have cradle-to-grave responsibilities for all of the nuclear weapons in the U.S. stockpile. However, these responsibilities cannot be met without talented and trained personnel, and we cannot sustain nuclear competence without healthy and active WRD&T programs.

Although the decline in WRD&T resources is an issue of undeniable concern and although the Laboratory's Weapons Program is facing many uncertainties, we are completely dedicated to fulfilling our responsibilities in maintaining a reliable, safe, effective nuclear weapons stockpile that provides the deterrence on which the country still relies. In spite of these impediments, the Weapons Program continues to produce many individual technological accomplishments of outstanding quality. The articles that follow summarize a few of the many outstanding achievements of LLNL's Weapons Program and illustrate the strong research and development program we still possess.

Contact: W. F. Scanlin (415) 423-6810.

High-Explosives Applications Facility

We are working to produce energetic materials with both higher performance and improved safety properties.

LLNL's new High-Explosives Applications Facility (HEAF) was occupied in the spring of 1989 (Figure 1). HEAF laboratories designed for synthesizing, formulating, and testing of high-energy materials are now operational. The remaining laboratories, designed for larger-scale high-explosives testing (up to 10 kg TNT equivalent) in containment tanks, including a facility for a four-inch-bore gun, became operational during May 1990.

Synthesis Efforts

Our current work in new high-energy materials focuses on synthesizing two classes of compounds: insensitive high explosives that perform better than TATB (1,3,5-triamino-2,4,6-trinitrobenzene) and high explosives with more energy than HMX (1,3,5,7-tetraazacycloctane). During the past year we marked progress in the latter area, successfully synthesizing a poly-nitroamino cyclic compound with a calculated performance better than that of HMX (Figure 2). An 800-g sample of this material, formulated with 5% Viton A, was pressed to 96.5% of its theoretical density. We evaluated its performance with cylinder tests; the results showed a detonation velocity of 8.81 km/s and a detonation pressure of 38 GPa. This formulation has 2 to 3% more energy than comparable formulations of HMX. Its shock sensitivity is much greater than that of HMX, however, thereby limiting its use as a general explosive.

Formulation Activities

Our current formulation effort is aimed at developing a material that has a higher energy than TATB and that also meets the Department of Energy's protocol for an insensitive high explosive. We are working with mixtures that contain TATB, HMX, and high-density energetic binders. Preliminary results indicate that the energy—but not the sensitivity—of such formulations depends linearly on HMX concentration. We are studying five HMX-based formulations that are highly likely to pass shock-sensitivity tests. Such materials have many applications in nuclear weapons.

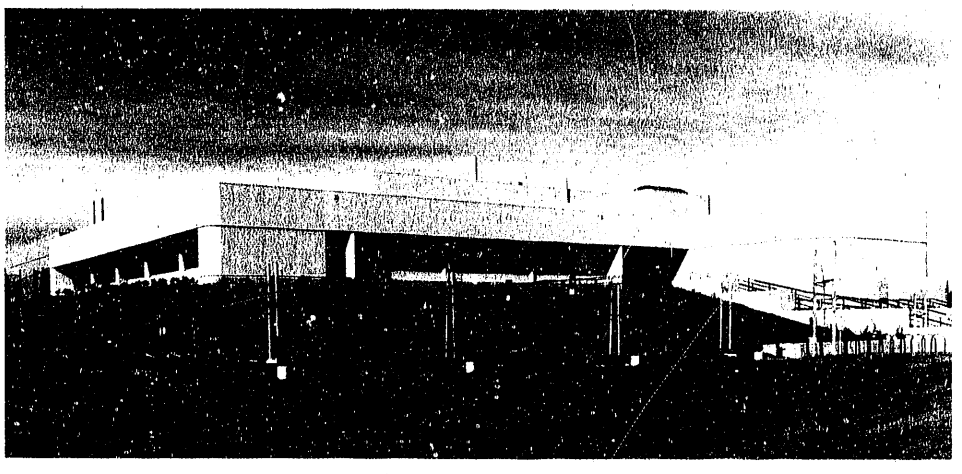


Figure 1. *Office section of the HEAF, looking northwest.*

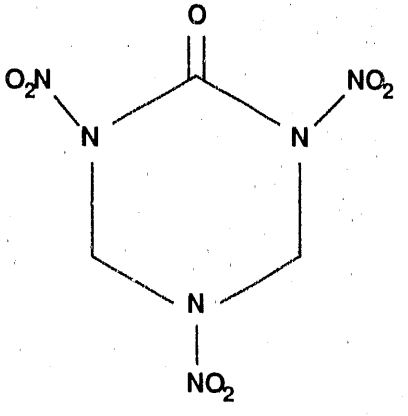


Figure 2. *A newly synthesized high explosive, 2-oxo-1,3,5-trinitro-1,3,5-triaza-cyclohexane, that has 2 to 3% more energy than HMX.*

Work on Composites

We are working to extend our understanding of composite high explosives (materials consisting of a mixture of fuel and oxidizer). Such materials have properties that make them useful in special applications. We have added aluminum to PETN (pentaerythritol) to determine whether energy is transferred from the exothermic formation of aluminum oxide rapidly enough to improve the performance of the composite over that of PETN alone. Results indicate that the energy released from mixtures of aluminum and PETN can be tailored to specific applications. We plan experiments with mixtures of RDX and aluminum, and TNT and aluminum, in the near future.

Separable Insensitive Binary Explosives

We are investigating the practicability, for both nuclear and nonnuclear weapons applications, of a high explosive composed of two separable components, neither of which can be detonated without the other. Such binary explosives are potentially safe, environmentally sound, and—because component ratios can be readily altered—easily tailorable to specific applications.

The concept is to isolate the components—fuel and an oxidizer—in separate containers, mixing them immediately before detonation. This type of explosive has been known for over one hundred years; mixtures of nitric acid and nitrobenzene have been used in limited applications by the mining industry. However, difficulties in handling nitric acid, a highly toxic and corrosive substance, precluded its extensive use.

We have conducted our first feasibility test, detonating a mixture of nitric acid and dinitrobenzene in a cylinder experiment. The results showed that the performance of the explosive is close to that of LX-17, a widely used solid high explosive. This preliminary result encouraged us to continue development of binary high explosives.

Issues remaining to be resolved include optimizing performance, establishing efficient mixing of the components, and engineering a system that is suitable to large bombs as well as small ballistic systems.

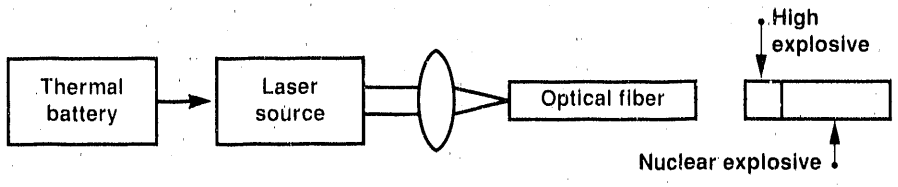


Figure 3. *A high-power, short-pulse chemical flashlamp laser can detonate a high explosive either directly or by driving an optically propelled slapper. A lens focuses the light from a battery-powered laser into an optical fiber that transmits it to the explosive. We hope to package the system in less than 500 cm³.*

Laser Initiation of High Explosives

We are investigating the feasibility of using a chemical flashlamp laser to detonate high explosives (Figure 3). By isolating a high explosive from spurious electrical impulses, this type of detonator promises significantly more safety than conventional designs. A short pulse (<30 ns) from a high-power (1 GW/cm^2) laser can be used either to initiate a high explosive directly or to drive an optically propelled slapper. Of the possible approaches, the chemical flashlamp laser has the highest potential for compact packaging.

The first phase of the project will demonstrate a brass-board package that meets performance, size, volume, reliability, and environmental requirements. We expect to package the compact design in no more than 500 cm^3. In the second phase, we will study the reliability of laser initiation in several common high explosives. We are also starting research and development on improved options. Our current objective is to build a prototype design that is reliable, compact, and rugged.

Contact: R. Alire (415) 422-2419.

W89 Engineering Development Program

The W89 warhead for the short-range attack missile embodies major performance improvements.

We are developing the W89 warhead for the Air Force's new short-range attack missile (SRAM II); the SRAM II missile will be carried by the B-1B bomber. The W89 will replace the W69 warhead now deployed in strategic bombers on the older SRAM A missile.

The SRAM II will embody major performance improvements over the SRAM A. Equally important, its W89 warhead will incorporate the latest safety features designed to prevent accidental nuclear explosion or dispersal of plutonium in the event of an accident. Of special note is its use of insensitive high explosive (IHE). IHE is virtually immune to accidental detonation and is being incorporated in other modern strategic air-carried warheads such as the B61-7 and B83 bombs and the W80-1 warhead for the air-launched cruise missile. In addition, the W89 is designed to prevent dispersal of plutonium in an aircraft fuel fire.

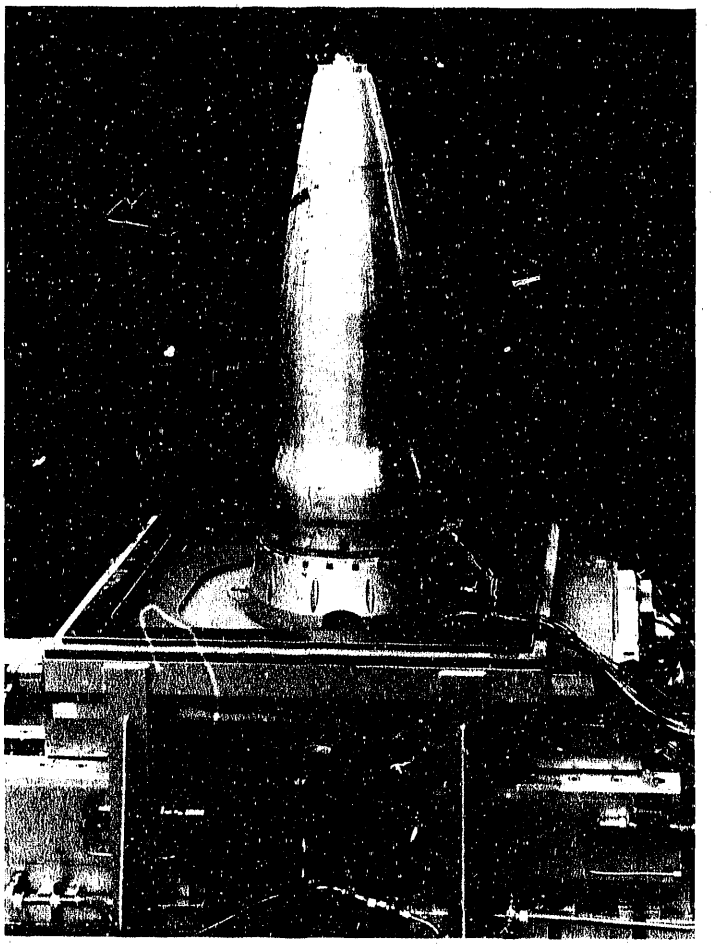


Figure 1. *Mock W89 warhead, instrumented with accelerometers, mounted on a shaker table to determine the warhead's resonant vibration frequency. A simple computer model of the warhead's vibrational behavior was constructed from these data and delivered to Boeing for use in their calculations. The results confirmed that the warhead's vibrational properties are acceptable.*

LLNL was assigned the task of developing the W89 in November 1986. Development engineering (Phase 3) began in January 1989. The first production unit (Phase 5) is scheduled for July 1993, and first asset delivery to the Air Force is planned for April 1994. While we are developing the warhead's nuclear explosive package, Sandia National Laboratory, Livermore, is working on nonnuclear components (such as the detonator firing set) and structural components (such as mounts for attaching the warhead to the SRAM II). Boeing Aerospace and Electronics in Seattle, Washington, is the prime missile contractor.

During the past year, the W89 program has passed several programmatic milestones. The first was a successful preliminary review by the Department of Defense (DOD) Design Review and Acceptance Group (DRAAG), which determines whether the warhead design meets the DOD's requirements. In addition, the joint DOD/DOE Nuclear Weapon System Safety Group gave its initial approval to the safety of the overall weapon system (bomber, missile, warhead), and the DOE laboratories and Boeing signed the warhead/

missile interface control drawings (ICDs). Finally, the program has been approved for transition to Phase 4, in which the warhead design is firm enough to begin preproduction activities in the DOE plants.

One important warhead/missile interface issue resolved during the past year was the resonant vibration frequency of the warhead. Since the vibration properties of the warhead/missile system affect the missile's flight-control system, they are an important concern for Boeing. We measured these frequencies by constructing a realistic mock warhead and mounting it on a shaker table (Figure 1). Accelerometers mounted in the warhead measured the resonant response. From the data generated, we constructed a simple computer model of the warhead's vibrational behavior and delivered it to Boeing for use in their calculations. The results confirmed that the warhead's vibrational properties are acceptable. We have also conducted other ground tests of the warhead's survivability in thermal, vibrational, and shock environments.

A stockpiled warhead contains many diverse components that can interact chemically with one another over its lifetime. We must demonstrate that during this time the warhead will not suffer adverse chemical reactions such as corrosion. To do this we constructed ten "core sample" units. These are small, sealed cylinders containing portions of the various warhead components that can react chemically. To simulate in several months the effects of several years in storage, we accelerate the chemical reactions by raising the ambient temperature. We are now opening and evaluating units that have been in storage since October 1989. As part of its continuing program to reduce hazardous waste in nuclear-weapon production plants, the DOE is requiring the replacement of some chemicals traditionally used in warhead production. Because we must continue to assess the chemical compatibility of new materials as they are introduced, we may need to repeat some of these sample core tests in the future.

We have constructed an instrumented mock W89 warhead that will be carried in the B-1B's bomb bay during captive-carry flight tests. The mockup will also be ejected from a bomb bay into a padded catcher box while the aircraft is parked on the ground. These tests are intended to evaluate operational environments while the missile is in the bomb bay and during ejection. The ejection tests began recently, and preliminary data match our expectations. Other mock warheads containing telemetry equipment will be tested in missile flights. In these tests, LLNL supplies components to Sandia, which installs the telemetry and completes assembly of the test warhead. With LLNL support, Sandia has begun ground tests to certify the performance of the special flight-test warheads. Flight tests are scheduled for the fall of 1991.

During the development program, we maintain close coordination with the DOE production plants to identify and eliminate potential production problems and to reduce production costs. During the past year, we have been able to dispense with two components and two production processes. One of the components would have been very difficult to fabricate and assemble. In addition to reducing risk, these improvements have significantly reduced cost. Nonnuclear high-explosive tests at LLNL's remote Site 300 were instrumental in enabling us to eliminate the components. These tests are also used to evaluate the effect of changes in Sandia components on warhead performance.

We are continuing the development engineering of the W89 warhead, paying special attention to operational environments, to production risks and costs, to coordinating our design with Boeing and Sandia, and to preparing for the approaching missile flight tests.

Contact: J. V. Tyler (415) 423-1307.

Cost-Effectiveness of Modernized U.S. Strategic Forces

We are applying a cost-effectiveness methodology to illuminate issues and options for U.S. strategic forces in an era of shrinking budgets.

The Strategic Modernization Program, initiated during the Reagan Administration, has produced substantial improvements in U.S. strategic forces. Among these are the development and deployment of the Trident-I submarine, the B-1B bomber, and the silo-based Peacekeeper missile, together with upgrades of strategic command, control, and communications systems. Future plans include deployment of the Trident-II submarine, the B-2 bomber, and less vulnerable ICBM forces. However, pressures building since the mid-1980s to reduce defense spending have put some of these programs at risk. As a result, difficult choices must be made.

If U.S. strategic forces are to undergo rational restructuring, modernization options must be sorted out: which programs should be pursued on schedule, which ones delayed or stretched out, and which ones canceled? Detailed plans will require careful scrutiny of the entire Department of Defense budget, with a weighing of how much particular systems contribute to our deterrence strategy, assessment of technical risks and opportunities, and analysis of costs and schedules. Within the spectrum of policy issues, we have focused our analysis on the issue of cost-effectiveness. We have developed a methodology for examining the cost-effectiveness of modernized strategic forces and have applied it to open-literature data on system costs and performance.

The measure of merit in our studies is the number of "effective weapons" per dollar invested. For a weapon to be effective, it must survive a Soviet first strike, launch reliably, and penetrate Soviet defenses to reach its target. This measure—the number of effective weapons per dollar spent—is a better gauge of utility than the number of weapons deployed or their payloads as it reflects two desired features for strategic retaliatory forces: survivability and deliverability.

We have used three cost measures: 20-year life-cycle cost, 20-year marginal cost, and 10-year forward cost. Each conveys important information to a decision maker, and together they provide a balanced perspective on system costs. The 20-year life-cycle cost comprises research, development, testing, and evaluation (RDT&E) costs, procurement costs (including military construction), and operational costs over a 20-year lifetime. This measure provides a useful characterization of an entire program and puts it in perspective with other programs at different stages in their history. The 20-year marginal cost describes the cost-effectiveness of each additional system procured beyond the planned program. It is more useful in considering systems for which RDT&E is essentially complete and the issue is whether current production plans should be extended or curtailed. Finally, the 10-year forward cost neglects sunk program costs and includes only RDT&E, procurement, and operating costs over the next 10 years.

We have used our methodology, together with cost and effectiveness data, to examine in some detail the investment issues for strategic forces squeezed by tight budgets and negotiated reductions (as in the ongoing Strategic Arms Reduction Talks, or START). We include proposed START constraints for two reasons. First, they will limit the number of weapons deployed and will impose a significant constraint on the total number of intercontinental and submarine-launched ballistic missiles (ICBMs and SLBMs) that can be deployed. Second, the survivability of some elements of the U.S. strategic forces depends on what other forces the U.S. and the Soviet Union have deployed. The Small ICBM, for example, cannot be studied in isolation because its survivability depends on the size of the threat and the number of other U.S. forces that can be attacked.

Figure 1 illustrates the kind of results produced by our methodology. The calculations were based on the 20-year program cost. Results are shown for two different alert conditions: one with generated forces (in a high-alert condition) and one with ungenerated forces (on day-to-day alert). Several features of the results are noteworthy. First,

strategic submarines are relatively cost-effective for both alert postures because a considerable fraction of the force is at sea at all times. Second, the cost-effectiveness of ICBMs depends on assumptions about how these systems are used in response to a nuclear attack. We have assumed here, for the sake of illustration, that silo-based ICBMs on day-to-day alert ride out an attack while those in the high-alert condition execute a prompt response. For bomber forces, cost-effectiveness depends critically on their alert posture, as comparatively few bombers are on day-to-day alert.

Our studies have identified some key issues facing decision makers. The two most important of these are (1) the value of a high alert rate at the time of an attack and (2) the need for force diversity in the face of uncertainties in a future threat spectrum. In future studies, we will consider additional force options and will update cost estimates of our earlier studies. Although our cost-effectiveness methodology cannot resolve for Congress and the Executive Branch the difficult choices presented by shrinking budgets, it can help to illuminate the issues and options.

Contact: P. L. Chrzanowski (415) 422-6522.

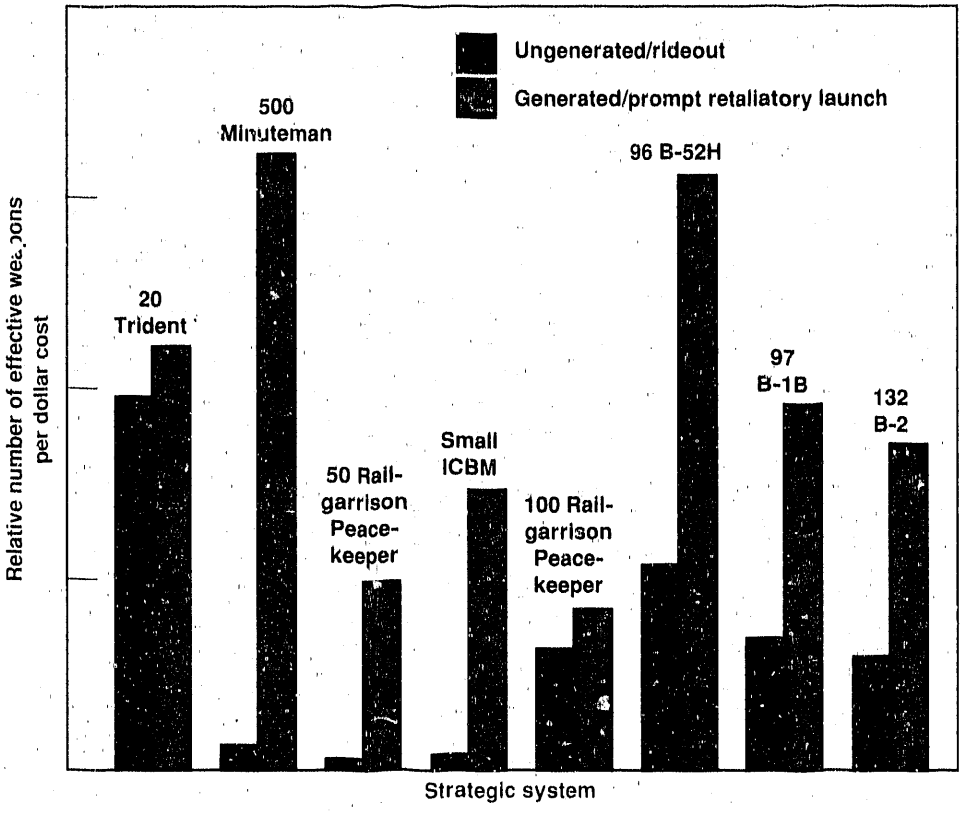


Figure 1. *Life-cycle cost-effectiveness of selected strategic options. Results are shown for eight strategic systems: 20 Trident submarines with D-5 missiles, 500 Minuteman ICBMs in silos, 50 Peacekeeper ICBMs with rail-garrison basing, 500 Small ICBMs on hard mobile launchers, 100 Peacekeeper missiles with rail-garrison basing, 96 B-52H bombers with air-launched cruise missiles, 97 B-1B bombers (with 16 weapons each), and 132 B-2 penetrating bombers (with 16 weapons each). Cost-effectiveness is shown for two alert conditions: (1) generated forces (high alert) and prompt retaliatory launch of IBCMs, and (2) ungenerated forces (day-to-day alert) and rideout of the attack with silo-based ICBMs and undispersed Peacekeeper missiles.*

Numerical Simulation of Electromagnetic Effects in Realistic Geometries

We are developing techniques to add geometric realism to simulations of electromagnetic waves and plasmas.

Computer simulation is an indispensable tool in plasma physics, the field of physics that seeks to understand the complicated properties of highly ionized gases. Simulation techniques also find many applications in electrical engineering, where it may be necessary to study the behavior of electromagnetic waves in waveguides, in dielectric (nonconducting) media, and as waves are scattered from conducting obstacles. One challenge common to both domains is to find an efficient and accurate method of handling geometric boundaries in problems dealing with electromagnetic fields, especially when the boundaries are irregular or complex.

There are several approaches to designing field-solvers for complicated geometries. The most natural is to transform to a set of boundary-fitted coordinates in which one or more coordinate lines are coincident with the boundary of the problem. The field equations in the new curvilinear coordinate system are again solved by finite-difference methods. Unfortunately, this approach is well-defined only when the grid is at least piecewise logically rectangular and can prove cumbersome for complicated domains.

We are developing methods of simulation in geometrically complex domains that are based on finite elements and finite volumes. Such methods offer greater generality and flexibility than boundary-fitted coordinates. Our aim is to produce a truly geometry-independent method. Here we present some results from our work with finite elements.

Electromagnetic Problems

Traditional approaches to solving Maxwell's equations (which describe the behavior of electromagnetic fields) in the time domain employ finite-difference methods on regular grids to replace the use of differential operators. Although these methods are both accurate and robust, they prove awkward for complicated boundary shapes, often replacing smoothly curved or slanted boundaries with stair steps.

The enormous geometric flexibility of finite-element techniques makes them very effective for solving mechanical engineering problems. The domain of application is first divided into simple subdomains—usually triangles or quadrilaterals with sample points or nodes coincident with the vertices. The subdomains may be constructed in any convenient way so that, in general, the nodes form an unstructured grid (that is, the connectivity of the nodes cannot be mapped onto a logical grid structure). In such a grid, the nodes may be placed anywhere one chooses. This latitude in placement can be an enormous advantage in optimizing calculations: local regions can be refined either *ab initio* or dynamically without affecting the resolution in other parts of the calculation, and, of course, there is no problem in fitting the boundaries.

Finite-element methods have enjoyed recent success in computational fluid dynamics, in part because of their use with a new class of weighted residual techniques called Taylor-Galerkin methods. Because of the formal similarity between the Euler equations of fluid flow used in fluid dynamics and Maxwell's equations of electromagnetics (both essentially hyperbolic systems of partial differential equations), it seems natural to apply these new methods to simulating electromagnetic phenomena.

A model calculation illustrates the ease with which finite-element methods can incorporate a complicated boundary shape into an electromagnetic simulation. Figure 1a shows a two-dimensional unstructured grid surrounding a boundary that resembles an armored tank. The grid was generated automatically from boundary data alone. Note that the unstructured grid enables us to use very small zones to resolve the electromagnetic waves under the turret and gun while using much larger zones elsewhere. In this example, the electric field lies in the plane of the simulation and the magnetic field is out of the plane. We used the Taylor-Galerkin method to derive finite-element equations. Figure 1b shows the results of a calculation in which a two-cycle plane wave incident from the left boundary strikes the tank to produce the reflected wave seen in the color contours.

We have also obtained more quantitative results that include

calculations of electromagnetic modes in cavities and the transmission of plane waves through an array of fine wires. Comparisons with analytic results and with output of standard finite-difference codes have been quite favorable.

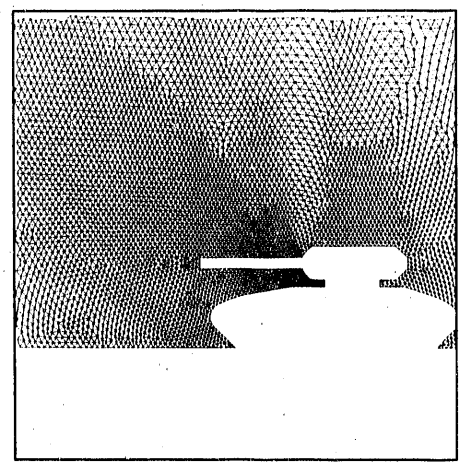
Plasma Problems

Plasma dynamics, an intrinsically nonlinear process and therefore difficult to treat mathematically, is best understood through a combination of analytical methods and numerical simulation. Many plasma simulations at LLNL and elsewhere are based on particle-in-cell (PIC) techniques. In PIC simulations, representative plasma particles sample forces from a fixed grid of field points and then move across the grid, where they deposit their charge and currents to update the fields. This Lagrangian-Eulerian hybrid technique has proved to be a very effective aid to understanding kinetic processes in plasmas.

Plasma simulations with realistic boundaries are needed in such applications as the design of electron guns and ion-beam diodes. In these devices, small errors in the curvature of the emitting surface can drastically change the focusing characteristics of the beam. In plasma simulations, we must incorporate particles into the calculations.

An immediate challenge in using particles on anything other than a rectangular grid is to locate a particle on the grid so that it can contribute its charge or current density. We have developed a simple search procedure that uses the properties of interpolating functions on triangular or quadrilateral elements to trace the particle across the grid. After a particle is pushed, we use interpolation to check whether it is still in the element where it was last located. If not, the interpolating functions associated with the nodes of the element indicate where to continue the search. Particles are usually localized in three attempts or less. We have vectorized the search procedure to produce impressive vector-to-scalar speedups.

(a)



(b)

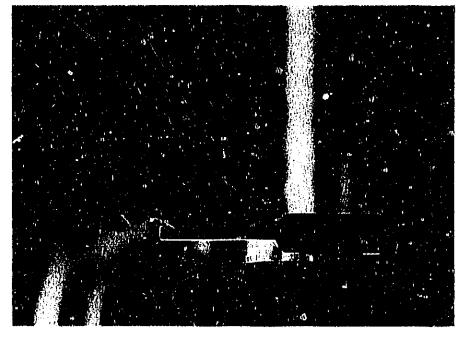


Figure 1. *(a) Unstructured grid around an armored tank. (b) Calculated magnetic field produced when the tank scatters a two-cycle plane wave incident from the left. The electric field lies in the plane of the simulation, and the magnetic field is out of the plane.*

Figure 2 shows particles traced across an unstructured grid surrounding an electric gun. This example is just one step away from a simulation of a self-consistent plasma. We first propagated an electromagnetic wave down the waveguides at the upper and lower left to produce an accelerating electric field on the grid between the cathode and anodes. We then used this imposed field to accelerate test electrons. In a self-consistent calculation, the particles and fields would be advanced together.

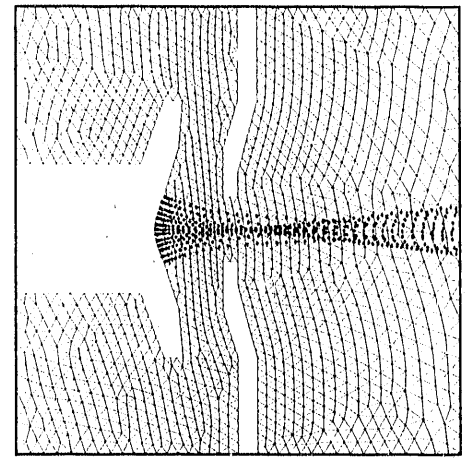


Figure 2. *This calculation traces test particles across a grid in the electric field of an electron gun.*

Summary

We have obtained promising results in developing an electromagnetic simulation code for arbitrary geometries based on finite elements. During the coming year, we will perform self-consistent simulations of particles in two dimensions and will extend our electromagnetic field propagator to three dimensions. These techniques should be of great value in designing electron guns and ion diodes, simulating the lethality of high-power microwaves, calculating radar cross sections, and other applications.

Contact: J. Ambrosiano (415) 423-6634.

Three-Dimensional Calculations of Material Strength

We have shown that the rapid deformation of a tantalum shape is best described by a rate-dependent model.

Our work on chemical-energy warheads emphasizes sophisticated two- and three-dimensional computer codes, together with material-response models, to predict a warhead's performance. Calculations are validated by comparing them with a carefully planned and well-diagnosed experiment. To examine the sensitivity of the dynamics of a tantalum plate to the assumptions of the model used, we have done a series of calculations based on three different constitutive-response models. Such a model embodies the properties of a material's strength and its variation as the material deforms.

Accurate calculation of the material response of tantalum to explosive loading has been of interest for several years. The standard mathematical model describing such behavior, known as the Steinberg-Guinan model (our "full-strength model"), was developed at LLNL. This constitutive model is valid for high deformation rates but does not accurately predict the final shape of the tantalum. Typically, the material appears too stiff, and the calculated final shape does not undergo as large a degree of folding as is observed in experiments. A practical measure, adopted by some workers to provide better agreement with experiment, is to reduce the yield strength of tantalum by a factor of two. This model (our "half-strength model") provides better agreement between calculation and experiment in some instances but lacks any material-property or theoretical basis.

More recent efforts have produced a comprehensive constitutive model of tantalum, known as the Steinberg-Guinan-Lund model (our "rate-dependent model"), which includes a dependence on strain rate and has proved useful for strain rates from 10^6 to as low as 10^{-4} s^{-1}. The Steinberg-Guinan-Lund model was generated by amending the standard Steinberg-Guinan model to include a thermally activated portion of the yield stress that is a function of strain rate and temperature. As the strain rate in the tantalum varies from high values during the explosive loading to moderate values during the folding process, the effective yield strength varies from a high of 1.60 GPa to a low of 0.20 GPa.

The foregoing three models provide an interesting set for calculational purposes, allowing one to compare their relative effects on the predicted formation dynamics and final shape of an explosively formed tantalum plate. Our tantalum plate was used as the liner in a generic explosively formed penetrator (EFP) warhead. Although the size and geometry of the baseline design are relevant to actual warhead designs, we selected this one for reasons of convenience, availability, and known performance.

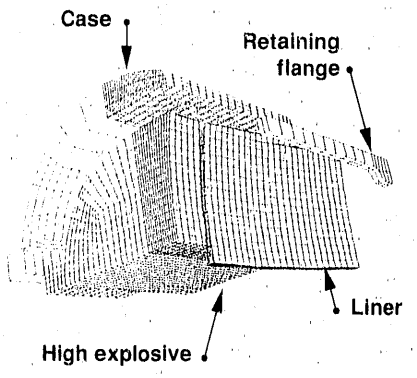


Figure 1. *Exploded view of warhead configuration.*

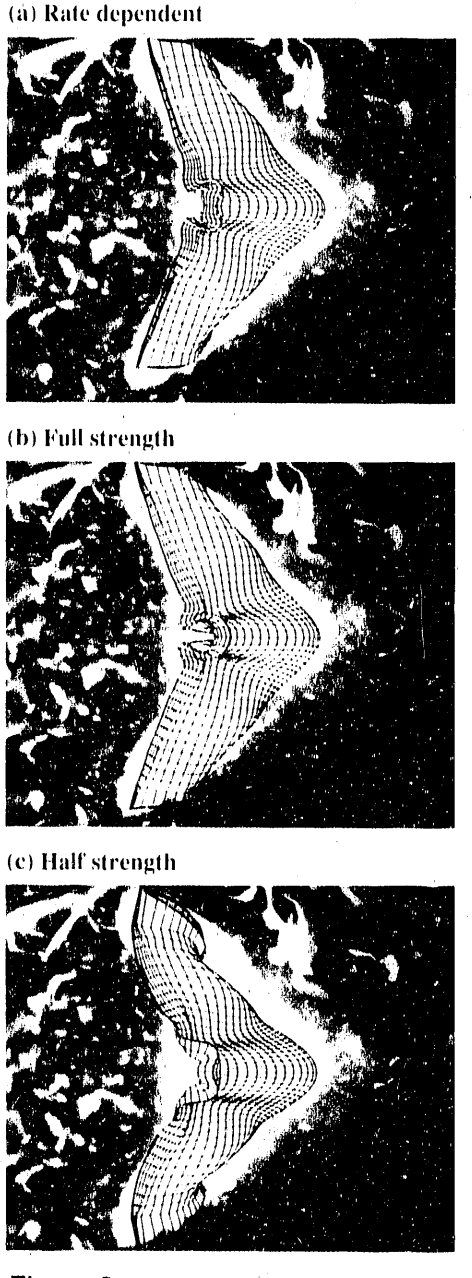


Figure 2. *Results of the three model calculations superimposed on pulsed radiographs of the deforming EFP at 100 μs: (a) rate-dependent model, (b) full-strength model, and (c) half-strength model.*

Figure 1 shows our basic configuration as represented by the computer mesh. In this exploded view, only one-quarter of the warhead is shown, as the symmetry of the configuration makes it unnecessary to calculate the entire EFP. The cylindrical charge is 105 mm in diameter and about 139 mm long. Nestled in the warhead body and oriented laterally outward from the axis of the cylindrical body is a concave, rectangular tantalum liner with a uniform thickness of about 2 mm. The EFP is intended to operate in a fly-over, shoot-down mode; the explosive charge forms the tantalum liner into a rearward-folding, long-rod penetrator.

To evaluate the models, we needed experimental data on the shape of the liner at various times during the deformation process. We performed two warhead tests using pulsed radiography of liner deformation and optical observation of the exploding charge to obtain the data. Our primary diagnostic was three radiographs. Three 450-kV x-ray tubes were programmed to shadowgraph the liner at 100, 150, and 380 μs. The 100- and 150-μs times encompassed the deformation and folding of the liner, and the 380-μs view showed the fully formed, final shape.

Our calculations were done with a modified version of the DYNA3D code that incorporated the three tantalum models. Figure 2 shows radiographs obtained at 100 μs overlaid with the results of calculations based on the three models. Although at this point there are no dramatic differences, the degree of forward folding of the wings is clearly greater in the half-strength calculation than in either of the others. It is evident that the half-strength result is the poorest of the three.

At 150 μs (Figure 3), the half-strength result is deviating further from the experiment while the two others remain similar. At this point, the rate-dependent calculation appears in best agreement with experiment.

Finally, after the liner has completely collapsed at 380 μs (Figure 4), the calculated shapes of the deforming EFP are vastly different. Now, only the rate-dependent model agrees well with the observed shape.

Our comparisons of model with experiment demonstrate that the accuracy of the calculated deformation of the tantalum sample is indeed sensitive to the constitutive model used to describe it. Moreover, the rate-dependent model provides the best agreement with experiment during the deformation process. Because the EFP is initially deformed at high strain rates and assumes its final shape at moderate strain rates, our calculations provide a significant test of a constitutive model, especially for a rate-dependent material such as tantalum.

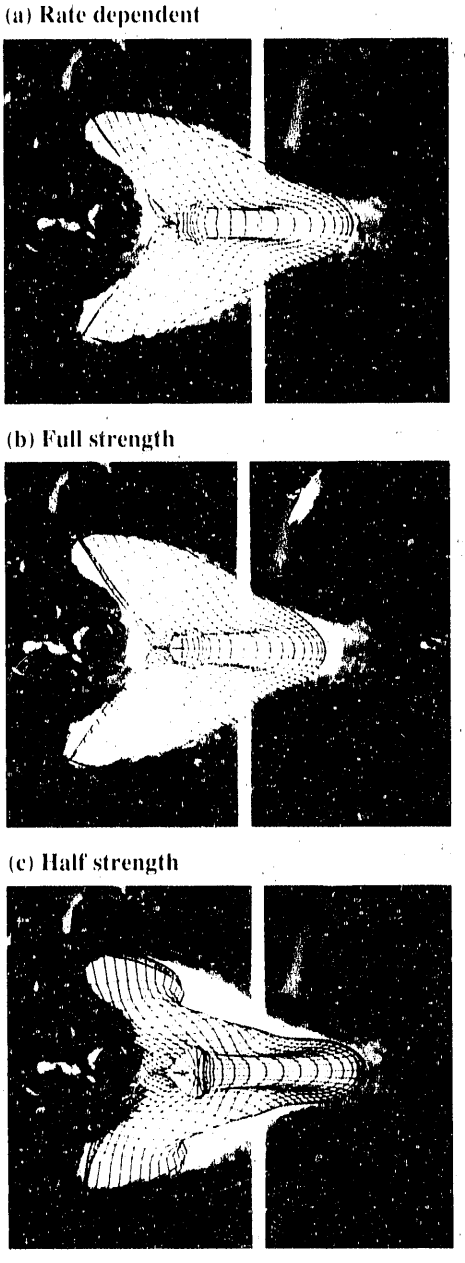


Figure 3. *Same calculations as in Figure 2 at 150 μs: (a) rate-dependent model, (b) full-strength model, and (c) half-strength model.*

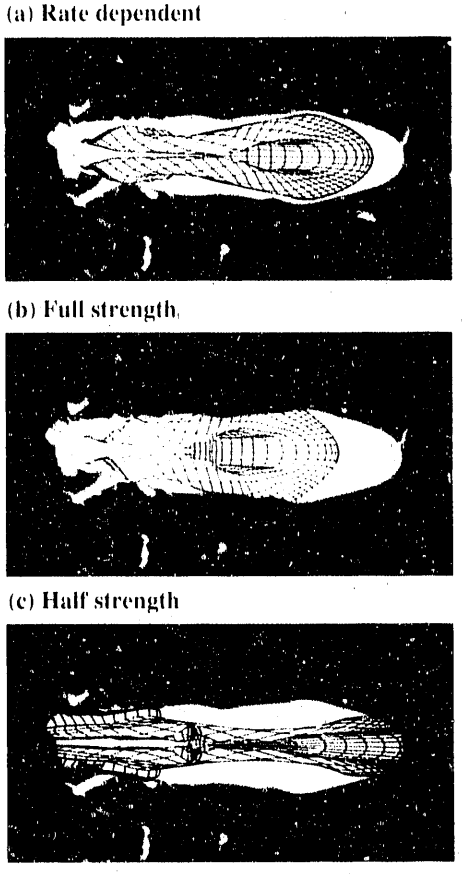


Figure 4. *Same calculations as in Figures 2 and 3 at 380 μs: (a) rate-dependent model, (b) full-strength model, and (c) half-strength model.*

Contact: D. W. Baum (415) 423-2236.

Opacity Experiments with the Nova Laser

Measurements with the Nova laser are providing data on plasma opacity.

The opacity of a high-temperature plasma to x rays depends strongly on its ionization state, or the degree to which its constituent atoms are stripped of their electrons. Knowledge of how the x-ray opacity of a material changes with its ionization is of fundamental interest in astrophysics, in studies of laser-produced and magnetically confined plasmas, and in the design of nuclear weapons.

We are using the Nova laser as an energy source to create highly ionized plasmas on which we make detailed, spectrally dependent measurements of opacity. These experiments are a collaborative effort between the U.K.'s Atomic Weapons Establishment and LLNL's Nuclear Test, Nuclear Design, and Laser Programs.

The technique used to make plasma opacity measurements is called point-projection spectroscopy. The key elements are a point x-ray backlighter source and an imaging crystal spectrometer (Figure 1). The sample, contained in a multisegment sandwich, is heated and ionized to a plasma state by a 1-ns laser pulse from eight of Nova's ten beams. Nova's other two beams generate the 100-ps backlighter x rays. The multisegment sample enables the simultaneous measurement of the spectral features of the backlighter source, the x rays transmitted by the sample, and scattered backgrounds (see Figure 1). A Bragg crystal diffracts the x rays from the sample to produce a spectral image. Analysis of the spectrum provides data on the energy-dependent x-ray transmission of the sample and thus on its opacity.

Measuring Plasma Density and Temperature

The opacity of a plasma varies as a function of its density and temperature. To meaningfully compare opacity calculations with the experimental data, then, we must first know the density and temperature of the plasma sample. We have recently measured the time

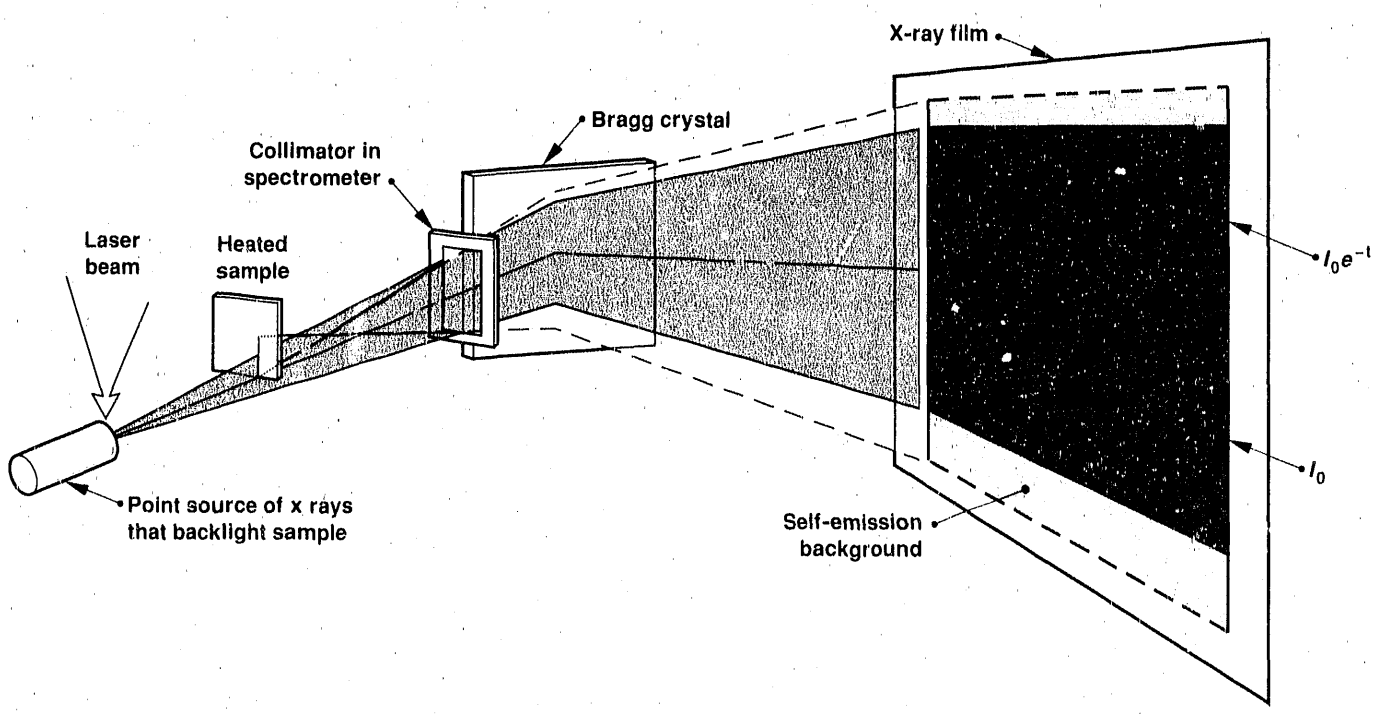


Figure 1. *In point-projection spectroscopy, some of Nova's laser light illuminates the sample material to generate a plasma and some is used to illuminate a point source of backlighting x rays. After passing through the plasma, the x rays are diffracted to produce an absorption spectrum that can be analyzed to determine the plasma's opacity. (I_0 is the unattenuated backlighter spectrum and t is the transmission coefficient determined by the opacity.)*

dependence of the density in a Nova laser experiment using the Wolter 22× microscope whose output was recorded by a streak camera (Figure 2). The expansion of the plasma enables us to turn on the backlighter at different times in successive experiments to learn how opacity depends on density.

We determine the time-dependent temperature of the sample by measuring its x-ray emission between 0.1 and 3.0 keV. Nova's Dante x-ray spectrometer, equipped with x-ray diodes (K- and L-edge-filtered), measures the total energy emitted by the plasma sample as a function of time. If the sample is in thermal equilibrium, the total energy is uniquely related to temperature. The shape of the output spectrum, also measured by the Dante spectrometer, indicates the degree of equilibrium. By comparing the measured temperatures and densities with hydrodynamic calculations, we can understand the state of the plasma sufficiently to enable us to analyze the opacity data.

Experimental Results

Our initial experiments have concentrated on aluminum. We chose aluminum because its atomic kinetics are relatively simple and are accurately described by computer models. Experiments with aluminum were thus used to confirm the validity of our techniques (see Figure 3). We are modifying the experiment to eliminate the problems of debris and crystal imperfections. These improvements will also increase the spectral resolution of the instrument by a factor of three. Within the present resolution of the experiment, the data agree well with theoretical calculations for aluminum, thereby validating our experimental technique.

Contact: T. S. Perry (415) 423-2065 or P. T. Springer (415) 423-9221.

Figure 2. *Streak-camera image of an exploding foil. Time increases in the rightward direction. The sample was initially too small to be resolved by the 22× microscope, but after a few nanoseconds it has expanded to the point where its thickness can be determined to a few percent. Somewhat later, the expanding sample collides with the frame that encloses it, reversing the expansion. This process can be seen at the far right of the streaked image, where the boundary marking the upper edge of the sample begins to slope downward.*

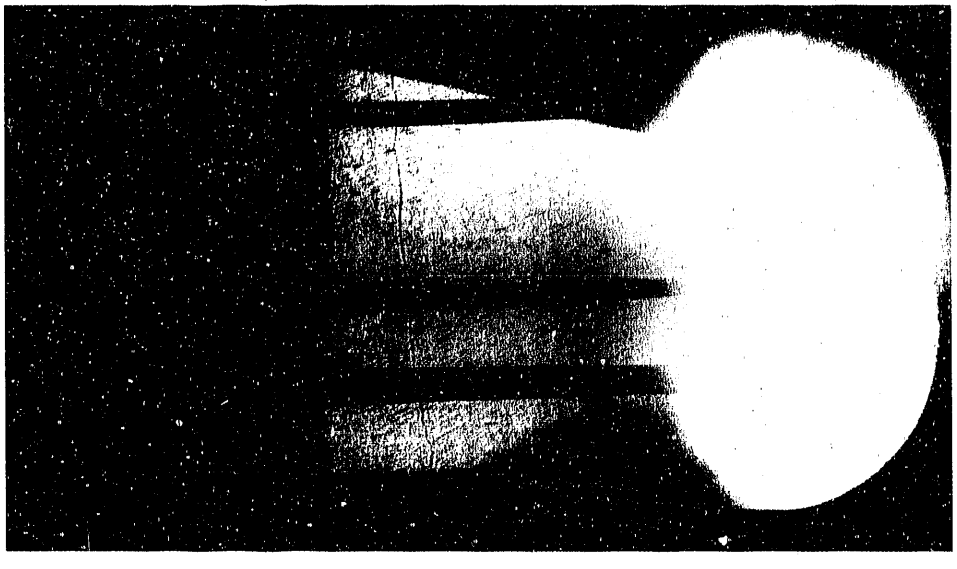


Figure 3. *Actual film record of an aluminum opacity experiment illustrates the kind of data our technique returns. The cluster of vertical dark lines starting at the top of the image and extending about halfway down are absorption lines produced by highly ionized aluminum. The thicker black horizontal lines, used to provide a reference for subtracting film fog, are from a support structure in front of the film. The gray horizontal stripe was produced by a filter containing aluminum, silicon, and yttrium. These materials have x-ray absorption edges that provide fiducials for calibrating the wavelength scale. The bright spot at the far right was caused by debris from the sample that broke through the light filter in front of the film. The fainter, irregular diagonal and vertical lines arise from defects in the Bragg diffraction crystal.*

New Streak Cameras

In the Contact Event we successfully tested several new streak-camera designs that greatly increase our data-gathering capabilities.

The contribution of underground nuclear testing to national security is commensurate with the quantity and quality of data we can extract from an experiment. Shrinking test schedules have stimulated demands for a greater volume and precision of data, making it imperative to develop better instruments and to devise innovative techniques that meet the needs of experimenters. State-of-the-art techniques used to record data in the laboratory are now often being applied to underground tests. In particular, downhole streak cameras, a basic and essential diagnostic in nuclear experiments, are now returning orders of magnitude more data than previously.

In the recent Contact Event (June 1989), for example, we used streak cameras to gather more than 90% of the data. The 16 streak cameras fielded in that event were able to record about 4000 data channels. Records were as short as a few tens of a nanosecond and were synchronously timed to within less than one nanosecond. As might be expected with a system of this size and complexity, our instruments pioneered a number of advanced designs and novel techniques. The result was the most successful application of downhole streak cameras to date.

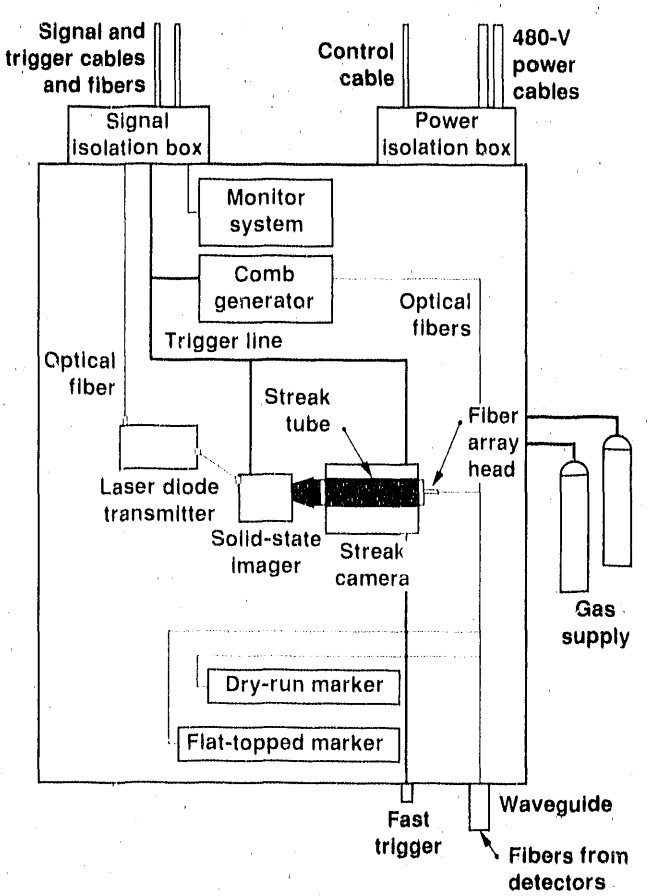


Figure 1. *In the Contact Event, light from the detectors was channeled up bundles of optical fibers that transmitted it to an array of streak cameras, one of which is illustrated here. Sixteen streak cameras embodying a variety of designs were fielded in the Contact Event.*

The Streak Camera

In the typical streak camera (Figure 1), light from an optical source is swept very rapidly across a phosphor surface to produce a streak-like image whose intensity varies in space as the intensity of the source varies in time. The light may come from a spectrometer, an imaging diagnostic, or any of a variety of other instruments. The resulting image on the camera's output phosphor is next amplified by a microchannel-plate image intensifier and then captured as a single frame by a solid-state imaging camera. The image frame is then digitized and transmitted uphole on a high-speed data-communications link to a trailer on the surface, where the bit stream is stored in a recording device for subsequent recovery and analysis. Figure 2 shows a simulated streak-camera image.

Contact Event

In the Contact Event, we used a total of 16 cameras with three different models of streak tube that embodied several technology variations. One camera, the latest LLNL/EG&G design, was significantly smaller than earlier models, a reduction achieved by separating the power supply from the tube. (The smaller each camera, the more cameras we can field in a given volume.) Circuitry improvements also make this design less susceptible to electromagnetic interference, thus providing a better image.

We also fielded a commercial streak camera manufactured by Kentech, Inc. In addition to being less vulnerable to electromagnetic interference, the Kentech design has an image intensifier located within the streak tube itself, thereby eliminating the need for an external microchannel-plate image intensifier. It is also much more compact than current streak cameras. Two of these were used successfully on the Contact Event.

A key to the high data density achieved on the Contact Event was spatial multiplexing; each camera is fed two bundles of input fibers instead of one, one above the other on the photocathode. Careful control of the photoelectron beam within the tube produces two complete streak records on the output phosphor, each with half the time duration of a single-input image, to provide higher spatial resolution of the image. We used 13 of these multiplexed cameras in addition to the three nonmultiplexed cameras described above to give a total of 29 views of the data, each with a sweep duration of 30 ns.

In addition to transmitting physics data, the optical-fiber arrays for every view also contained fibers that carried downhole calibration and test signals. We used a dry-run system to test the streak cameras downhole. The intensity and temporal position of the light pulses on the streak camera's readout verified proper operation of the entire system.

Downhole Module

The cameras and their support systems were mounted in a heavy-walled steel module measuring about 1.7 × 1.7 × 2.4 m located at the top of the diagnostic cannister about 21 m from the nuclear device. The module was insulated against electromagnetic interference. The fiber arrays carrying optical signals from the various experiments to the streak cameras entered the module through cutoff waveguides at its bottom (Figure 1).

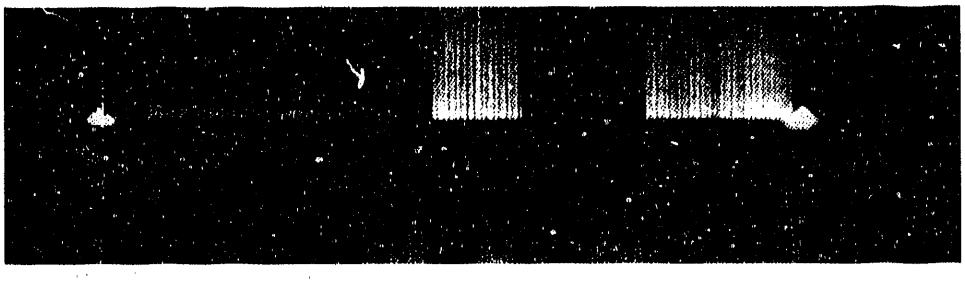


Figure 2. *Simulated image of a spatially multiplexed (duplexed) streak-camera system. The image is viewed through a microchannel-plate intensifier and the downhole imaging camera.*

Calibrating the Cameras

To simulate the responses of the streak cameras to actual data, we taped masks photoetched with precise patterns to the optical-fiber entry windows of the cameras and illuminated them with a light source. The masks enabled us to test for temporal and spatial resolution, gain at various microchannel-plate settings, dynamic range, aberration, and the relations among all these parameters.

Final sensitivity calibrations were carried out in the field with either a combination of a flashlamp and integrating sphere or a pulsed-laser/phosphor system. In the flashlamp/sphere system, the source consists of two coupled, diffusely reflective integrating spheres that provide a spatially uniform, pulsed light source well suited to "flat-field" calibrations. The light was guided to the streak camera by a fiber array. Because the amplitude of the light pulse is essentially constant for the brief duration of the streak, the consistency of a streak's intensity with respect to time reflects the system response. A typical downhole calibration test of a camera consists of four to six flat-field streaks recorded at different intensities.

The pulsed-laser/phosphor system provides a similar flat-field source but can be pulsed on after the camera sweep starts. This eliminates "blooming" in the output of the spatially multiplexed cameras, an undesirable effect that can occur with the flashlamp/sphere system, in which the flashlamp is turned on well before the sweep begins.

We used the downhole calibration data, together with the laboratory test data, to correct for any system idiosyncrasies that might distort the data from the nuclear test. To ensure timely evaluation of the downhole data, we entered them into a spreadsheet program that plotted them and analyzed the results in the field. This quick-look analysis was essential to quality control of the calibration process, providing a good set of performance data for each streak-camera system.

Summary

The streak-camera diagnostics used on the Contact Event were the largest and most complex ever fielded. They were also the most successful in the quantity and quality of vital physics data they acquired. We are continuing to develop new and innovative equipment and techniques needed to calibrate and support these essential systems in the harsh field environments to which they are subjected.

Contact: J. J. Ronchetto (415) 422-3795.

Applying Nuclear Testing Technology to ES&H Issues

We are applying nuclear-chemistry technologies developed for nuclear-weapon testing to important environmental, safety, and health (ES&H) issues.

Throughout the history of nuclear testing, the science of nuclear chemistry has provided experimental data critical to understanding the performance and reliability of nuclear weapons. The need for new experimental data on the behavior of individual parts of a nuclear-explosive device during the explosion has stimulated the steady development of a strong technology base for measuring radionuclides and stable isotopes. Today, radiochemical diagnostics for a single nuclear test may require us to measure more than a hundred nuclear species.

During the 1980s, we actively applied measurement technologies originally developed for nuclear-test diagnostics to nuclear safeguards, environmental monitoring, and risk assessments from the migration of radionuclides at the Nevada Test Site (NTS) and elsewhere as well as to the study of issues concerning nuclear-waste management. The DOE's new emphasis on environmental, safety, and health (ES&H) issues presents fresh opportunities to expand the application of nuclear-chemistry technology. We describe here some current examples.

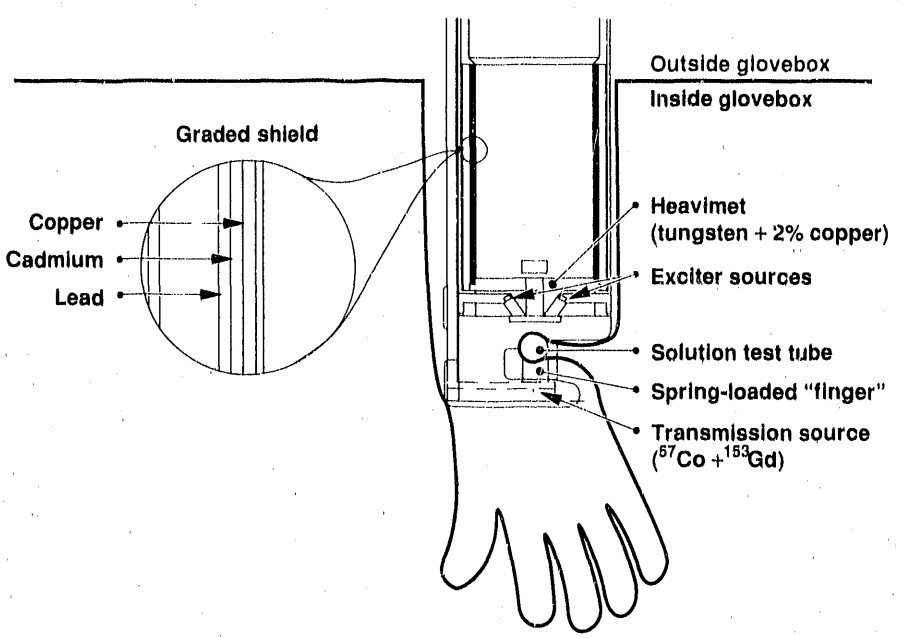


Figure 1. *The portable XRFA instrument inserted into a glovebox. The solution to be analyzed is placed in a test tube or cell located in a glove and is held in place by mechanical "fingers." The gamma-ray source excites x-ray fluorescence from uranium and plutonium in the solution.*

Portable X-Ray Fluorescence System

We have applied our expertise in gamma-ray and x-ray spectroscopy to develop an advanced, nondestructive means of analyzing special nuclear material (an accountability category that includes plutonium and enriched uranium). The result is a prototype portable x-ray fluorescence analysis (XRFA) instrument that enables safeguards inspectors to perform on-site analysis of plutonium and uranium solutions.[1] This innovation avoids the costly and time-consuming alternative of shipping samples from inspection sites back to central laboratories for analysis.

Because sampling is done in a glovebox, we designed the portable XRFA to be insertable into one of the gloves (Figure 1). With the instrument in place, solution samples in test tubes can be analyzed without removing them from the glovebox. The test tubes are pressed against the glove sleeve, and a spring-loaded mechanical "finger" holds them in the proper position. They are exposed to cobalt-57 gamma-ray sources that induce K x-ray fluorescence from uranium and plutonium. The x-ray spectrum is measured with a high-purity germanium detector, and the data are analyzed with a computer code to determine uranium and plutonium concentrations. A combined cobalt-57 and gadolinium-153 source is used for transmission measurements to correct the observed x-ray intensity for sample self-attenuation effects.

Consequently, only one solution is required to calibrate the XRFA instrument for an analytical precision of 0.3% over a broad range of concentrations (0.1–300 g/liter).

Tracing Lead Contamination

Mass spectrometry is routinely used in nuclear-test diagnostics to measure isotopic abundances of uranium and plutonium as well as other actinide elements, such as neptunium and americium, remaining in the test debris. We have adapted this technology to make high-precision measurements of lead isotopes in environmental samples. Our objective is to use characteristic signatures of isotopic composition to identify and trace pollution sources.

Lead has four naturally occurring, stable isotopes with nearly independent sources. Three of the lead isotopes—206, 207, and 208—are produced by radioactive decay of the isotopes uranium-238, uranium-235, and thorium-232, respectively. The fourth lead isotope, 204, is not a decay product but is present only in native lead. The isotopic signature of a lead-ore deposit therefore is determined by the relative contributions of these four sources.

In a preliminary study of lead contamination in surface waters of the Great Lakes, we have found that spatial gradients are clearly evident in both lead concentrations and isotopic compositions.[2] The predominant pathway for lead contamination in the Great Lakes is atmospheric deposition, primarily from automobile exhausts. We find that Canadian and U.S. sources of industrial lead are isotopically distinct. Both sources contribute significantly to lead pollution in the Great Lakes, and the distribution of lead from each source conforms to the expected atmospheric distribution of aerosols from industrial and population centers. Future studies using this isotope-signature technique may include other aerosol-borne toxic metals and acid rain.

New Measurement Technologies

During 1989, the Secretary of Energy called for an aggressive research and development plan for environmental restoration and waste management at DOE sites. We responded by undertaking a new initiative called the Nevada Environmental Applied Research (NEAR) project. In this effort, we are focusing on environmental problems at the NTS and are using the site as a testbed for environmental assessment techniques and cleanup strategies.

As part of the NEAR project, we are investigating the use of trace-element patterns measured by inductively coupled plasma mass spectrometry (ICP-MS) to identify and map specific aquifers in NTS groundwaters. In this technique, first used in 1985 for nuclear-testing applications, a fine mist of an aqueous sample solution is sprayed into a plasma torch. A mass spectrometer analyzes the distribution of atomic masses in the sample. Trace concentrations of over 60 chemical elements can now be rapidly and simultaneously measured.[3] ICP-MS has already found applications in laser isotope separation, environmental protection, hazardous waste management, and several other LLNL programs.

Photoacoustic spectroscopy—another new technology—is one of the most sensitive for detecting actinide species and identifying their oxidation states in solution. This capability is important in monitoring sites that may be contaminated by radioactive wastes. The actinide species present in a sample solution are measured by illuminating the sample with a pulsed, tunable light source and then detecting the acoustic waves generated when a species absorbs optical energy at a characteristic wavelength. We have demonstrated that an optical fiber can be used to transmit the excitation light.[4] This technique can detect submicromolar concentrations of most actinide species, a sensitivity greater by a factor of 1000 than is possible with conventional absorption spectroscopy. We hope to demonstrate the optical-fiber approach in remote measurements of actinide species in NTS monitoring wells and then apply this technique in the DOE's environmental restoration and waste-management plan.

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Contact: D. A. Leich (415) 422-6609.

Arms Control and Treaty Verification Activities at LLNL

We are providing technical support to a broad and varied spectrum of ongoing arms-control negotiations.

During the past year, LLNL's activities in arms control and treaty verification have broadened and intensified. Current negotiations supported by LLNL advisers include the Nuclear Testing Talks (NTT), the Strategic Arms Reduction Talks (START), Conventional Forces in Europe (CFE), the Chemical Weapons Convention (CWC), the Conference on Disarmament (CD), and defense and space talks. With the Administration seeking ratification of the Threshold Test Ban and Peaceful Nuclear Explosions treaties this fall and seeking to complete the NTT and START treaties in early summer, and perhaps the CFE treaty this year, our responsibilities are expected to continue to expand for the foreseeable future. Major new policy initiatives, as well as the unprecedented complexity of recent arms control agreements, require both analytical studies and the development of new technologies.

Analytical studies are needed to determine the monitoring provisions to be negotiated, the mix of monitoring measures to be developed at a given time, and the decision process to be used to evaluate compliance. New technologies are needed to deal with such issues as in-country seismic monitoring, weapons inventory control, detection of nuclear payloads, and chemical sampling. We also make forecasts of future technology requirements, support the Washington community and negotiators with information on what technologies can and cannot be expected to accomplish, and prepare to respond rapidly when specific system requirements are identified. Our work focuses on merging analysis and state-of-the-art technology developments in the context of verification schemes.

LLNL also provides technical staff support of arms-control activities to several agencies of government: the DOE's Office of Arms Control, the Secretary of Defense's START Policy Office, and, in non-proliferation issues, the State Department. We also contribute to many related workshops and symposia.

Nuclear Testing Talks

We supported the NTT, both in Geneva and in Washington, D.C. In this role, we helped define options and examined their impacts using statistics and decision-analysis tools. Laboratory researchers lead the scientific community in applying these tools to treaty verification issues; the results have contributed to the selection of specific treaty options.

Our work on the Local Seismic Network (used in verifying some provisions of the Peaceful Nuclear Explosions Treaty) has been brought to maturity and successfully adapted to a self-contained, portable system for seismic monitoring of the Threshold Test Ban Treaty or other verification applications.

Chemical Weapons Convention

The Laboratory's verification responsibilities have recently been expanded to include the CWC. For the past ten years, the U.S. has been involved in complex, multilateral negotiations sponsored by the United Nations and in bilateral negotiations with the Soviet Union to draft a comprehensive arms-control treaty covering chemical weapons. The treaty would prohibit the production (including key chemical precursors), stockpiling, transfer, and use of such weapons. The current draft agreement, which will be implemented by an international agency, includes reporting requirements, on-site monitoring by instruments, and on-site inspections.

We have been working closely with the DOE's Office of Arms Control to help define an effective plan for developing the necessary monitoring technology for such a treaty. We have also participated in planning and evaluating the National CW Trial Inspections. This effort included mock inspections of commercial chemical companies to identify those producing or capable of producing treaty-limited precursor chemicals.

Our ongoing CW work includes the evaluation and development of sensitive chemical analysis

techniques for possible use in remote monitoring and on-site inspections. Sensitivity, specificity, and portability are key concerns here, as the techniques must be both effective and easy to apply.

Strategic Arms Reduction Talks

We continue to develop and evaluate START verification regimes and the technologies for verifying them. In this work, the Laboratory's intelligence efforts and decision-analysis capabilities play a central role. Together, these disciplines provide useful tools for identifying the most effective verification procedures in the context of the evasion opportunities that are available to the Soviet Union.

One START-related technology involves tags and seals. These are unique, nonreproducible identifiers that can be permanently attached to a treaty-limited item. The objective is to identify the item for purposes of inventory control and to ensure that it was legally produced. LLNL has established a "red team" to evaluate possible flaws or means of cheating or spoofing tags developed at other DOE laboratories. We are also pursuing the development of various tagging concepts.

Another major technology area is radiation detection. We are researching concepts for use in several possible applications including nonvisual identification of the number of warheads mounted in the payload section of a ballistic missile, discrimination of cruise missiles carrying nuclear and conventional warheads, detection of solid-fuel rocket propellant at permanently monitored production facilities, and control of warheads should START require the destruction of special nuclear material.

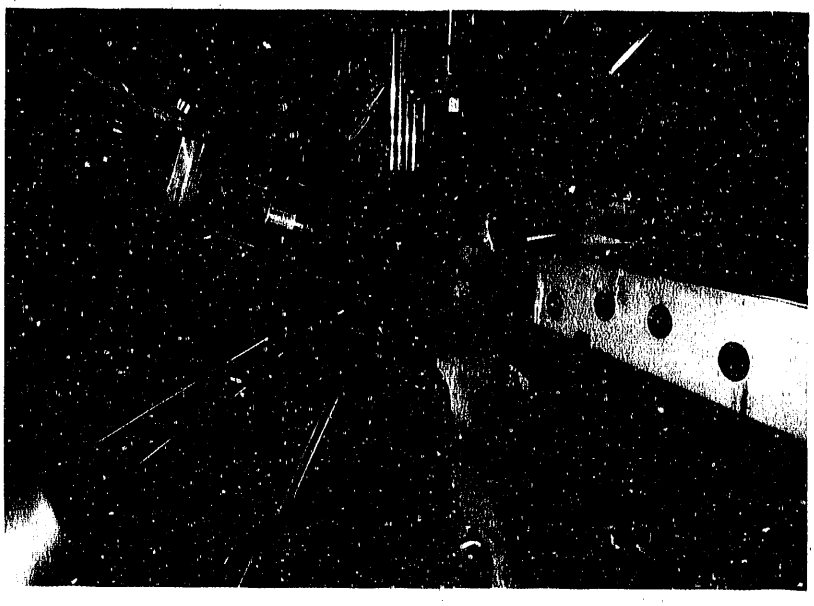
Conventional Forces in Europe

The outcome of the fast-moving CFE talks may demand much less in the way of sophisticated verification technologies than either a START or a CWC agreement. However, because of the mobility of the conventional forces and treaty-limited items involved, the large number of bases and storage sites, and the vast extent of the geographical area that must be monitored, the DOE Office of Arms Control is conducting a framework analysis of the issues. This fast-track effort will evaluate which issues, if any, will require technology advances either to improve the effectiveness of verification or to reduce the costs of inspection.

The U.S. may also begin negotiations on a Short-Range Nuclear Forces (SNF) agreement, perhaps in conjunction with the CFE talks. To prepare for this prospect, we have initiated a comprehensive program that comprises several elements. We will analyze force structures, likely areas of instability, and potential routes of circumvention. In addition, we will develop and evaluate verification technologies as appropriate, including application scenarios and requirements. The Intermediate-Range Nuclear Forces (INF) Treaty and START constrain the destructive power of arsenals indirectly by controlling surrogates (the missile and its launcher) rather than by eliminating warheads themselves. In contrast, in a CFE or SNF treaty, where most delivery systems have both a nuclear and conventional mission, it may be necessary to control and possibly to eliminate nuclear warheads per se. Such a policy will have many ramifications for the DOE requiring Laboratory support.

Contact: D. W. Dorn (415) 294-4704.

Laser Research



Inside the experiment chamber of the Nova laser, a technician sets up the tiny target.

Laser research at LLNL is divided into five major programmatic areas: inertial confinement fusion (ICF), uranium atomic vapor laser isotope separation (U-AVLIS), special (plutonium) isotope separation (SIS), laser technology, and advanced applications. We have made important progress this past year in each of these areas.

The continuing objective of the ICF program is to understand and develop the science and technology of ICF so that its full spectrum of capabilities and benefits can be realized. Our near-term goal is to apply ICF technology and facilities to provide a better understanding of the physics of nuclear weapons. A longer-term goal is to explore the feasibility of ICF as a clean and inexhaustible source for commercial electric power production. Our Nova laser is the latest in a series of ever more powerful laser facilities at LLNL. This year, we continued to use Nova to study inertial confinement fusion, laser-plasma interaction physics, weapon physics, and laser science. We also made advances in the theory and design of targets, in target fabrication and materials science, in laser and optics research, and in diagnostics. Substantial progress was made in the development of concepts and technologies for the next higher power laser facility for ICF.

Improved Nova performance also has contributed to continued progress in the development of laboratory x-ray lasers. In 1989, the LLNL laboratory x-ray laser team produced amplified spontaneous emission (i.e., lasing) at 4.48 nm in nickel-like tantalum. This is a significant step toward the ultimate achievement of an x-ray laser source for holographic microscopy of living biological cells.

Also in 1989, the laser isotope separation program was reorganized to facilitate the near-term deployment of AVLIS technology to production plant operation. Dedicated SIS and U-AVLIS program offices were formed to direct the numerous technical, regulatory, and administrative functions required to transfer the AVLIS and associated materials-processing technologies to plant operating contractors. To support laser development and engineering for both programs, a separate laser technology organization was formed. Many years of effort have gone into the development of the AVLIS technology. In order to make full use of this extensive technology base, the National Academy of Science, at the direction of the Secretary of Energy, is reviewing the AVLIS programs for potential additional applications.

The U-AVLIS program's mission is to assist the Department of Energy in revitalizing the U.S. uranium enrichment enterprise and in restoring this country's competitive

position in the multibillion-dollar international enrichment market. The U-AVLIS program is tasked with demonstrating and transferring the AVLIS technology to the commercial sector. In January 1990, the DOE submitted to Congress a detailed plan for the demonstration, transition, and deployment of U-AVLIS. Following the successful completion of a final major demonstration of the integrated AVLIS process at Livermore, scheduled for late 1992, the Secretary will decide whether to authorize plant construction at a specific site. To provide the data for this crucial decision, the U-AVLIS program is designing and constructing next-generation hardware to demonstrate a significant level of uranium enrichment capability with plant-scale lasers and separators. These demonstration tests will bound the economic and performance uncertainties of building a production plant. A commercial deployment contractor, yet to be selected by the DOE, will participate in the AVLIS demonstration tests and will manage the design, construction, and initial operation of the first U-AVLIS plant increment.

The mission of the SIS program is to develop and demonstrate the principal technologies—AVLIS and plutonium processing—to be used to isotopically tailor fuel-grade plutonium to weapon-grade material. This year, the SIS program conducted a major series of tests using surrogate (i.e., nonplutonium) material to demonstrate the technical basis for SIS plant systems. During these tests, the separator system was installed, activated, and integrated with the process laser and auxiliary laser systems. Isotope-separation demonstrations using plutonium were placed on hold by the DOE when they decided not to request plant deployment funds for the 1991 fiscal year. SIS development, including laser system development and operation, separator development, plutonium processing and dose reduction, physics point design, and process flowsheet preparation, is to be completed and documented in 1991.

The laser technology section has a broad charter to support research, development, and deployment of the SIS and U-AVLIS processes and to pursue alternate applications of laser technologies. This includes the copper lasers, the process dye lasers, the laser-system computers, networks, and controls, and special projects. During the past year, significant progress was made in the development and demonstration of advanced and more-powerful copper lasers, more-powerful dye laser chains, and the associated computer and control systems. We are continuing to collect operating reliability data for a plant-prototypical copper laser system; more than 1.4 million device hours of copper laser operation have been accumulated. In addition, alternate applications of AVLIS technology are being investigated for next-generation microlithography and materials processing.

The advanced applications program is developing advanced laser, electro-optics, and signal processing and imaging technologies for national security applications. Many of these technologies are finding important civil applications as well. A major effort is the development of high-power semiconductor laser diodes for use primarily as optical pump sources for solid-state lasers. These small, high-efficiency, lightweight, intense light sources are making possible the development of novel solid-state lasers of interest to the Department of Defense (e.g., for communicating with submarines).

Research is also continuing to develop both high-power glass lasers pumped by conventional flashlamps and high-repetition-rate crystal lasers pumped using an innovative arc lamp. Major demonstrations of both efforts were completed this year. These lasers have application in materials processing and as point sources for x-ray lithography.

In addition, sophisticated signal-processing techniques were developed and applied this year to the reconstruction of optical images perturbed by the atmosphere and of radar images of the ocean surface. These techniques have application to space surveillance and antisubmarine warfare. A project was also initiated this year to demonstrate that two-stage gas guns can provide a means for the low-cost launch of objects into low earth orbit.

Over the past 18 years, the scope of laser research at LLNL has grown immensely. The small-scale, low-power laser systems of our early days have given way to high-power, high-reliability, record-breaking laser facilities of plant-prototype scale. Initially, our investigations focused primarily on the feasibility of ICF; today, our efforts have expanded to include a broad range of national security and commercial applications. Numerous LLNL-developed laser technologies have attracted a broad customer base within the Departments of Energy and Defense, and others have been transferred to private industry. We expect that within the next three to five years, our research efforts will culminate in the commitment to construction of a uranium-enrichment production plant, a major upgrade of the Nova laser facility to make it capable of producing ignition of deuterium-tritium fuels, and such potential technology transfer to x-ray lithography, submarine communications, and optical imaging applications.

Contact: J. I. Davis (415) 423-9818 or A. Levy (415) 423-8729.

The Nova Laser

We have increased the Nova laser's capabilities for generating substantially higher output energy and power and for delivering temporally shaped pulses of laser light to targets.

We continue to increase the productivity and flexibility of the Nova laser as an experimental facility for studying inertial confinement fusion (ICF), laser-plasma interaction physics, weapon physics, and laser science. During 1989, we fired 584 high-power shots to provide the drive source for 675 experiments. The energies provided by the laser (at a wavelength of 1.05 μm) ranged from <1.0 kJ to >120 kJ. Pulse durations varied from 10 ps to several nanoseconds. Temporal pulse shapes included square, Gaussian, and specially shaped pulses designed to improve target performance. Figure 1 shows the input/output characteristics of Nova and illustrates the range of energies provided during the year on shots using all ten beams.

In parallel with our target experiments, we improved Nova for future experiments. Last year, we reported on the installation of new platinum-particle-free laser glass in the output amplifiers.[1] This year, we used this high-damage-threshold glass to demonstrate record output energy and power at both 1.05 μm and the third-harmonic wavelength of 0.35 μm, which couples more efficiently to implosion targets. We also began a two-year program to increase our control of the output power, pulse shape, and focusing of Nova's ten beams.

To reduce the risk of optical damage to components when the laser is operated at high output energy, we improved the spatial uniformity of the beam by making several changes in optical staging. The beam size at the input to each of the Nova amplifier chains was previously defined by a circular aperture. Gibbs diffraction phenomena, resulting from spatial filtering of the flat-topped beam beyond the aperture, produced an undesirable intensity modulation on the beam. By replacing our original apertures with specially serrated apertures, we substantially reduced this modulation. In addition, we changed the magnification of a mid-chain spatial filter and reoriented one 31.5-cm amplifier to reduce abberations and improve spatial uniformity of the gain.

The Nova laser system was designed to provide 80 to 120 kJ of output energy at 1.05 μm and to convert this output to 40 to 70 kJ at 0.35 μm. After installation of the new glass, improvements in staging, and extensive testing of one beamline, we gained confidence that we could safely meet or exceed the laser's design goals at both wavelengths. In April 1989, we performed a series of shots to demonstrate the capabilities of the laser system at 1.05 μm and three pulse durations of interest:

- 2.5 ns, where damage to output optics is of concern.
- 1.0 ns, where output power and energy are close to that of greatest interest for ICF experiments.
- 0.1 ns, where output power is limited by beam breakup from self-focusing.

We measured the energy of each beam in a full-aperture calorimeter and measured the pulse temporal shape with a streak camera (which obtained its signal from the beamline output sensor). In a 2.5-ns square temporal pulse, we obtained up to 125 kJ of output energy; in a 1.0-ns square pulse, we obtained up to 82 kJ; and in a 0.1-ns Gaussian temporal pulse, we obtained up to 126 TW of output power, all with 2% or less rms spread in energy among Nova's ten beams. These tests clearly demonstrated that Nova can safely exceed its original 1.05-μm performance goals.

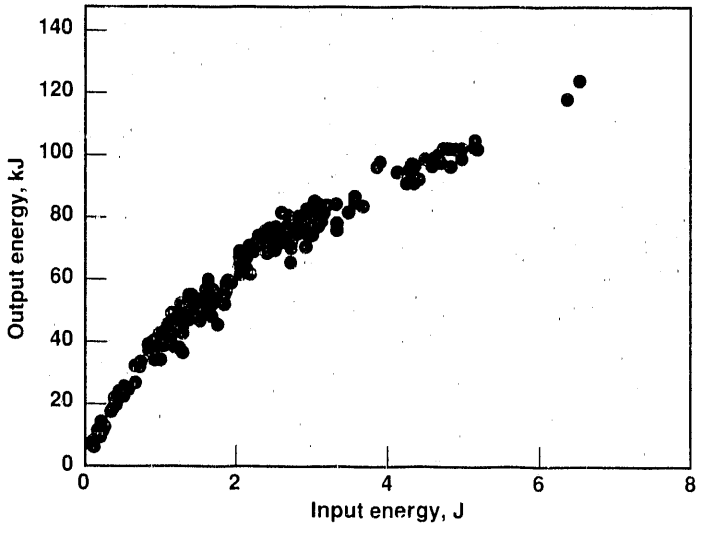


Figure 1. *Output energy from the Nova amplifier system at 1.05 μm vs energy input to disk amplifiers for ten-beam shots between April 1, 1989, and February 1, 1990.*

Later in the year, we performed a series of shots to demonstrate that Nova can deliver more than 40 kJ of 0.35-μm light to a target. In this test series, the Nova laser provided 100 kJ of 1.05-μm output in a 2.0-ns square temporal pulse to the frequency-conversion arrays on the ten-beam target chamber. We frequency-chirped the laser pulse to prevent stimulated Brillouin scattering in the fused-silica focusing lenses. (We had found previously that Brillouin scattering by high-energy third-harmonic pulses produces bulk damage in fused-silica optics.[2]) The frequency-conversion arrays performed as expected and converted 50% of the 1.05-μm output to 0.35 μm. Approximately 85% of this output was transmitted by the optics into the target chamber. Five shots in the series produced more than 40 kJ of 0.35-μm energy in the target chamber. On the highest-energy shot, calorimeters in the target chamber recorded 45.3 kJ. Careful inspection of the most threatened optics in the laser and target chamber after both series revealed no damage.

Imploding ICF targets to high density with Nova requires shaped laser pulses that are temporally tailored to reduce entropy addition to the fuel by shock waves, instantaneous power imbalance among the ten beams at the target (<5%), and placement of the beams on the target to within 30 μm. We made considerable progress toward these goals by starting target-irradiation experiments with shaped laser pulses, assessing the energy balance, and initiating improvements in our diagnostics that measure third-harmonic power at the target.

Figure 2 shows an example of a shaped third-harmonic pulse we recently used for an implosion experiment. The solid line represents the average, instantaneous, third-harmonic power as a function of time provided by a single beam. These data were calculated from streak-camera records of 1.05-μm output pulses from the ten beams and the measured efficiency of the frequency-conversion array on each beam. The dashed lines are displaced by one standard deviation, calculated from the scatter in the data from the ten beams. The scatter is dominated by noise in the streak-camera data; thus, the actual power balance may be better than that shown. The rms spread in power of 20% in the low-power foot of this pulse is far short of our goal of 5%. At present, we are able to balance output energy more precisely than output power. The rms spread in third-harmonic energy measured by calorimeters on the ten beams on single shots is routinely less than 3% for these pulse shapes. The variations in power arise because of differences in third-harmonic conversion efficiency among the beams, which requires us to have different 1.05-μm drive energies and, hence, different saturated pulse shapes when we balance the third-harmonic energies. These pulse-shape differences will be easily correctable in the future by changing the beam areas when we have better pulse-shape diagnostics to assess the effect of the changes. We have provided pulses of the generic shape shown with third-harmonic energies ranging from 25 to 40 kJ at the target. Providing third-harmonic pulses that are precisely tailored to target requirements is possible because of a flexible pulse-shaping system at the master oscillator[3] and computer codes that accurately calculate the pulse shape necessary at the master oscillator to obtain the desired output pulse.

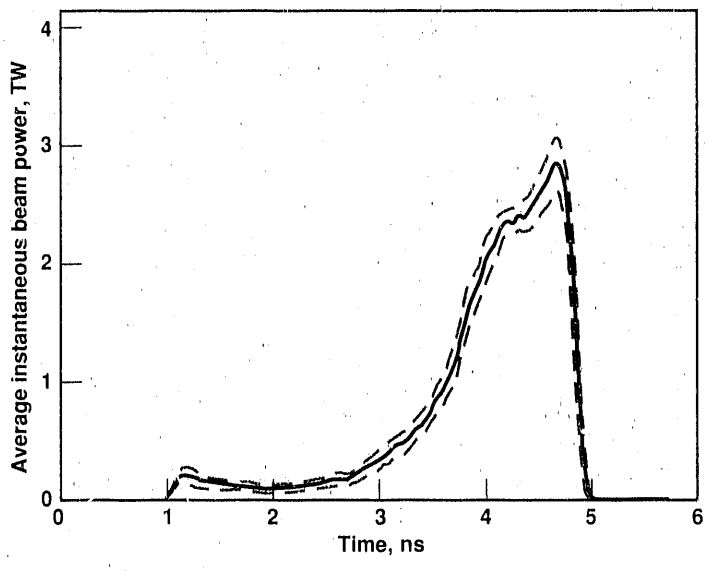


Figure 2. *Instantaneous power vs time of a 0.35-μm shaped pulse used for ICF implosion experiments. The solid line represents average single-beam power; the dashed lines are displaced one standard deviation as calculated from differences among the ten beams.*

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Contact: D. R. Speck (415) 422-0681.

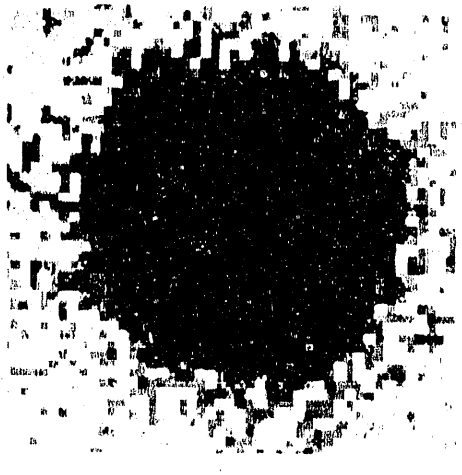
Pulse-Shaped Implosions on Nova

We have imploded ICF targets using a drive pulse tailored to match a theoretical pulse that produces reduced shock heating of fusion fuel, a requirement for reaching high gain.

In inertial confinement fusion (ICF), a small pellet containing deuterium and tritium (DT fuel) is imploded to high densities (~10 to 100 times the density of solid lead). The central temperature of such fuel is raised to several thousand electron volts (or about 50 million degrees Celsius). Under these conditions, thermonuclear fusion reactions begin and rapidly consume most of the fuel. It is important that the fuel be first compressed and then heated. Hot fuel is difficult to compress, and heating prior to compression would require a very large driver (in terms of energy) to attain fusion conditions. We refer to an ideal compression as adiabatic (no heat added to the fuel) or isentropic (no change in entropy of the fuel). To achieve this type of compression, we must prevent shock waves from being generated and propagating into the fuel before it reaches the final high density. This, in turn, requires that a target be "pushed" inward in a prescribed manner: gently at first and, as the target implodes, with ever-increasing force. The inward push in ICF targets is generated by ablating in rocket-like fashion the outer part of the pellet. Ablation is caused by either directly shining the Nova laser beams on the target or by converting the beams to x rays that strike the target. In either case, we control ablation pressure by carefully controlling laser power as a function of time. We shape the laser pulse on Nova with an electro-optic modulator, known as a Pockels cell. (Our work on pulse shaping is described in the previous article; Figure 2 of that article shows one of the pulse shapes we used for our experiments.)

To measure the performance of ICF targets, we add a small amount of argon gas to deuterium fuel that contains no tritium (DD fuel). Argon emits copious x rays when it is compressed and heated. Detailed measurements of these x rays tell us the fuel density, size, and temperature at peak compression.[1] In addition, measurements of emitted DT neutrons give us the fuel density-size product (DD fusion reactions produce tritium and a secondary DT neutron). These many measurements provide strong constraints on, and a severe test of, hydrodynamic modeling codes. The multiple independent measurements are self-consistent and provide good evidence that we are interpreting our data correctly.

(a) Square pulse



(b) Shaped pulse

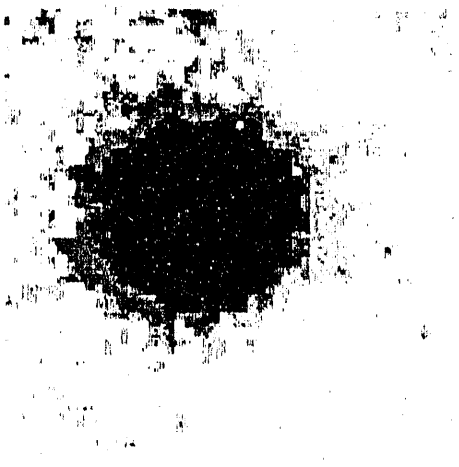


Figure 1. *Time-resolved x-ray images from the fuel region of imploded ICF targets driven by (a) a square pulse and (b) a shaped pulse.*

Our first experiments have been successful, and our measurements are in good agreement with predictions. Figure 1 shows time-resolved x-ray images, taken at peak compression, of the argon emission from two similar targets that absorbed the same total drive energy. One target was driven by a square pulse whereas the other was driven by a shaped pulse. The shaped pulse drives the target to a noticeably smaller final core size and, therefore, to a higher density. Although this pulse shape is better than a square or unshaped pulse, it does not produce a perfectly adiabatic implosion. Such an implosion requires a shape with a lower power early in time, then increasing more gradually to attain final high peak power. Our next step is to use this more optimum pulse shape to investigate ICF targets.

Reference

1. See "The Nova Laser," in the July/August 1989 issue of *Energy and Technology Review* (UCRL-52000-89-7/8), pp. 26–31.

Contact: R. E. Turner (415) 422-8112.

Multiframe Gated X-Ray Image Camera: The Fastest Movie Camera in the World

Using a new gated microchannel-plate camera, we have obtained an unprecedentedly fast and clear sequence of images of a laser-target implosion.

X-ray imaging diagnostics are essential for understanding the performance of laser-imploded target capsules, laser-produced plasmas, and the lasers themselves. Such devices must function on very fast timescales (picoseconds, or billionths of a second). In addition, we would like to obtain a series of images, not just a single snapshot. In collaboration with the University of Rochester, New York, we have developed a multiframe gated x-ray camera that may well be the fastest movie camera in the world.

Gating of an MCP (microchannel-plate) detector works simply by applying a pulsed voltage to an MCP. X rays that are incident on the coated front of the MCP produce photoelectrons that are amplified when a voltage pulse is applied to the MCP. The amplified cloud of electrons at the output of the MCP is accelerated by a dc voltage into a phosphor, and the light is recorded on film.

Electrical gating of MCPs can produce shutter times of <100 ps. Previous MCP cameras have used several different microstrip lines coated on an MCP, each with independent electrical gating, to obtain several image areas on a single MCP. We have simplified this concept by using a continuous microstrip line, coated as a meander on an MCP, to obtain an unprecedented sequence of fourteen 80-ps shutter-time x-ray images of laser-target implosions.

In our device, the gating voltage pulse is produced by the avalanche breakdown on a p–n diode and then propagated along a microstrip formed in a 6-mm-wide meander. The strip is separated by 3.5 mm to avoid crosstalk and to minimize reflections at the corners. To image target implosions, we used a 150-ps, ~1-kV electrical gate pulse. Because of the extreme nonlinearity of gain with voltage of the MCP, the x-ray gate time was two to three times shorter than the electrical gate, producing x-ray gate times of <100 ps.

In this experiment, the camera was filtered to be sensitive to 2-keV photons. Fourteen x-ray images were projected by fourteen pinholes onto the meander microstrip, with an image spacing of 7.5 mm. The 50-ps voltage pulse propagated along the serpentine, sequentially triggering each image, with delays of 50 ps. We took a series of images of a target implosion driven directly by the University of Rochester's Omega laser. The target was a deuterium-filled glass shell (~250 μm diameter, 5-μm wall thickness); it was imploded by uniform irradiation with 1.2 kJ of 0.35-μm laser light in 650 ps from 24 laser beams.

The images obtained are shown in Figure 1. The initial images (upper left) show the shell of x-ray emission from the glass heated by the irradiating laser. By the fourth frame, the ball has clearly started to implode. By the ninth frame, an implosion core formed by the gaseous fuel has become visible. The implosion reaches its minimum size by the final frame (lower right).

The advantages of multiple frames are clearly evident. The time separation of the images (50 ps) provides as much information on the image as does a streak camera, but these images are two dimensional (unlike the one-dimensional streak-camera records). There is no uncertainty in the sequencing of the images; one simply follows the serpentine path. In addition, the large number of images makes it possible to record many details of the implosion.

Contact: J. Kilkenny, (415) 423-4213.

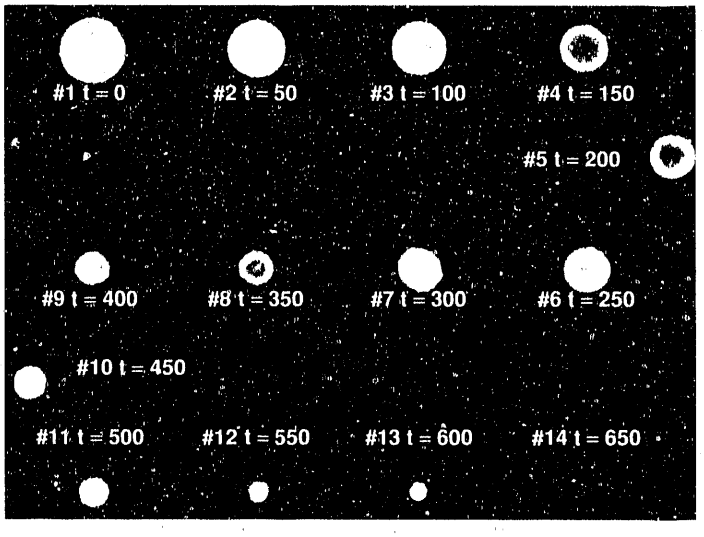


Figure 1. *Series of x-ray images (starting at upper left and ending at lower right) from a direct-drive x-ray implosion of a deuterium-filled glass-shell target using the University of Rochester's Omega laser. The sequence and time (in ps) of each image are shown.*

Damage-Resistant Optical Materials

We are developing new damage-resistant optical materials for high-peak-power lasers and have improved the damage performance three- to fivefold for some optical materials.

Optical materials that are resistant to laser-induced damage are essential for the successful operation of high-peak-power laser systems. Damage resistance of optics affects both laser performance and overall system cost. Cost is affected because the more light that can pass through a given optic, the smaller and, hence, less costly that optic can be to handle a given laser-energy output. For future fusion research, a laser system's overall cost is a major constraint, and optical materials are needed with damage thresholds two or three times higher than those of the current Nova materials (Table 1). We define damage threshold as the minimum laser fluence (in joules per square centimeter) that produces a permanent change in an optical material when viewed under 100× magnification.

A typical laser-output optical chain for transporting a high-power laser beam to a target requires damage-resistant coatings for highly reflective (HR) mirrors, polarizers, and antireflective (AR) surfaces; bulk materials, such as lenses and frequency-conversion crystals; and polished optical surfaces, such as lenses and debris shields. Two material types have proven particularly troublesome: multilayer dielectric coatings that either reflect or polarize the beams, and the bulk crystal used to convert the laser beam from 1.06 to 0.35 μm.

We have pursued two avenues of research to improve coating damage resistance. First, we have developed a method for processing current coatings that improves the damage threshold by as much as a factor of five. By illuminating the coatings with slowly increasing laser powers, we can "condition" defects in the coating, preventing them from damaging until higher powers are reached. Although the mechanism for this process remains elusive, we have begun to use the technique to improve HR coatings used on Nova.

Table 1. **Operating wavelengths of current Nova laser components and recent improvements in laser damage thresholds.**

Component	Mirror	Polarizer	Frequency converter	Focusing lens
Operating wavelength, μm	1.06	1.06	1.06, 0.53, 0.35	0.35
Damage threshold, J/cm² at 10 ns:				
1985 Nova technology	7–10	7–15	15 at 1.06 μm 3–6 at 0.35 μm	25–30
Present technology	40–50	40–60	60–65 at 1.06 μm 25–30 at 0.35 μm	25–30
Improvement factor	~5×	~3×	~4× at 1.06 μm ≳5× at 0.35 μm	No change

Second, we have developed completely new coating materials and processes. For example, we are extending our single-layer sol-gel AR-coating process to make multilayer HR coatings. To date, we have prepared mirrors with excellent damage resistance and sizes up to about 10 cm in diameter. Sol-gel processes are inexpensive compared to other commercially available coating methods ($500/m² vs $15,000/m²). We are also developing a new coating process that uses plasma-assisted deposition at high temperatures (>1000°C). Initial coatings prepared by this process have the highest damage thresholds of any coating we have tested. Moreover, we can use this process to prepare a completely new class of coatings that may make it possible to design new, less-costly laser-system architectures. Our major technical challenge will be to scale this process to larger sizes.

We also have continued to develop new frequency-conversion materials and methods to improve the damage resistance of those currently in use. In our search for new materials, we have found that salts of some amino acids (specifically, l-arginine) give high damage thresholds and improved conversion efficiency. We also continue to develop processes for growing our current frequency-conversion crystal material, potassium dihydrogen phosphate (KDP), to eliminate damage-causing defects. We have found that continuous filtration of the crystal-growth solution down to 50 nm yields an improvement of greater than a factor of five in damage threshold.

Contact: J. Campbell (415) 422-6497.

Laboratory X-Ray Lasers

We are using two arms of the Nova optical laser to demonstrate lasing at 4.5 nm—100× shorter than visible light and optimal for imaging live biological microstructures.

In 1984, we first demonstrated lasing at a soft-x-ray wavelength of 20.6 nm, which was some ten times shorter than emission from any previous laser.[1,2] In that work, we used two beams of the high-power Novette optical laser as a pump on a thin selenium foil. Our recent work has focused on inventing and demonstrating x-ray lasers with more power, better coherence, and, most important, shorter wavelengths. One of our principal objectives is to use such lasers in biological applications.

A hologram of a live (wet) biological microstructure, such as a large protein, can be made by scattering the coherent output from an x-ray laser off the protein and then recording the scattered pattern. Only x-ray lasers have sufficient brightness to record the hologram over a timescale that is short enough (~50 ps) to freeze the motion of a biologically active sample. Nevertheless, a problem arises from the x rays that are absorbed rather than scattered by a sample. Such x rays heat protein and expand it, blurring the image. To minimize this problem, we recently performed a landmark study to identify the optimal wavelength for an x-ray laser that causes the least absorption per scattered, or signal, photon.[3] We concluded that the optimal wavelengths for imaging biological samples in aqueous solution are slightly longer than the 4.37-nm carbon K-edge, as shown in Figure 1. At these wavelengths, the required exposure times to minimize blurring are well matched to achievable x-ray laser-pulse durations of 50 ps.

Thus, our goal has been to achieve lasing at wavelengths five times shorter than 20.6 nm, our original breakthrough wavelength. During the past year, we realized that goal by using two beams of the Nova laser. We irradiated a thin foil of tantalum, heated it to a temperature of about 1 keV, and stripped off about 45 of its 73 electrons, leaving a closed 3d (nickel-like) shell.[4] Further excitation of the electrons populates the $n = 4$ levels. However, the strong 4p–3d radiative transition leaves the 4p shell empty, leading to a 4d–4p population inversion and lasing at 4.48 nm, close to the optimal wavelength that we seek. As shown in Figure 2, the exponential growth of the signal demonstrates the lasing action.

We anticipate that further experiments using mirrors for multiple-pass amplification and mode selection for purer coherence will allow us to obtain actual biological holograms. Thus, we are at an exciting juncture in the development of laboratory x-ray lasers and in bringing the promise of their applications to fruition.

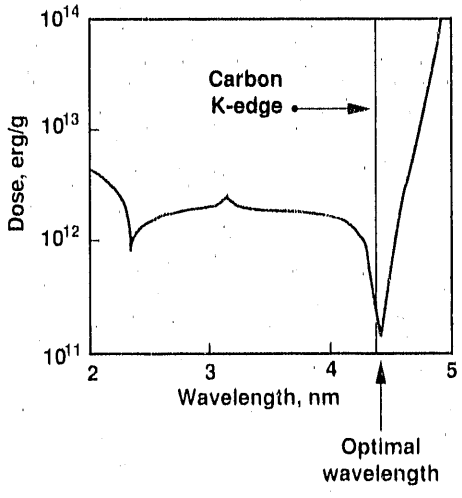


Figure 1. *Dose absorbed by a biological sample vs wavelength of the illuminating x-ray laser. For each wavelength, the incident fluence required to create a hologram and achieve 30-nm resolution is computed, and then the absorbed dose is found. The optimal wavelength is slightly longer than that of the carbon K-edge, where scattering is maximized and absorption is minimized.*

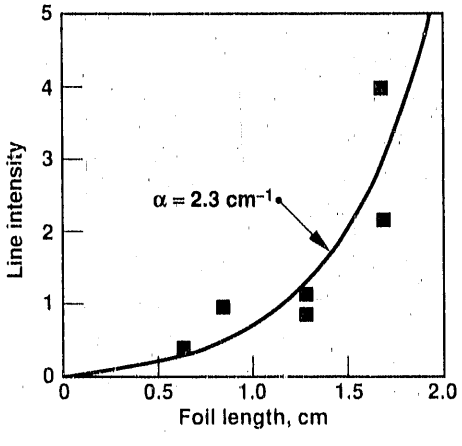


Figure 2. *Growth of a 4.5-nm laser signal as length is varied of the thin tantalum-foil x-ray laser target illuminated by two beams of the Nova laser. Exponential signal growth demonstrates lasing action.*

References

1. M. D. Rosen et al., *Phys. Rev. Lett.* **54**, 106 (1985).
2. D. L. Matthews et al., *Phys. Rev. Lett.* **54**, 110 (1985).
3. R. A. London, M. D. Rosen, and J. L. Trebes, *Appl. Opt.* **28**, 3397 (1987).
4. B. J. MacGowan et al., *Bull. Amer. Phys. Soc.* **34**, 2097 (1989).

Contact: M. D. Rosen (415) 422-5427 or D. L. Matthews (415) 422-5360.

Subpicosecond 7-TW Tabletop Laser

The pulses of our small-scale, subpicosecond neodymium:glass laser can exceed 7 TW in peak power. Focused intensities greater than 10^{18} W/cm^2 make it one of the brightest laser sources in the world.

Small-scale, high-power (terawatt), short-pulse lasers are being developed for research applications in multiphoton processes, dense plasma physics, and extreme-ultraviolet lasers, as well as for weapons research and research in support of inertial confinement fusion. Although the large-gain bandwidth of dye lasers yields subpicosecond pulses, their low saturation fluence and short storage time limit the available fluence to a few millijoules per square centimeter, thus severely limiting peak power. The bandwidths of excimer-based systems can support pulses as short as 200 fs and saturation fluences on the order of 10 mJ/cm^2. However, excimer lasers require large-aperture amplifiers to produce pulses of more than a few tens of gigawatts.

Broadband solid-state laser materials such as neodymium:glass, titanium:sapphire, and alexandrite exhibit saturation fluences on the order of joules per square centimeter. However, since the intensity-dependent refractive index produces beam filamentation, short pulses cannot directly access this large stored energy density. Chirped-pulse amplification (CPA) circumvents this problem in solid-state lasers. A chirped pulse is a broadband laser pulse whose frequencies (colors) are generated at different times; when the color sweeps from red to blue with time, the pulse is positively pulsed. CPA compresses a comparatively long pulse to a short pulse only after amplification. Thus, intensity in the amplifiers is kept below the beam filamentation level.

We have used CPA to produce a small-scale neodymium:glass laser that yields subpicosecond pulses with almost the same peak power as a Nova beamline (7 TW) in a nearly diffraction-limited beam. A mode-locked Nd:YLF (neodymium: yttrium-lithium-fluoride) oscillator produces 50-ps pulses at a 76-MHz repetition rate. One pulse selected from the mode-locked train is coupled into a 1-km single-mode, fused-silica fiber, within which self-phase modulation produces a broadband, chirped pulse. Adjusting fiber length and power input produces a linearly chirped 4-nm pulse at the fiber output.

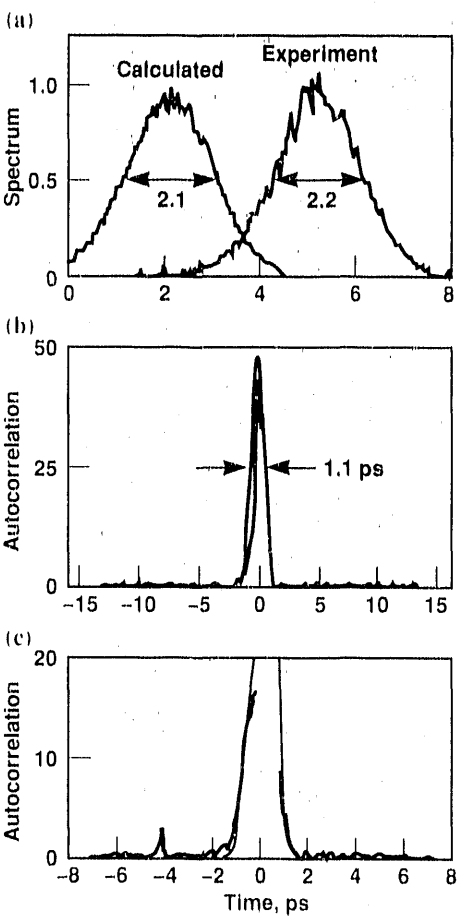


Figure 1. *Calculated and experimental results for a shaped 2.5-J laser shot: (a) spectra, (b) single-shot autocorrelation trace of 750 ± 65 fs (autocorrelation FWHM = 1.1 ps), and (c) expanded autocorrelation trace showing the absence of "wings."*

Fully exploiting the solid-state laser requires pulse stretching. Since chirped-pulse frequency components (colors) arrive at different times, a device that disperses the components can stretch or compress the pulse by speeding up or delaying the red part relative to the blue. Diffraction gratings stretch the pulse to 350 ps before amplification.

A ring regenerative amplifier (the heart of the laser system) produces a net gain of 10^7 from a single laser amplifier while maintaining diffraction-limited beam quality. The pulse energy is increased from 1 nJ (fiber output) to 10 mJ while gain-narrowing of the chirped spectrum is minimized. A series of single-pass amplifiers further increases the pulse to 10 J, and a pair of gold diffraction gratings compresses it to 1-ps duration. Spectral shaping techniques compress final duration to 0.75 ps (Figure 1) with peak power greater than 7 TW. Focused intensities exceeding 10^{18} W/cm^2 make this laser one of the brightest laser sources known.

A small-scale system with the peak power of a Nova beamline will allow us to perform new types of experiments in physics and to support inertial confinement fusion research. Such experiments will begin soon.

Contact: M. Perry (415) 423-4915.

AVLIS Laser Technology for the Next Generation of Microlithography

Fabrication of faster, more complex integrated circuits demands technologies that can deliver high-power, short-wavelength light. We are applying the laser technology developed for atomic vapor laser isotope separation (AVLIS) to this challenge.

Complex integrated circuits are manufactured by microlithography, and the size and number of features (e.g., transistors, resistors, diodes) determine the capability and cost of such devices. The wavelength of the light used in their manufacture is becoming a fundamental fabrication limitation. Present-day microlithography can produce a minimum feature size of slightly less than 1 μm, sufficient for fabricating 1-Mbit memory circuits. For the next generation of circuits, the minimum feature size must be decreased, and this means, among other things, that shorter-wavelength light will be required for the microlithography process.

At present, 1-Mbit direct random-access memory (DRAM) chips are fabricated by optical projection techniques using the blue lines of high-pressure mercury arc lamps (Figure 1). Soon, 4-Mbit DRAMs will be available, fabricated by optical projection using near-ultraviolet (UV) lines and quartz masks. Circuits with 16- and 64-Mbit capacity are in the early stages of development and will be available in a few years. The lithographic technique of choice for these circuits most likely will be deep-UV projection lithography. Future DRAMs with greater capability will require such a small minimum feature size that x-ray lithography in either a near-contact mode (proximity mode) or with an advanced version of demagnifying optics (projection mode) will be necessary.

The copper/dye laser system developed for AVLIS is the highest-average-power laser system of its type in the world today. This system, in modified formats, can produce the variety of photon sources for advanced microlithography:

- Deep-UV projection lithography. The deep-UV source must have a stable, narrow spectral width. AVLIS copper lasers frequency-doubled to 255 nm can provide a stable source with narrow bandwidth and with the reliability of a production system.
- X-ray proximity lithography. This technique promises to dominate the next decade of DRAM production. It requires wavelengths of 0.8–1.4 nm, which are presently available in high fluxes only from large, expensive synchrotron machines. However, the AVLIS copper/dye laser system with a modified pulse format can produce the required spectrum of x radiation through laser-generated plasmas in an economical and efficient manner.
- X-ray projection lithography. For ultrahigh resolution, this technique requires soft x rays in the 10-nm range together with multilayer optics (already developed at LLNL as part of our work in inertial confinement fusion). AVLIS copper lasers alone can generate laser plasmas that radiate efficiently in this wavelength regime, again providing an attractive alternative to synchrotrons.

We are adapting the AVLIS laser systems for these lithographic applications, with support from the Laser Program and the Institutional Research and Development Program. The first step is to improve beam quality and to shift the green and yellow light produced by the copper lasers into the UV. Next, we will develop pulse-compression schemes that will allow the laser pulse to be matched efficiently to the task of x-ray production. Once these modifications are made, the technology will be transferred to industry. Thus, it will soon be possible to produce the advanced lithographic light sources required to fabricate the next generation of microprocessors and memory chips.

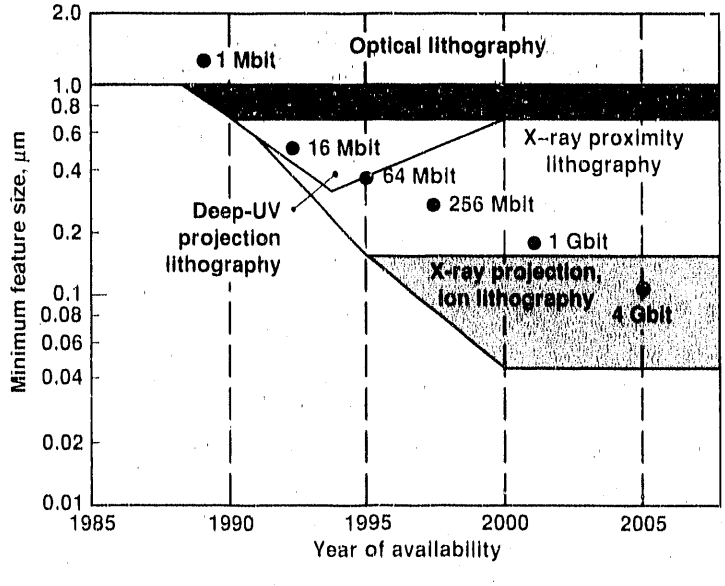


Figure 1. *Estimated time scale for the production of future generations of dynamic random-access memory (DRAM) chips, their minimum feature size, and the applicable lithographic techniques.*

Contact: H. W. Friedman (415) 422-2257 or E. R. Ault (415) 422-6209.

Advanced Laser Applications

Among our achievements this year, we set a world record for high-average-power linear and two-dimensional diode laser arrays, placing LLNL at the forefront in the design and fabrication of highly efficient, compact, solid-state lasers for commercial and military applications.

We are tailoring and extending LLNL optical technologies to meet new challenges in the use of advanced lasers. For example, we are developing high-average-power solid-state lasers and semiconductor diode arrays for laser pump sources. We have begun to use such laser systems in commercial and military applications, including x-ray lithography and detection of mines near shore in ocean surf. We are also applying the imaging technologies developed in our laser research to overcome atmospheric distortion, making it possible to resolve images of manmade satellites and astronomical objects from the ground.

High-Power Diodes and Diode-Pumped Solid-State Lasers

During the past year, we achieved several milestones in the areas of diode-pumped solid state lasers and high-power diode laser array packaging. These accomplishments place LLNL in the forefront in the design and fabrication of highly efficient and compact solid-state lasers.

Last year, we fabricated the first truly high-power laser diode arrays. This year, we expanded our capability and performance in the areas of semiconductor laser fabrication and packaging; our goal is to produce large quantities of high-performance diode arrays designed specifically for pumping high-average-power solid-state lasers. Recent progress in the fabrication and testing of semiconductor pump arrays includes the demonstration of extremely robust, long-lived, high-power arrays, the development of ultrathin stackable arrays that incorporate void-free large-area bonding of silicon to silicon, and our demonstration of high-yield, large-batch production of narrow-linewidth, high-power diode bars suitable for the pumping of crystalline lasers.

Also this year, we produced world-record high-average-power linear and two-dimensional diode arrays, in large volume and at low cost, for use in a broad range of applications. When these arrays were assembled, microchannel cooling techniques were used to provide for the removal of waste heat. These arrays (Figure 1) are now being processed in volume for the assembly and production of high-average-power diode-pumped solid-state lasers. The peak-power cost is approximately \$7/W, and the average power cost is approximately \$35/W.

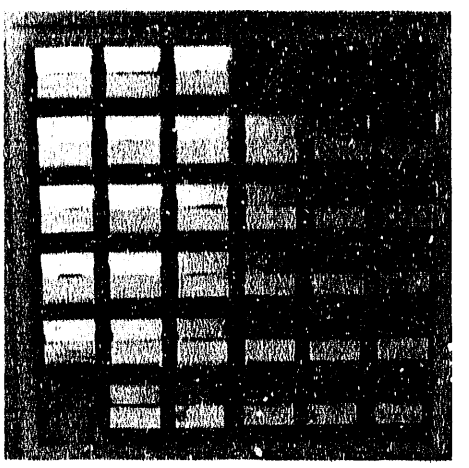


Figure 1. *High-power laser diode arrays, which can now be fabricated in quantity at LLNL, have achieved world-record power levels.*

Life tests to date on our high-power stackable diode bars (10–20 W/cm) indicate that, under constant-light-out conditions, we can expect a lifetime of as much as 3×10^{11} shots, which corresponds to operating for 10 years at 1 kHz. These are the longest lifetimes ever reported for high-power aluminum-doped gallium arsenide (AlGaAs) lasers in either pulsed or continuous-wave tests. We are integrating these arrays with solid-state crystalline storage media to produce efficient, high-repetition-rate (3.5-kHz), high-average-power (50-W), 532-nm radiation lasers for our Department of Defense sponsors.

High-Average-Power Nd:Solid-State Lasers

High-average-power, solid-state laser technology is essential for x-ray lithography, laser radar, and materials processing. Solid-state lasers can produce extremely high peak-power pulses of light that can be focused on high-atomic-number materials to generate x rays, to illuminate distant satellites, and to machine tough metals and ceramics. The solid-state laser has the unique capability of achieving high levels of performance within a compact, efficient, and lightweight package. These performance features have been demonstrated independently, and the next step is to integrate them into a single device.

We have demonstrated new levels of advanced laser system

performance during the last year with the completion of a high-average-power Nd:glass laser system. This system uses revolutionary materials and components integrated into a new compact architecture. With it, we have produced 10-J, near-diffraction-limited, gigawatt pulses of light. This level of performance was demonstrated at pulse-repetition rates of 10–30 Hz with an overall system efficiency of 1%.

In addition, we have activated a crystal slab laser testbed, from which we have obtained encouraging new data. Initial tests have produced an average laser output power of up to 490 W.

Thermo-optic distortions we observed in these glass and crystal lasers were analyzed with the aid of three-dimensional computer simulations of the thermal fields, stresses, and surface displacements. We have simulated the intense pumping required and its effects on laser propagation. The results of our observations and simulations emphasize the importance of uniformity in pumping and cooling to achieve high-quality laser-output power.

Demonstration of a Ground-State-Depletion Laser

Supported by the Defense Advanced Research Projects Agency, we conceived and demonstrated a new class of diode-pumpable solid-state laser, which we refer to as the ground-state-depletion (GSD) laser. This novel laser is a quasi-three-level system in which the terminal lasing level is the ground electronic state. Until now, these lasers were very inefficient when operated in a Q-switched mode; efficient operation required liquid-nitrogen temperatures.

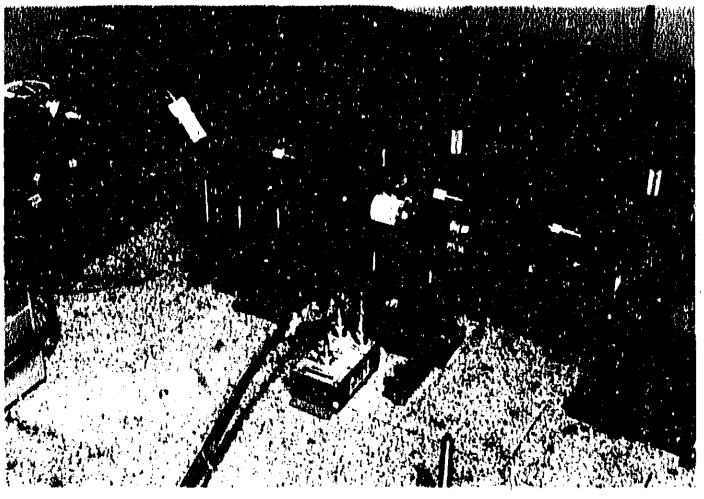


Figure 2. *Our new frequency-doubled GSD laser generates 455-nm light to match the cesium resonances. This laser/filter combination is of considerable interest for such undersea applications as submarine communications.*

Our concept results in a highly efficient room-temperature Q-switched laser. The increased efficiency is due, in large part, to the removal of ground electronic state ions that would otherwise absorb the laser radiation and form a large loss term.

This GSD laser has been demonstrated to be as efficient as a conventional Nd:YAG laser operating at 1.06 μm; it has been Q-switched to generate a power of 0.5 J/pulse. The laser shown in Figure 2 has been frequency-doubled in critically phase-matched $KNbO_3$ to produce blue radiation. The host material used is yttrium orthosilicate (YOS) grown for us by D. Brandle of Bell Laboratories. This new laser material is grown core-free in diameters greater than 2 cm and in lengths of several tens of centimeters. The material is highly damage-resistant, with a bulk damage threshold for 10-ns pulses in excess of 42 J/cm^2. This damage threshold is comparable to that for high-quality fused silica.

Our new GSD laser operates at 911 nm and can be frequency-doubled to 455 nm to achieve resonance with the well-known cesium atomic absorption filter. This laser/filter combination is of interest for a number of undersea applications, such as submarine communications.

Radar Ocean Imaging

We are investigating the use of air- and space-borne radar systems to image ocean-surface features (e.g., ship wakes) and have developed a numerical-simulation capability for modeling microwave scattering from the ocean. This year, we participated in the Loch Linnhe 90 Radar Ocean Imaging Experiment, a joint U.S./U.K. experiment in Scotland. We provided the ground-based synthetic-aperture radar (SAR) processing capability. The system processed data from the NASA-JPL DC-8 Airborne SAR and included integration of the high-density digital tape unit, data reformatting software (developed in cooperation with the Jet Propulsion Laboratory in Pasadena, California), several image-reconstruction algorithms, and image-analysis tools.

Contact: E. V. George (415) 423-3939 or K. R. Manes (415) 423-6207.

Industrial-Scale AVLIS is Approaching its Deployment Goals

Atomic vapor laser isotope separation (AVLIS) technology has achieved levels of performance and reliability that are sufficient to justify its deployment on a commercial scale.

The goal of the Atomic Vapor Laser Isotope Separation (AVLIS) Program is to develop a laser-based process for changing the naturally occurring isotopic ratios of various elements. The most important and economically viable application for this process is the enhancement (by enrichment and/or depletion) of the elements uranium and plutonium (uranium is a fuel for commercial nuclear reactors, plutonium is used primarily in military applications). This application of laser technology is one of the most demanding ever undertaken. Although we employ powerful lasers comparable to those used for industrial welding operations (tens of kilowatts), the laser light we generate must be in the ultraviolet or visible ranges of the spectrum. The color and optical qualities of the light must be controlled precisely, and the laser systems must be reliable, economical, and able to operate continuously, 24 hours per day, under commercial production conditions.

During the past several years, the AVLIS research team has defined the basic laser system architecture, projected its ultimate performance capabilities, and estimated the cost of a deployed operating system. This team includes researchers from LLNL and our two industrial participants in the development program, Martin Marietta Energy Systems, Inc., and Westinghouse Idaho Nuclear Co.

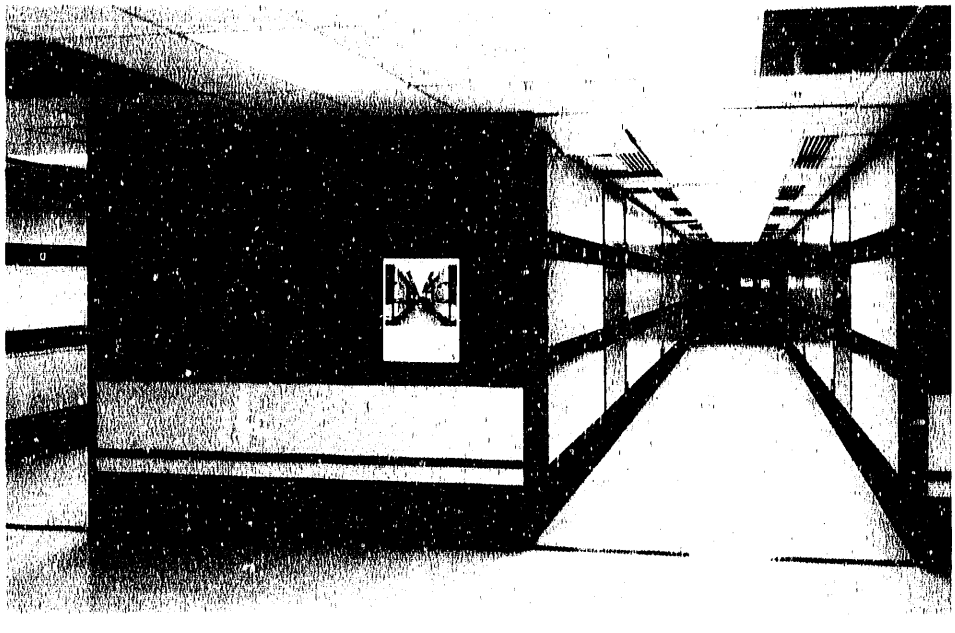


Figure 1. *Copper-vapor-laser amplifier chains are operating around the clock in the Laser Demonstration Facility at LLNL. Each chain comprises a 20-W oscillator and three amplifiers, each rated at 300 W of optical power.*

AVLIS's Multiple-Laser System

Two types of lasers are used in the AVLIS process. High-power copper-vapor lasers were chosen for their ability to efficiently convert electricity into optical power in the green and yellow ranges of the spectrum. Dye lasers, using common fluorescent dyes (similar to those found in paints and clothing), are then used to convert this fixed-color laser light to light frequencies that can be continuously tuned to match the atomic levels of the element being processed. Initially, both the copper-vapor and dye lasers were research-scale devices capable of delivering only a few watts of optical power. We have only recently developed industrial-scale devices that have the reliability needed for AVLIS. Now that this capability has been developed, many other applications of the AVLIS technical base are being studied. Among them are the purification of semiconductor materials, more efficient lighting, x-ray sources for semiconductor lithography, and direct laser material processing (cutting and welding).

A key factor in the successful development of the AVLIS lasers is their modular architecture. Each system is reduced to subsystems that are independently developed and

optimized. At this level, rapid progress can be made by several teams working independently. All subsystems are connected periodically to ensure their continued compatibility. Unlike the series approach, where components are developed one after another until the whole system is integrated and tested, our parallel approach allows the system to be tested early in the development phase so that unexpected technical issues that arise can be resolved in a timely manner. During operation, the modular system is highly accessible and can be repaired or modified readily without shutting down the entire system. The modular approach also allows us to rescale the system as necessary to respond quickly to varying market demands and mission requirements.

We are continuing to develop the lasers and their subsystems (computer controls, active alignment systems to steer the laser beams, diagnostic systems, and optical coatings). We are confident that we will be able to achieve the further refinements in performance and reliability that are needed to keep pace with the progress of isotope separation technology as we approach plant deployment.

Figure 2. *A portion of the dye laser system. Green laser beams from the copper lasers excite the dye lasers to produce the yellow light shown.*

Laser Demonstration Facility: Highest Average Power

Operating 24 hours a day, the AVLIS Program's Laser Demonstration Facility (LDF) system of 60 individual copper-vapor lasers has attained more than 1,000,000 device-hours (Figure 1). A total-system optical power of 7500 W is now being produced on a steady-state basis, and we expect to reach our goal of 8000 W by September 1990. Also this year, we succeeded in producing more than 1000 W of optical power in a single dye-laser amplifier chain and have proven the dye lasers' ability to operate for hundreds of hours (Figure 2). The LDF continues to be the highest-average-power visible laser system in the world.

In addition to its role in the development of AVLIS lasers, LDF supported a series of full-scale isotope separation experiments for the Special Isotope Separation (SIS) Program this year. Using a surrogate (nonradioactive substitute) element in place of plutonium, we conducted critical, long-duration tests of the total AVLIS process, including integration and testing of plant-scale hardware. Detailed measurements confirmed our process projections and provided support for our performance and cost projections of the SIS plant design.

In the coming year, we will continue to upgrade the LDF and improve its performance. All systems are being configured for integrated plant-scale experiments of uranium isotope separation, scheduled for 1991 and 1992. These complex and challenging experiments will provide the design verification needed to proceed with the next phase—deployment of the first AVLIS uranium enrichment plant—which is scheduled for the late 1990s.

Contact: E. R. Ault (415) 422-6209.

Uranium AVLIS Program

U-AVLIS is potentially the lowest-cost technology for enriching uranium to the level needed to fuel commercial nuclear power reactors. A decision by the DOE to complete the U-AVLIS demonstrations and begin predeployment activities will send a clear signal that the U.S. is determined to be a competitive force in the international market.

In January 1990, the Secretary of Energy submitted to Congress the Department of Energy's *Plan for the Demonstration, Transition, and Deployment of Uranium-AVLIS Technology*. This detailed program plan leading to the construction of an atomic vapor laser isotope separation (AVLIS) plant for uranium enrichment clearly demonstrated the DOE's commitment to maintaining the U.S.'s competitive position in the international uranium market.

For the past 16 years, the Laboratory, in collaboration with Martin Marietta Energy Systems and its predecessor Union Carbide, has developed, engineered, and demonstrated the AVLIS system at continually increasing scales. LLNL is now preparing for a final series of major tests that will demonstrate the hardware, performance, and costs required to establish the economic basis for beginning plant construction.

U.S. Uranium-Enrichment Policy Objectives

The U.S. role in the international uranium-enrichment market influences this country's energy security, technological and business competitiveness, balance of trade, safeguards and nonproliferation policies, supplies of special nuclear material, and employment. Until 1974, the U.S. was the sole supplier of uranium enrichment services to the free world. By 1987, the U.S. was still the single largest free-world supplier, but its market share had been reduced to 50%. It is now obvious that enrichment cost will be the dominant factor for capturing future sales. Since the U.S. gaseous diffusion plants are becoming less competitive with time, the U.S. market share will be lost by about the year 2000 without the modern, competitive enrichment capability that AVLIS provides.

The international market in enriched uranium is highly competitive and is expected to remain intense for many years to come since demand growth is slow and the current worldwide capacity exceeds annual demand by about 30%. In addition, foreign suppliers are expanding their capacity in anticipation of a growing future demand and are aggressively marketing their capabilities. Typical of this cost-competitive market is the announcement by Urenco of their plan to begin construction in 1992 of a centrifuge enrichment plant in the U.S. with U.S. partners. The Soviets have also announced a very aggressive pricing strategy of $60–75 per separative work unit (SWU)[1] in an evident attempt to take advantage of their excess enrichment capacity (estimated at between 3 and 10 million SWUs per year) to obtain hard currency and to stimulate continued expansion of trade with the West. The recent political changes in Eastern Europe will probably make the Soviets an acceptable supplier to most utilities, including those in the U.S.

It is clear then that if the U.S. wishes to regain and retain a significant share of this market, there is a pressing need for a new, low-cost U.S. enrichment capability. Since U-AVLIS is potentially the lowest-cost enrichment technology, a prompt commitment by the DOE to complete the U-AVLIS demonstrations and to begin predeployment activities will send a clear signal to the international market: the U.S. is determined to exploit the technological lead the U.S. now enjoys in AVLIS and will be a strong competitor in the expanding cost-competitive market of the late-1990s. This in turn will strengthen the DOE's position with existing customers and enhance its ability to attract new customers in the near term. Fortunately, the technological status of the national U-AVLIS program is well positioned to face the competition and to meet the needs of the marketplace.

U-AVLIS Technology

The U-AVLIS technology consists of three major subsystems: lasers, separators, and uranium chemical processing. Copper lasers optically energize the tunable dye lasers; the wavelengths of the light from the dye lasers are precisely set to photoionize the uranium-235 isotope in the separator. The uranium-235 is then collected as product, and the non-ionized uranium-238 is collected as tails. After removal from the separator, the product is chemically

processed into a form acceptable for fuel for commercial nuclear reactors.

During 1987 and 1988, the integrated laser and separator technologies were demonstrated at large scale, providing a sound basis for predicting U-AVLIS enrichment performance. By September 1989, the copper lasers in the Laser Demonstration Facility had achieved more than a million unit-hours of operation. They are currently producing more than 7500 W of power continuously (24 hours a day), a 25% increase in the last year and a sevenfold increase since 1985. We are testing the next-generation copper laser and expect that it will be able to produce approximately triple the power per unit at about 40% of the cost per watt of the first-generation lasers. In its first tests, this new laser has already demonstrated twice the unit power of the earlier designs.

Also this year, we have proven the durability of the dye lasers. They have been operated for long-term demonstrations of hundreds of hours, and more than 1000 W of high-quality tunable power has been produced in a single dye-laser amplifier chain.

Results from these demonstrations serve as the technical basis for the current U-AVLIS plant design. Using factory production costs of lasers and separators, extrapolated from those demonstrated on existing hardware designs, we project uranium-enrichment production cost of approximately $25 per SWU. This is well below the $60 per SWU price level necessary to be competitive in the global market.

A demonstration of the AVLIS process with plant-scale subsystems is currently scheduled for 1992. After this demonstration, the Secretary of Energy will decide whether to continue to deploy AVLIS according to plan. A positive decision will accelerate predeployment activities, leading to the start of plant construction by March 1993 and to first production by January 1997 (Figure 1).

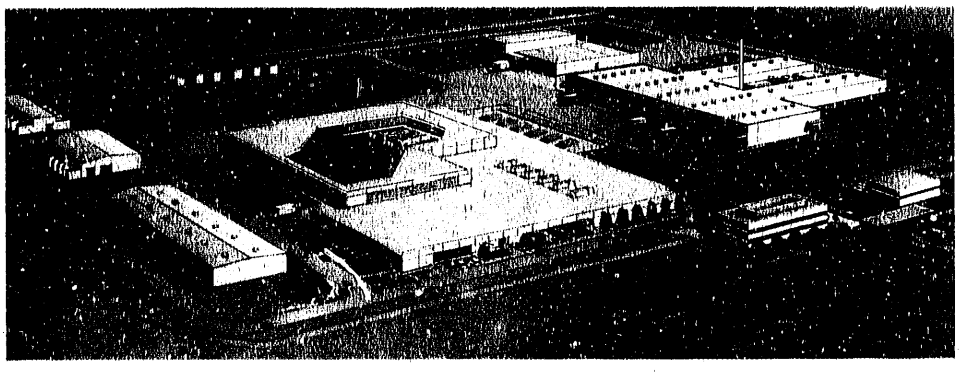


Figure 1. *Artist's rendering of the proposed U-AVLIS plant, which could begin enrichment production in early 1997.*

Overall U-AVLIS Program Plan

We are constructing the Uranium Demonstration System (UDS). This system will allow us to demonstrate large-scale, integrated uranium enrichment in a multi-unit separator with laser light in a plant-like operating environment. This demonstration and the engineering data derived both from its construction and from its operation should provide the information needed to evaluate the economic and technological competitiveness of U-AVLIS and for the DOE to make a final deployment decision.

An overall U-AVLIS program plan has been developed in response to the market needs, the current technology status of AVLIS, the overall program objectives, and the demonstration goals. This plan calls for the UDS to be completed as soon as reasonably possible, preserving the option to start first enrichment production in early 1997. While the UDS tests are proceeding, we will also complete the predeployment activities (including site selection, completion of the conceptual design report and the environmental, health, and safety compliance assessments, and licensing activities) so that plant construction can begin in mid-1993. At this time, the LLNL U-AVLIS program will provide technical support for the plant construction project and will continue development and demonstration activities to reduce plant operating costs and improve process performance.

This plan and schedule take fully into account the significant progress made recently in AVLIS lasers, separators, and uranium processing. Concurrent demonstration and deployment could keep overall U-AVLIS program costs down and thereby minimize the economic uncertainties involved in proceeding decisively to U-AVLIS plant deployment.

Note

1. The separative work unit or SWU (in kilograms) is a measure of the value of enrichment services and is used as the unit of exchange for such services to utilities.

Contact: R. W. O'Neil (415) 422-6222.

Plutonium Laser Isotope Separation

In late January of 1990, the Secretary of Energy decided not to construct the SIS plant for separating plutonium isotopes using the Laboratory-developed AVLIS process. As a result of the decision, we are closing out and documenting the SIS plant construction project and are working with the DOE production complex to transfer the SIS technology and equipment.

The Special Isotope Separation (SIS) Program is developing and demonstrating the principal technologies required to process reactor-fuel-grade plutonium into weapon-grade plutonium using the atomic vapor laser isotope separation (AVLIS) process developed at LLNL. We are preparing to conduct process performance verification (PPV) tests to demonstrate the performance of all major unit process elements at or near plant scale.

In early January 1989, the Idaho National Engineering Laboratory was selected by the Department of Energy (DOE) as the site for the proposed SIS plant. This plant is designed to derive weapon-grade material from DOE-owned reactor-fuel-grade plutonium and to recover plutonium from existing residues; it will provide a contingent supply of weapon-grade plutonium, thereby reducing dependence on DOE's reactors and permitting flexibility in response to changing plutonium supply requirements. The AVLIS process also offers technical diversity in that this technology differs significantly from the conventional reactor-based production processes. Currently, the Hanford N reactor is on standby, and the Savannah River reactors are shut down pending repairs; consequently, the U.S. is presently unable to produce weapon-grade plutonium.

In late January 1990, the Secretary of Energy announced his decision to not construct the SIS plant given current budget problems and funding priorities within the DOE. He also stated that it is important to develop a thorough understanding of SIS technology for national security and other purposes. He therefore proposed to complete research and development experiments for SIS (excluding plutonium testing in the Engineering Demonstration System) and to provide for completion of the research program in an orderly fashion. A National Academy of Sciences review of SIS technology has been instituted by the DOE to identify alternate applications such as waste minimization and isotopic purification of other elements. The results of this study should be available in 1991.

We are currently closing out and documenting the SIS production plant construction project, a task that will be completed by the end of fiscal year 1990. We plan to complete the development and demonstration work directly supporting the SIS project by the end of the 1991 fiscal year.

The SIS Program has participated extensively in the evolution of the production plant design that was described in the 1987 preliminary design report. The proposed SIS plant is being designed to meet modern DOE specifications and all applicable Nuclear Regulatory Commission (NRC) and State of Idaho requirements and guidelines. The laser facility and plutonium facility designs are currently 60% and 40% complete, respectively.

In incorporating plutonium processing technology, we have taken particular care to select and develop processes and equipment designs that enhance worker safety and reduce waste generation. Pyrochemical processes are used to prepare feedstock for the AVLIS process from plutonium oxide, the principal form of feed to the SIS plant. Nitrate-based aqueous processes are used to recycle scrap and recover plutonium from the salts employed in the pyrochemical processes. With the demonstration facilities at LLNL, we are developing all the major pyrochemical and metallurgical processes. The key aqueous processes for plutonium scrap recovery and waste processing are being demonstrated at the Pacific Northwest Laboratory (PNL) in Hanford, Washington. These processes incorporate a catalytic-electrolytic plutonium oxide dissolver (CEPOD), an advanced dissolver that improves cycle time and plutonium recovery rate compared with conventional dissolvers.

Recently, the Laser Demonstration Facility (LDF), which serves both the uranium and plutonium AVLIS programs, was upgraded to more than double its available process power. This was accomplished by improving copper laser performance and by constructing a second corridor of copper lasers. Current average performance of the copper lasers is 85% of SIS production plant requirements per corridor (each corridor contains six MOPA or master oscillator/power amplifier chains); individual MOPA chains have demonstrated power levels of >100% of plant requirements. We have also upgraded the dye laser system to provide the full suite of colors necessary to fully demonstrate plutonium AVLIS.

This year, we also completed the installation of Engineering Demonstration System (EDS) hardware in the LLNL plutonium facility and operated the system using surrogate (i.e., nonradioactive) materials. The EDS linebox is essentially a glovebox containing multiple separator units; a full-scale production prototype separator has been operated in the EDS using surrogate materials. In tests conducted in the Triton system (an offline separator development facility also located in the plutonium building), this separator was shown to satisfy the throughput requirements for projected SIS plant operating cycles.

The pyrochemical processes for plutonium processing are being demonstrated in the Materials Processing Laboratory (MPL; see Figure 1). These processes are used to prepare plutonium metal feed for the AVLIS process, to recover the plutonium product and prepare it for weapon production, and to prepare the byproduct plutonium for storage; they include calcining, direct oxide reduction, molten salt extraction (to separate ^{241}Am), casting, hydriding/dehydriding, and electrorefining to remove chemical impurities. We have shown that these processes do indeed meet plant yield, purity, and plutonium utilization requirements. An important aspect of this work is to demonstrate processes and equipment that minimize waste generation and reduce operator radiation exposure.

To date, we have demonstrated the pyrochemical processes in fixed furnaces. An important element of the SIS Program has been the development of a tilt-pour furnace. The proposed SIS production plant design will use a tilt-pour furnace for direct oxide reduction, molten salt extraction, electrorefining, and salt scrub (to recover residual plutonium). Use of the tilt-pour furnace improves operability, minimizes operator dose, reduces scrap production, and requires less plant floor space than a fixed furnace of equivalent capacity. We have built an engineering prototype tilt-pour furnace and tested it using surrogate materials to ensure its mechanical function. More than 300 cycles have been completed using common salts and surrogate metals in a nonradioactive glovebox environment. We are installing a prototype tilt-pour furnace, incorporating upgrades suggested by the results of this first test series, in the MPL to demonstrate its performance with plutonium.

Figure 1. *The Materials Processing Laboratory in the LLNL plutonium facility, where the pyrochemical processes for plutonium processing are being demonstrated.*

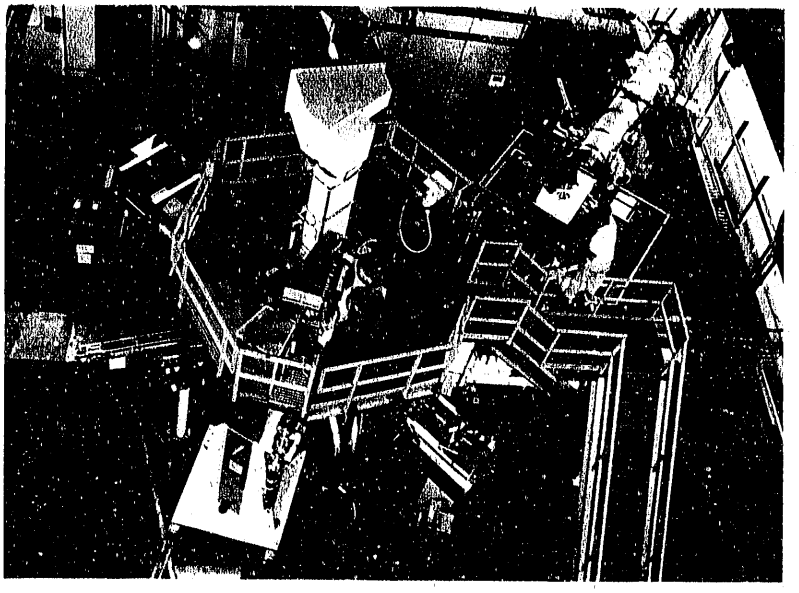
We have operated the LDF and the EDS as an integrated system using surrogate materials and have verified system integration by measuring photoionization performance. Up to three separator units have been operated simultaneously as part of these operations. We are planning further tests with surrogate materials to complete process performance verification pending a DOE decision of no significant environmental impact due to this work.

As part of the overall SIS effort, we are developing materials-handling and automation technology to enhance worker safety in the SIS plant. The major thrust in this area is to take an overall systems view of plutonium processing, integrating the processes, processing equipment, and handling equipment. Working with experts from IBM, Los Alamos, Sandia, and the U.K. (Harwell), we are adapting commercially available robotics and automation technology to plutonium-processing glovebox operations.

We are actively working with the DOE production complex to transfer the technology and equipment developed for SIS.

Contact: J. G. Harri (415) 422-6157.

Magnetic Fusion Energy and Beam Research



The Alcator-C tokamak has been installed at LLNL as part of the MTX, an experiment to study the interaction of intense millimeter-wavelength radiation with magnetically confined plasmas.

Research in magnetic fusion was one of the Laboratory's earliest activities. Our broad objective today is to contribute to the development of the physics understanding and the technology base required to harness the awesome potential of thermonuclear fusion for energy production. LLNL plays a leading role in the development of millimeter-wavelength sources for electron-cyclotron resonance heating, superconducting magnets, and computational methods for modeling the complex processes that occur in a magnetically confined plasma.

Intense beams of charged particles play an important role in magnetic fusion technology. LLNL has pioneered the development of the induction linac, a linear particle accelerator concept that is uniquely suited to the generation of intense pulses of energetic particles. In recent years, the LLNL Beam Research Program has led the nation in research on the induction-linac-driven free-electron laser (IFEL). In this device, the energy from an intense electron beam is converted to coherent electromagnetic energy, at frequencies ranging from millimeter wavelengths to visible light. The Beam Research Program is applying induction linac technology to applications in defense, energy, and particle physics research.

The Magnetic Fusion Program comprises activities in theoretical and computational physics, experimental plasma physics, and fusion technology. The theoretical effort is strongly linked to the analysis of experimental results obtained at LLNL and at major experimental facilities around the world. In our computational effort, we have developed a new and efficient approach to modeling the complex processes that govern the transport of energy in magnetically confined plasmas. Relying on more efficient computational algorithms as well as on increases of machine capabilities, we hope soon to be able to model tokamak experiments with a previously unobtainable degree of physical realism.

Our experimental research is conducted both at LLNL and at

General Atomics (GA), in San Diego. At GA, our experimental team has primary responsibility for the physics of the edge region of the plasma. It has recently become apparent that control of the boundary conditions at the plasma edge is critical to obtaining satisfactory confinement of the plasma. Here at LLNL, we have established a tokamak facility, called the Microwave Tokamak Experiment (MTX), to examine the interaction of intense pulses of millimeter-wavelength radiation with a magnetically confined plasma. In these experiments, we can supply millimeter-length waves from either conventional gyrotron sources or from an IFEL. The Japanese Atomic Energy Research Institute (JAERI) has developed a diagnostic package for the MTX, and a team of JAERI researchers is participating in the experiments.

The next generation of magnetic fusion devices will require superconducting magnets. We have established FENIX, a facility to test large, superconducting magnetic coils. In addition, we are working with industry to develop techniques to improve the production of superconducting materials.

Production of energy from magnetic fusion is an international goal. In 1987, the U.S., Japan, the Soviet Union, and Euratom, under the auspices of the International Atomic Energy Agency, established a joint project to develop, design, and construct an experimental power reactor. This project, called the international thermonuclear experimental reactor (ITER), is headquartered in Garching, near Munich, West Germany. LLNL has the responsibility for planning and coordinating the U.S. effort supporting ITER. In 1990, the ITER team will complete the conceptual design of the facility. If the project participants agree to proceed to the engineering design, the device could be operating and producing net fusion power early in the next decade.

The induction linac technology pioneered by the Laboratory's Beam Research Program has broad applications. LLNL maintains the primary research facility in the U.S. for studies of the propagation of intense beams of charged particles. This facility, the Advanced Test Accelerator (ATA), located at Site 300, has also provided a superb test bed for the development of IFEL technology. In 1990, under sponsorship of the Defense Advanced Research Projects Agency, we completed our studies of particle-beam propagation on ATA.

A newer facility, the Experimental Test Accelerator (ETA-II), is now operating at the Livermore site. It is equipped with a magnetic wiggler for FEL operations. In addition to its use for FEL development studies, funded through the Strategic Defense Initiative Organization, the ETA-II facility is used to generate millimeter-wavelength pulses for the MTX. In 1989, we successfully generated intense millimeter-wavelength pulses in the ETA-II and transmitted them to the MTX tokamak for experiments on plasma absorption and scattering. We are currently upgrading the ETA-II facility to accommodate high-repetition-rate operation of both the accelerator and the FEL.

LLNL maintains a strong capability in computational modeling of induction linac and FEL devices. These computational tools are validated by close comparison with experimental results, and provide a basis for the design and analysis of future systems. We are currently examining a number of new applications of induction linac technology, especially in the area of energy research. The high-power microwaves generated by an IFEL can be used, in turn, to produce an intense field for accelerating a bunched electron beam. Called a relativistic klystron, this is one approach to the design of the next generation of high-gradient accelerators for elementary particle physics research. In collaboration with the Lawrence Berkeley Laboratory (LBL) and the Stanford Linear Accelerator Center, we are investigating the use of an induction-linac-driven relativistic klystron to produce high-power microwaves.

The induction linac is also seen as the primary approach to the generation of intense pulses of heavy ions for use as an inertial fusion driver. This year, a joint effort was established, with participants from the Beam Research Program and the Inertial Fusion Program at LLNL and the Heavy Ion Accelerator group at LBL, to explore conceptual improvements in heavy-ion fusion technology.

With the Compact-Torus Accelerator Project (known as RACE, for ring accelerator experiment), we are working to accelerate, compress, and focus plasma rings confined by compact toroidal magnetic fields. This project is supported by the Laboratory's Institutional Research and Development Program. Our plasma ring acceleration experiments have demonstrated qualitative agreement between predicted and measured internal structure, and have shown that focusing and soft-x-ray generation are possible. This technology has applications in defense, inertial confinement fusion, and magnetic fusion energy.

Contact: A. J. Glass (415) 422-9804.

Microwave Tokamak Experiment

Our initial studies of plasma heating using a free-electron laser (FEL) were very successful. We injected 100-MW, 140-GHz microwave pulses from an FEL and measured microwave transmission through the plasma. We saw no indication of nonlinear effects at high power; this result is consistent with theory, which predicts that such effects will appear only at very high powers of ~1 GW.

The Microwave Tokamak Experiment (MTX) is a fusion research facility for investigating plasma heating, confinement, and control; it is part of the national Magnetic Fusion Energy Program. In these experiments, we inject microwave radiation into a high-magnetic-field tokamak. Electron heating is accomplished by selecting the frequency of the injected microwaves to be equal to the electron's resonant frequency (which is determined by the magnetic field of the tokamak); this heating process is called electron cyclotron resonance heating (ECRH). For the high (5–10-T) magnetic field of the MTX, these corresponding frequencies are 140 to 280 GHz. Microwave radiation is produced either by a free-electron laser (FEL), which generates a series of short (50-ns), very-high-power (1–2-GW) pulses, or by a gyrotron, which generates ~400 kW of continuous power. Both microwave systems are installed on the MTX so we can readily compare heating using the FEL-generated pulses with heating using the continuous-power gyrotron.

A major advantage of the FEL is that the frequency of the microwaves can be altered during the tokamak shot, thereby allowing us to change the heating zone in the plasma. With this localized heating, we can actively control various plasma processes and instabilities. Operation of the FEL can also be extended to higher powers and frequencies more easily than can the gyrotron. We are conducting these FEL experiments in collaboration with LLNL's Beam Research Program.

The objective of our 1989 research was to establish a good target plasma for ECRH experiments and then to conduct single-pulse FEL propagation experiments. We achieved routine operation at plasma densities greater than 10^{20} m^{-3}, electron temperatures greater than 1 keV, and plasma Z_{eff} near 1.5 (Z_{eff} is the average charge of the plasma; a plasma with $Z_{eff} = 1$ would be a pure hydrogen plasma). During the single-pulse FEL experiments, we generated intense microwave pulses (2-mm wavelength) of powers up to 0.4 GW at a frequency of 140 GHz. We compared the transmission of high-power microwaves with that of low-power (1-W) microwaves. We saw no indication of nonlinear effects at high power; this result is consistent with theory, which predicts that such effects will appear only at very high powers of ~1 GW.

The FEL consists of a high-current (2–3-kA), high-energy (6-MeV) electron accelerator (the ETA-II), and a pulsed wiggler (the ELF-II). Results obtained by the Beam Research Program in this collaborative effort demonstrate that the FEL output power is well predicted by theory, giving us confidence that we will be able to extrapolate FEL technology to future devices at higher powers and frequencies. The microwaves generated in the wiggler are transported through the windowless quasi-optical transmission line to the MTX tokamak. The transmission line consists of a large, evacuated tube that encloses mirrors that collect and focus the radiation and connects the FEL and MTX vacuum systems. Most important, no windows separate the FEL source from the tokamak. This transmission system is a significant advance for fusion devices, because the weakest link in high-power microwave technology is often the window separating the source from the load (e.g., gyrotrons usually have windows at their output). Our results clearly demonstrate that a transmission line of this sort can efficiently handle high-peak-power microwaves.

A principal diagnostic used to evaluate the interaction of the single-pulse microwaves with the plasma is a microwave horn, which is located on the inside wall of the tokamak and connected to a receiver. The power measured by this diagnostic is reduced by the plasma because of absorption at the electron cyclotron absorption layer and because of spreading caused by refraction by the plasma density gradient. We have made extensive computer calculations of these refractive effects; examples of ray tracing at three different electron densities are given in Figure 1. Coupled to these refractive ray-tracing calculations are algorithms to determine plasma absorption. We compare the results of these calculations with the experimental measurements to determine the

relative contributions of absorption and refraction and thus the transmission of the microwaves through the plasma. Figure 2 shows the experimental results of microwave transmission through the plasma (normalized) as a function of electron density. The overall trend with density is approximately what is predicted by theory and shows a "cutoff" of microwave transmission at high plasma density. We are comparing these results with our computer calculations, although measurement uncertainties during such single-pulse FEL experiments make detailed comparisons difficult. Most important, however, these results show no indication of nonlinear effects (e.g., very high transmission with no absorption) at this ~100-MW power level.

To prepare for future high-average-power experiments with multiple FEL pulses (i.e., several hundred pulses with an average power of 1–2 MW), we stopped the FEL experiments in November 1989 and began to install a multi-pulsed wiggler, the Intense Microwave Prototype. We are also upgrading the ETA-II accelerator to provide more stable operation. Upon completion of these modifications, we will perform long-pulse heating experiments with the FEL (a ~10-ms, 5-kHz stream of pulses at an eventual average power of 1–2 MW). In the interim, we are installing an experimental, fixed-frequency, 140-GHz gyrotron to heat the MTX tokamak with continuous microwaves at 0.4–1 MW. Results from these gyrotron experiments will allow us to compare electron cyclotron heating with gyrotrons and with FELs. With the multiple-pulse FEL experiments and the long-pulse gyrotron experiments, we will be able to make more quantitative

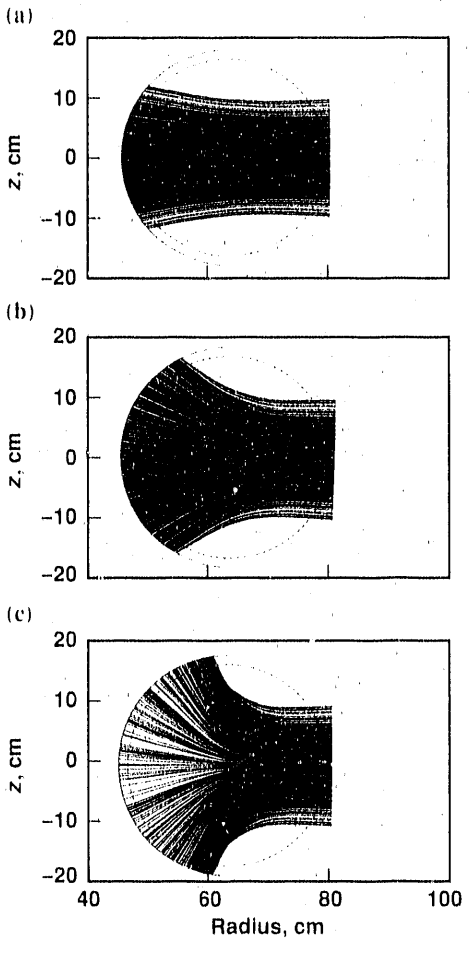


Figure 1. *Effect of plasma refraction on ray trajectories for peak densities of (a) 0.5×10^{20} m^{-3}, (b) 1.4×10^{20} m^{-3}, and (c) 2.2×10^{20} m^{-3}. The microwaves are incident on the plasma cross section (dotted circle) from the right. Note that at the highest density (c), the rays are bent significantly as they pass through the plasma.*

plasma measurements for comparison with theory than we could with the single-pulse FEL experiments discussed above.

We are also developing novel plasma and microwave diagnostics, particularly to obtain information about the input microwave-mode pattern, microwave absorption in the plasma, and electron energy

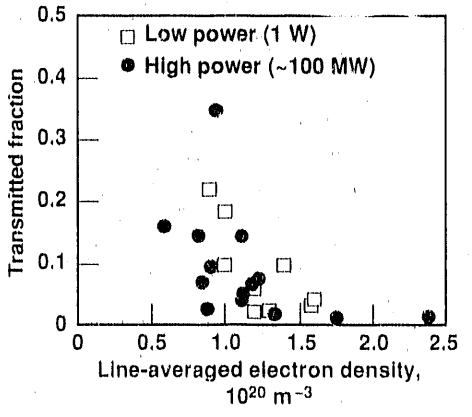


Figure 2. *Experiment measurements of the fraction of 140-GHz power transmitted through the MTX plasma as a function of electron density. The trend with density and the "cutoff" of microwave transmission at high plasma density is approximately what is predicted by theory.*

distribution. We recently installed a multichannel calorimeter to measure microwave transmission through the plasma as a function of position. A collaborative effort with the Japan Atomic Energy Research Institute (JAERI) has produced several new diagnostics, including a fast x-ray detector system, a fast neutron system, and a special microwave diagnostic station. Other diagnostics under construction include a diagnostic system to measure the electric field of the FEL in the plasma (another JAERI collaboration), fast measurements of the electron cyclotron emission of the plasma (a University of Maryland collaboration), polarimetry to measure the plasma current profile, and microwave reflectometry to measure pressure fluctuations.

Contact: B. Hooper (415) 423-1409 or S. Allen (415) 423-2676.

The International Thermonuclear Experimental Reactor

We are coordinating the overall U.S. technical effort to design the international thermonuclear experimental reactor and providing direct support in three key areas: systems and operational analysis, magnetics, and current drive and heating.

An LLNL team is coordinating an international collaboration including the United States, the Soviet Union, Japan, and the European Community to design the world's first experimental fusion reactor. The conceptual design of the International Thermonuclear Experimental Reactor (ITER), now in its third year, will be completed on schedule at the end of 1990 under the auspices of the International Atomic Energy Agency (IAEA).

ITER represents the largest worldwide fusion collaboration ever attempted, comprising about 400 person-years of design effort and about $100 million in validating research and development (R&D) work. Scientists and engineers from each of the participating parties are working together as a unified design team at the Max Planck Institut für Plasmaphysik in West Germany.

Design Philosophy

ITER is being designed as a tokamak device to demonstrate the scientific and technological feasibility of fusion power by confirming the physics necessary for a fusion demonstration reactor and by addressing the technologies essential to such a reactor. The device shown in Figure 1 represents the heart of the ITER facility; its principal parameters are listed in Table 1.

Table 1. **Principal parameters of the ITER tokamak.**

Plasma major radius (R), m	6.0
Plasma half-width at midplane, (α), m	2.15
Elongation, 95% flux surface	1.98
Toroidal field on axis (β_0), T	4.85
Nominal maximum plasma current (I_p), MA	22
Nominal fusion power (P_f), MW	1000

The ITER conceptual design is based on scientific knowledge, extrapolations derived from tokamak operations over the past decade, and the technical know-how that flows from the extensive R&D programs of the participating parties. The ITER design policy has been to (1) proceed on the basis of performance reached in the present generation of tokamaks, (2) provide the maximum machine performance consistent with prudent engineering practices and reasonable costs, (3) build in as much experimental and operational flexibility as practical in a machine of ITER's size, and (4) implement physics and technology R&D plans, using existing facilities, to validate the ITER design concept.

LLNL Contributions to ITER

LLNL is responsible for coordinating the U.S. technical activities, including all of the ITER-related R&D activities within the United States—at ten U.S. national laboratories, eight universities, and seven companies. LLNL is contributing 5 of the 11 full-time U.S. team members in Germany, including the U.S. managing director; we are also providing direct support to ITER through R&D in several key areas. A five-year engineering design phase is the next logical step.

In addition to managing the overall U.S. technical effort, we are providing direct support in three key areas: (1) systems and operational analysis, (2) magnetics, and (3) current drive and heating (CD&H). We are also providing information in divertor physics and developing new technologies that may be used for disruption control and fueling. In some cases, we are collaborating with other ITER participants.

In systems and operational analysis, we have been using the tokamak systems code to define ITER parameters and study possible parameter variations. We helped identify an optimum set of machine parameters for the conceptual design, and we have investigated operational scenarios.

In magnetics, we have provided free-boundary magnetohydrodynamic (MHD) equilibrium calculations to support the poloidal field (PF) magnet design. We have helped identify the optimal locations for the PF coils to meet engineering constraints while minimizing the stored magnetic energy and maximizing the volt-second capability of the PF system and control over the plasma configuration. We are currently examining ITER operation with a single PF null and divertor, investigating operating scenarios, and developing a design code for the vertical control system.

We are also developing high-field, radiation-tolerant magnet designs.

Much of the data for magnet component development comes from LLNL's high-field test facility. We are obtaining valuable engineering data on high-field (15-T), force-cooled magnets at ITER-relevant operating conditions from the design, construction, and operation of the conductor-performance-qualification coil and the proof-of-principle coil. The fusion engineering international experiment magnet facility being completed at LLNL will allow testing of ITER conductor alternatives at full design current and field.

In CD&H, we are performing the modeling effort required to define the physics requirements and support the engineering design for an ambitious CD&H system, including neutral-beam, lower-hybrid, and bootstrap currents. This baseline CD&H scenario is designed to provide full steady-state operation at low plasma density and will work with the PF system to provide long-pulse operation and control over the plasma current profile. We are coordinating efforts to design the neutral-beam system.

The electron-cyclotron part of the CD&H concept, which is important for start-up and disruption control, has been designed to allow real-time adjustment of the launch angle of the electron-cyclotron waves. We are developing disruption-control scenarios using this capability. LLNL's microwave tokamak experiment, in which an induction linear accelerator drives a free-electron laser, is demonstrating an alternative source for the ITER electron-cyclotron system.

A key physics issue for disruption control is the feasibility of using a localized electron-cyclotron current drive. We are performing electron-cyclotron experiments on the DIII-D tokamak at San Diego as part of our collaboration with General Atomics.

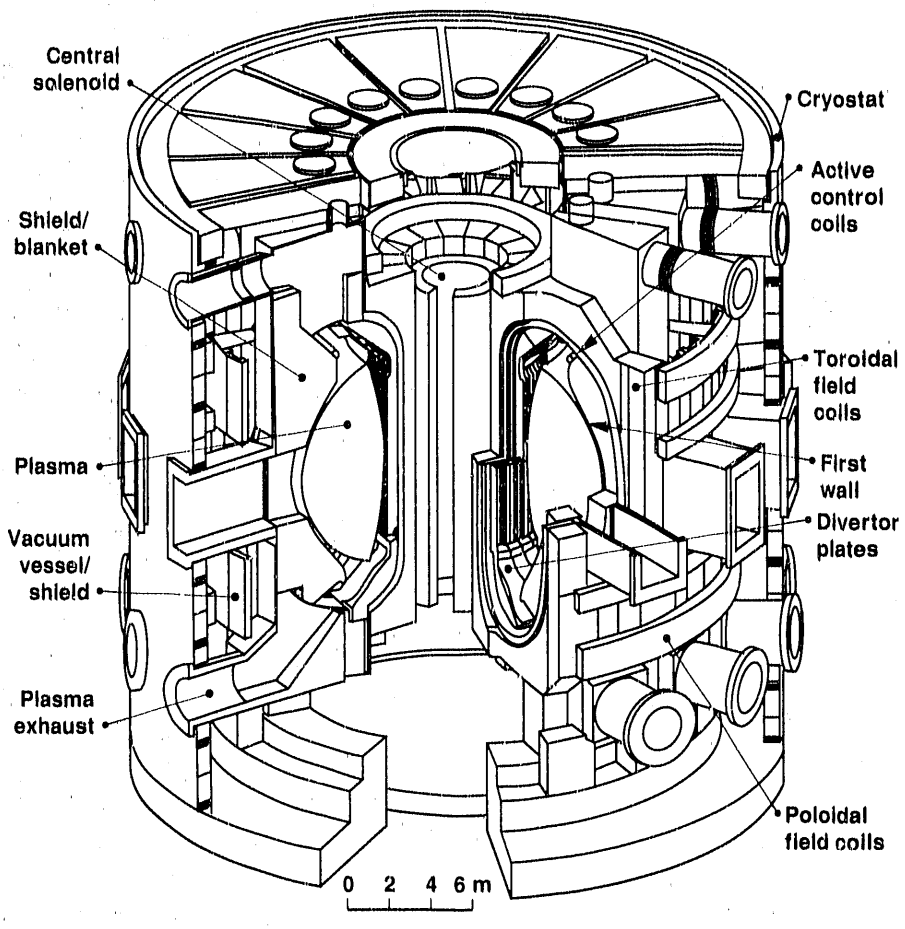


Figure 1. *Basic elements of the ITER tokamak.*

Another key physics issue is the behavior of the scrape-off-layer (SOL) and the power loading on the divertor plates. We are addressing this issue on the DIII-D, on which new divertor diagnostics have been installed. This year an advanced divertor will be installed on the DIII-D to investigate the effects of currents and poloidal electric fields in the SOL, pumping at the divertor plates, and the relative merits of an open vs a more closed divertor geometry.

A final issue is central fueling. In the ring accelerator experiment, we are developing the technology required to form and accelerate the high-field, high-density plasma rings that theoretical calculations say will be required for fueling the ITER.

Contact: C. D. Henning (415) 422-0235.

Free-Electron Lasers

This past year, we conducted two record-setting free-electron laser (FEL) experiments in which the wavelengths of the radiation produced (10.6 μm and 2 mm) differed by more than two orders of magnitude, thus demonstrating our understanding of FEL physics in two distinct physical regimes.

The free-electron laser or FEL (see Figure 1) is a source of coherent radiation in which kinetic energy from a relativistic electron beam is transferred to an electromagnetic (EM) field.[1] The electron beam is coupled to the radiation in a device called a wiggler, which creates a periodic magnetic field that is oriented perpendicular (transverse) to the motion of the electron beam. This magnetic field gives the electrons a periodic, transverse momentum aligned with the electric field of the radiation. If the proper phase in maintained between the electron beam and the radiation, the beam bunches and radiates coherently. The energy lost by the electron beam is converted directly into EM radiation. The wavelength of this radiation depends on several parameters, the most important of which is the kinetic energy of the electrons. By varying the electron energy, we can produce radiation of wavelength ranging from microwaves to perhaps x rays.

As the electrons lose energy in the wiggler, however, a condition called saturation is reached. At saturation, the electrons can no longer remain in phase with the EM radiation, and no more energy can be extracted from the beam unless the configuration of the wiggler is modified. In our wigglers, we accomplish this modification by gradually decreasing the magnetic field or "tapering" the wiggler. (It is possible, in theory, to accomplish this tapering by changing the spacing of the magnets in the wiggler, but this is much more difficult to achieve experimentally.)

The two record-setting FEL experiments conducted this past year are significant because they demonstrate our understanding of FEL physics in two distinct physical regimes, as the wavelengths of the radiation produced in the experiments differed by more than two orders of magnitude. In the first, we used a 10.6-μm input signal and tapered the wiggler to increase the energy extracted from the electron beam. In the second, we produced 2-mm radiation to heat a magnetically confined plasma.

For the 10.6-μm Paladin experiment, we used an electron beam produced by the Advanced Test Accelerator (ATA) at LLNL's Site 300. In previous experiments, we had concentrated on optimizing the exponential gain (the regime before saturation); we found that the FEL saturated at a level of 20–50 MW, depending on the input power from the master oscillator. This year, we carried out an experiment in which we injected a high-power signal (400 MW) from a carbon dioxide laser into the wiggler. This power (considerably higher than the saturated power level) caused the electron beam to bunch much more rapidly and allowed us to investigate the effects of tapering the wiggler. Using a 500-A, 46-MeV electron beam and a 17% linear taper on the wiggler, we amplified the 400-MW input signal to 610 MW, which corresponds to extracting 0.93% of the electron-beam energy as radiation.

In Figure 2, we compare the unperturbed electron-beam energy

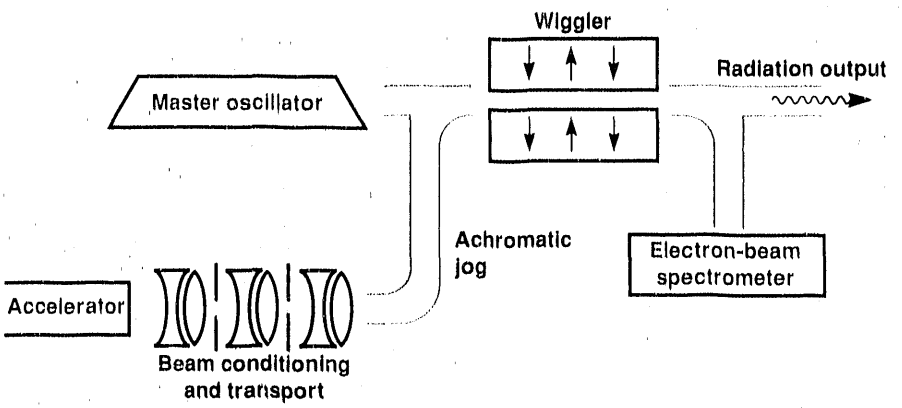


Figure 1. *Schematic diagram of a free-electron laser (FEL). An electron beam is accelerated and passed through a filter to remove electrons with excess random transverse motion. It is then transported to a parallel offset beamline by a series of dipole magnets (an achromatic jog). By offsetting the beam, we can match the input signal with the electron beam as it enters the wiggler. After the electrons exit the wiggler, they are swept out of the beamline by a dipole magnet; we measure their remaining energy with a spectrometer. The electromagnetic radiation generated by the FEL is transported to a diagnostic area where we measure power, energy, and mode profile.*

distribution (i.e., with no input signal from the master oscillator) with the electron-beam energy distribution with a 400-MW input signal. Figure 2b shows the effect of the FEL interaction, as the electrons have lost energy to the EM radiation. The net change in electron energy is 0.9%, in very good agreement with the optical-power measurement of 0.93%. Although this extraction efficiency was less than we had hoped for, it is, to the best of our knowledge, the highest efficiency ever achieved in the optical regime. In this experiment, the electron beam had considerable random transverse motion, which limited the wiggler performance and degraded the efficiency of the FEL. We expect that once this problem is overcome, we will be able to achieve even higher extraction efficiencies.

Our second FEL experiment was conducted at the Electron Laser Facility (ELF-II). This FEL used the 6-MeV electron beam produced by the Experimental Test Accelerator (ETA-II) and operated at approximately 140 GHz (at a 2-mm wavelength). The ELF-II demonstrated an overall gain of 70 dB, or about a 10-million-times amplification of the master oscillator; it produced a 10-ns microwave pulse every 2 s. With a 20-W input signal, the FEL saturated at 200 MW at a distance about 3.5 m into the wiggler (see Figure 3). This power level exceeded our 1987 record accomplishment (also at 140 GHz) by a factor of two. We propagated this FEL-produced radiation into a magnetically confined plasma in the Microwave Tokamak Experiment (see the article on p. 44).

Continued extraction of energy from the electron beam into the radiation field will require that we be able to taper the wiggler beyond saturation. In addition, to produce significant plasma heating, we must increase both the microwave pulse length and the pulse repetition frequency. Pulse length is currently limited by the time-dependent energy variation of the electron beam. Upgrades now in progress to ETA-II should greatly reduce this energy spread and allow us to produce pulses up to 30 ns long. A different wiggler magnet will be required to increase the pulse repetition frequency. At present, ELF-II uses a 4-m-long, pulsed electromagnet to provide the wiggler field; this magnet can operate no faster than one pulse every 2 s (otherwise, the magnet coils become too hot). We have a 5.5-m-long wiggler that we may be able to modify for future experiments.

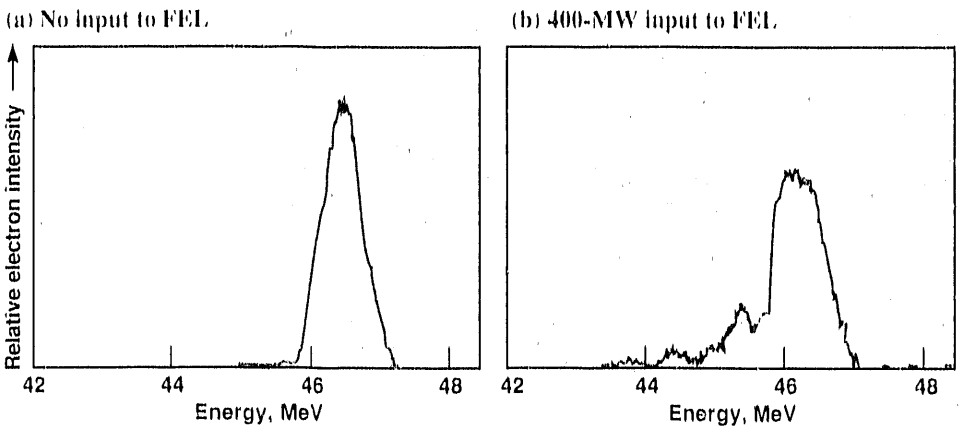


Figure 2. *Energy distribution of the electron beam in the Paladin experiment as measured by a spectrometer at the end of the wiggler (the resolution of this spectrometer was 0.2%): (a) the unperturbed electron distribution, and (b) with a 400-MW input signal to the FEL and a 17% linear taper of the wiggler. The net change in electron energy resulting from the FEL interaction as determined from these distributions is 0.9%, in excellent agreement with the optical-power measurement of 0.93%.*

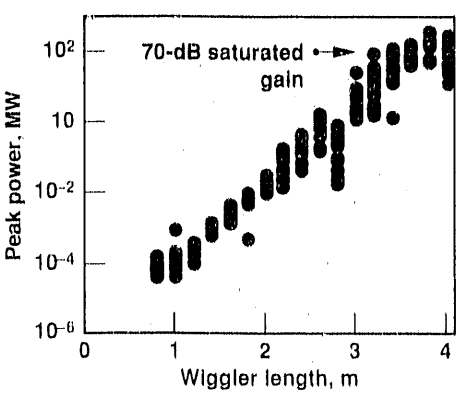


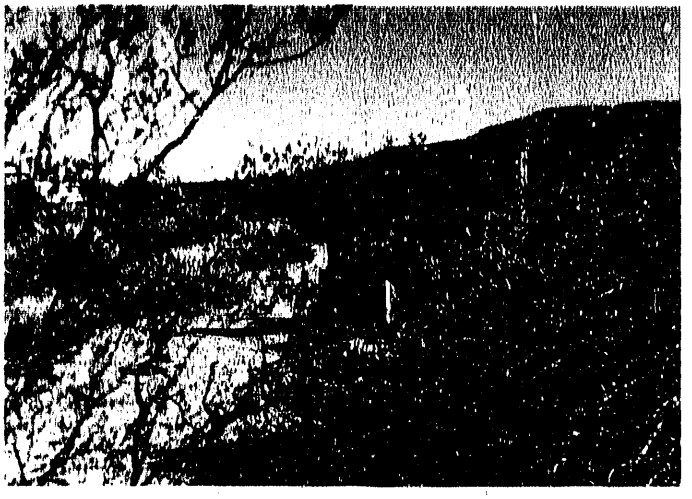
Figure 3. *Signal growth of 140-GW radiation in the ELF-II experiment. The FEL was saturated; that is no more energy could be extracted from the electron beam beyond a distance of about 3.5 m into the wiggler. The output power of 200 GW is twice as high as our previous record (set in 1987).*

Reference

1. For an overview of the physics of FELs and a review of previous Laboratory FEL accomplishments, see the December 1986 issue of *Energy and Technology Review* (UCRL-52000-86-12) as well as short articles in last year's July-August State-of-the-Laboratory issue of *Energy and Technology Review* (UCRL-52000-89-7/8), pp. 44-51.

Contact: T. J. Orzechowski (415) 422-6709 or M. K. Sheaffer (415) 422-6292.

Energy and Earth Sciences



A Laboratory scientist is measuring the force of gravity near the BREN tower at the Nevada Test Site as part of a test of Newton's inverse-square law of gravity.

The Energy Program oversees all nonfusion energy research at the Laboratory. Although the Program's emphasis has changed over the years, its mission has remained the same—to carry out research in a broad range of technical areas to help ensure that the nation will have adequate energy supplies at competitive cost in the future. The Energy Program draws its personnel from several departments, depending on the skills required. About half come from the Earth Sciences Department, which reports to the Energy Program Office while it also supports the Treaty Verification, Nuclear Test Containment, and Shock Physics portions of the Laboratory's Defense Program.

Targets for energy research are those promising technologies that are as yet unproven and have been avoided by the private sector because of the long lead time from the research effort to the entrance of the product or technology into the marketplace. Increasingly, environmental issues influence the directions taken by the Energy Program because they ultimately affect the cost of the product energy. This year, in addition to our continuing research in fossil, nuclear, and renewable energy, we began a concerted effort in advanced research for hazardous waste management and minimization.

Nuclear Energy

The Nuclear Waste Management Program is the Laboratory's largest nonfusion energy project. Its current major activity, begun in 1977, is the design and evaluation of a waste package for encapsulating high-level nuclear waste for permanent geologic storage in the repository proposed for Yucca Mountain, Nevada. Prototype engineering tests have been conducted at the Nevada Test Site. Predicting the performance of these repositories for their 10,000-year lifetimes requires a detailed understanding of the chemical and physical interactions of the container with the surrounding rock and water. We are using the computer codes EQ3NR and EQ6 to investigate the complex interplay among the processes that control these interactions.

Fossil Energy

Our largest fossil energy project deals with aboveground retorting of oil shale. We also have smaller projects related to conventional petroleum and the production of liquid fuels from methane and coal. For example, we are making progress in understanding the structure and function of natural enzymes associated with selected bacteria that can convert methane to methanol. We have gained valuable design information for mild-coal gasification from the operation of a small-diameter, 1-m-long screw pyrolyzer over a wide range of conditions.

Our understanding of how kerogen is converted to shale oil in a retort has proven to be useful in understanding how conventional petroleum (oil and gas) is generated in nature. During the past year, we demonstrated that chemical kinetics derived from laboratory experiments can indeed predict the time and temperature at which oil was

generated in the Maracaibo basin in Venezuela, one of the world's most prolific petroleum basins.

Understanding the flow properties of granular solids has broad applications ranging from soil mechanics to industrial process design and control. Our two-dimensional particle model has been valuable for designing our oil shale process. We recently extended our granular flow modeling to three dimensions for inelastic, frictional spheres in rapid shearing flows and in gravity-driven flows, and we are presently testing the predictions of this model against laboratory data.

To develop tools for monitoring the propagation of a steam front during enhanced oil recovery operations, we are using cross-borehole, audio-frequency, electromagnetic (EM) techniques to provide an image of the front. This year we conducted a successful field test at the South Belridge oil field, in California, in which we were able to monitor the encroaching steam front after successfully collecting the EM data through the steel well-casing.

Conservation and Renewable Energy

Our principal effort in promoting conservation—minimizing fuel use through improved efficiencies—has been in understanding combustion phenomena, such as knock (premature ignition) in internal combustion engines. Through chemical kinetic modeling, we have shown that the size of the hydrocarbon molecule and the types of carbon-hydrogen bonds in it play interrelated roles in the overall reaction in the fuel chamber.

Our geothermal project is designed to provide information that will ultimately reduce the cost of operation of a field. We are developing and demonstrating geophysical techniques such as seismic imaging to monitor subsurface processes. We completed the analysis of data from a network of three-component seismic stations in a 64-km^2 area within the Salton Sea geothermal field, in California; we found that there is an interlinked set of seismic zones that may act as major fluid pathways. We have since moved the network to the East Mesa geothermal field, also in California, and are collecting data at this new location.

Hazardous Waste and Environmental Restoration

We are taking an interdisciplinary approach to identify innovative ways to reduce waste in DOE process streams and to characterize and remediate DOE sites contaminated with hazardous waste. For example, fiber-optic chemical sensors have been developed for characterizing waste steams. We are also demonstrating waste cleanup technologies for volatile organic compounds at the DOE Savannah River site and at LLNL, and we are developing such cost-saving approaches to cleanup as *in situ* microbial filters.

We are also improving our ability to simulate the transport of contaminants in complex geological environments. This year, we developed a theory that describes contaminant infiltration in partially saturated, fractured porous media. We also implemented several reactive-transport computer codes and began the development of a particle-based simulator for reactive-transport problems in porous media.

Earth Sciences

The Earth Sciences Department has an active basic research program funded by the DOE's Office of Basic Energy Sciences and the Laboratory's Institutional Research and Development Program. In a joint project with the Physics Department, we are testing Newton's law of gravity by searching for deviations from it. As a part of the National Continental Scientific Drilling Program, we started field investigations at Katmai, Alaska—site of the largest rhyolitic eruption in 20 centuries. We also completed an important laboratory project, in which we constructed a large-volume split-cone apparatus that can reach pressures of 25 GPa (~25,000 atm) and temperatures of 2000°C; with this unique device, we will be able to experimentally assess conditions of pressure and temperature that are thought to exist in the earth's lower mantle (at depths greater than 600 km).

Our basic research program has been greatly enhanced by the rapid development of the Center for Geosciences in the Institute for Geophysics and Planetary Physics. The Center promotes collaboration between scientists at LLNL and at University of California campuses. Between 10 and 15 projects have been supported in recent years.

Support from the Defense Program represents about 35% of the Earth Science Department's activities. This past year, we provided support to the U.S. team negotiating the Threshold Test Ban Treaty protocol. For this, we drew on our expertise in nuclear testing and seismic and hydrodynamic monitoring to assess monitoring options and examine both the U.S. and Soviet positions. We also are conducting longer-range research related to monitoring possible future test-limitation treaties. This work requires an understanding of the interaction of nuclear explosions with geological materials, and much of what we know has been learned from computer simulations. This year, we successfully adapted DYNA2D, a state-of-the-art hydrodynamics code, so that it can handle all our nuclear-test containment and treaty-verification calculations. With this code we can now address emplacement conditions involving very complex geological characteristics.

Contact: R. N. Schock (415) 422-6477 or L. W. Younker (415) 422-0720.

Prototype Heater Test of the Environment around a Simulated Nuclear-Waste Package

We are evaluating the Yucca Mountain region as a possible site for a high-level nuclear-waste repository. Our testing and analyses of unsaturated fractured porous rock over the temperature range of interest are largely unprecedented.

Yucca Mountain, near the Nevada Test Site (NTS), is being considered as a potential site for the nation's first high-level nuclear-waste repository. In this project, LLNL is responsible for designing the waste package and for evaluating its performance and the geologic environment that will interact with it. Yucca Mountain is in an arid climate, and the proposed emplacement site is composed of fractured, porous, welded tuff. This year, to prepare for a series of field tests there, we performed the Prototype Engineered Barrier System Field Test. A principal objective of this test was to investigate the physical processes that should be incorporated into numerical models used to describe the hydrology and geochemistry in welded tuff.

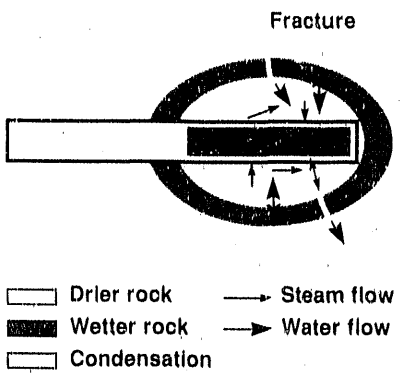


Figure 1. *Vertical cross section of a probable hydrologic scenario in partly saturated, welded tuff subjected to heating.*

A 3-m-long heater was placed in a borehole at the NTS to simulate the thermal effects of a spent-fuel package. During an accelerated heating test, we examined how the heating and cooling phases affected the rock mass surrounding the waste package over time. In the heating cycle, the region of boiling within the formation extended 0.6–0.7 m radially from the heater borehole wall, and the heating affected a volume of rock large enough to include several fractures. In the cooling cycle, we gradually decreased the heater power from 3 kW (the maximum power used) to zero. We measured such environmental parameters as rock moisture content, rock temperature, gas and liquid pressures, and rock permeability.

Many environmental conditions developed as expected (Figure 1). A dry zone developed around the heater borehole, and the degree of drying increased with proximity to the heater. A "halo" of increased moisture developed next to the dry region and migrated away from the heater when rock temperatures increased. Fractures near the heater borehole allowed hot, dry conditions to penetrate deeper into the rock mass, and pore gas pressure increased in regions where evaporation was vigorous. As we gradually reduced the heater power, the dry region around the heater cooled and slowly regained water.

Rewetting occurred fastest in rock above the heater and adjacent to fractures. In fact, fractures may accelerate rewetting. They may provide flow paths for humid air to contact the dry region so that capillary condensation occurs along the fracture face. They may also allow diffusion of the air humidity from the humid regions to the dry regions, and they may provide flow paths for water draining from the condensation region above the heater.

Before heating, our measurements along the heater borehole showed that the fracture system exhibits a strong heterogeneity in fracture permeability. After the heater was turned off, we found a measurable increase in air permeability for the rock that reached the hottest temperatures.

This test was a success in that the expected experimental conditions developed around the heater in the tuff. The test also showed which measurement techniques were effective under realistic environmental conditions and which ones might benefit from modification.

References

1. A. L. Ramirez et al., *Prototype Heater Test of the Environment around a Simulated Waste Package*, Lawrence Livermore National Laboratory Rept. UCRL-101693 (1989).
2. J. Yow, Jr., *Concept for Waste Package Environment Tests in the Yucca Mountain Exploratory Shaft*, Lawrence Livermore National Laboratory Rept. UCID-20450 (1985).

Contact: A. L. Ramirez (415) 422-6909.

Modeling Radionuclide Release from Nuclear Wastes

We have demonstrated that geochemical models successfully simulate important aspects of nuclear waste dissolution in fluids. We are using these models to evaluate the performance of proposed nuclear-waste repositories in various geologic environments over thousands of years.

Various long-term methods are being considered to dispose of nuclear wastes safely. One method is to use geologic repositories to isolate nuclear wastes from the environment. However, to meet the licensing requirements of the Nuclear Regulatory Commission, we must be able to predict how the repository components and the enclosing host rocks and fluids will be affected by temperature fluctuations, fluid flow, and other factors for up to 10,000 years. Therefore, we must estimate the rate at which radionuclides will be released from degrading nuclear wastes, how the composition of a fluid will change when it contacts different waste forms, and whether the precipitation of solid phases may limit the release of radionuclides into the environment. At LLNL, we are using the geochemical modeling codes EQ3 and EQ6 to simulate the interactions of nuclear wastes and fluids over thousands of years. Potential waste forms include glass and spent reactor fuel.

By integrating experimental programs with geochemical modeling of the dissolution process, we have developed process-oriented models of the kinetics of glass waste dissolution. Analytical studies of reacted glass surfaces revealed that residual gel layers and secondary precipitates are formed during the leaching of glass (Figure 1). Kinetic models suggest that the extent of disequilibrium between the gel layer and the adjacent fluid controls the rate at which glass dissolves. Also, the concentrations of elements in solution are controlled by secondary phases, such as clays and oxides, that precipitate on the glass surface.

We are using EQ3/6 simulations of spent reactor fuel dissolving in groundwater to identify the physical and chemical controls of radionuclide concentrations in solution. Figure 2 shows our results for uranium. Concentrations of uranium in solution are controlled by the uranium-bearing precipitate; the composition of the precipitate is determined by the availability of silicon in solution. If an adequate supply of silicon is available (e.g., as in a siliceous volcanic tuff repository), uranium silicates will precipitate, thus minimizing uranium concentrations in solution.

We will continue to refine these models to improve our predictions of the rates of nuclear waste dissolution and the controls of radionuclide concentrations in fluids. This will improve our ability to determine the long-term viability of isolating nuclear wastes in a geologic repository.

Contact: C. J. Bruton (415) 423-1936 or W. L. Bourcier (415) 423-3745.

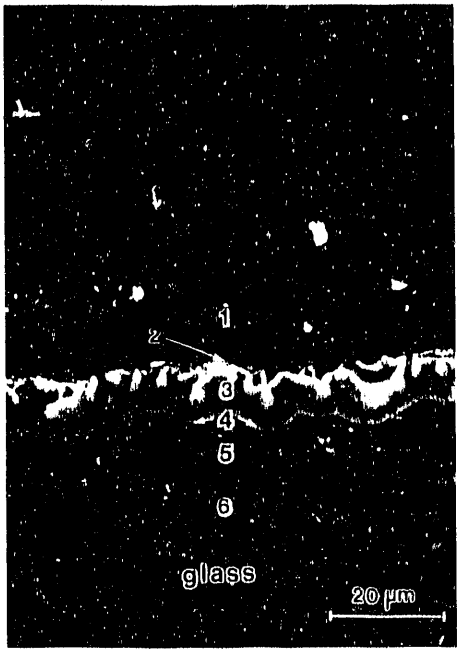


Figure 1. *Glass alteration layers that control solution composition during 90°C leaching of nuclear waste glass. Layers 1–5: permeable smectite, serpentine, and manganese oxide secondary phases. Layer 6: hydrous gel layer.*

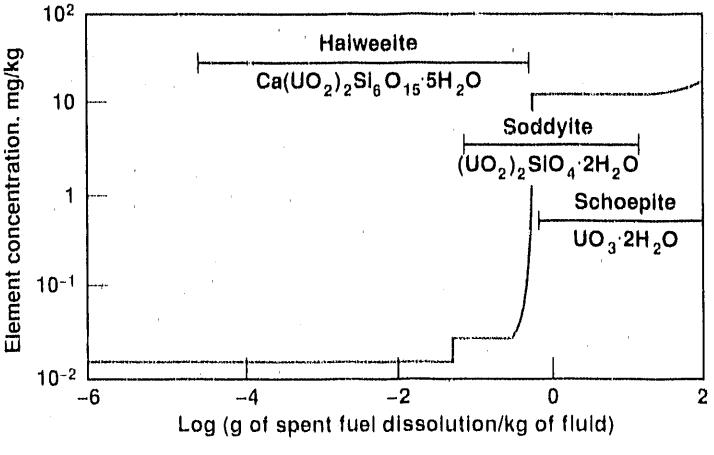


Figure 2. *Predicted stability ranges (horizontal bars) of uranium precipitates and corresponding changes in uranium concentration in solution (curve) during spent-fuel dissolution. Precipitation of uranium silicates minimizes uranium concentrations in solution.*

Hot-Recycled-Solid Retort for Oil Shale Processing

We have constructed a 4-tonne/day hot-recycled-solid retort for processing oil shale under rapid heating conditions in a continuous solid-recirculation loop. Operation of the retort will contribute to our understanding of pyrolysis and combustion chemistry, permit us to measure variations in oil properties with process conditions, and allow us to begin answering questions about handling bulk solids for a commercially sized plant.

We are studying aboveground oil shale retorting and have developed the LLNL hot-recycled-solid (HRS) process as a generic, second-generation, rapid pyrolysis retorting system in which recycled oil shale is the solid heat carrier. Last year, we upgraded our laboratory pilot plant to process 4 tonne/day of commercially sized shale. This will allow us, for the first time, to study pyrolysis and combustion chemistry using the full particle size and to produce enough oil for detailed characterization studies. Our previous 1985 experiments, which used a 1-tonne/day retort, produced oils with better stability and lower viscosity than previously thought possible. If we can reliably obtain oil of this quality as we scale up the process, we may be able to avoid expensive on-site hydrotreating of the oil and, thus, significantly reduce the overall cost of producing shale oil. Using our 4-tonne/day facility, we will continue our investigation of oil quality versus retorting conditions to determine performance at larger scales.

Unlike most chemical and petroleum processes, oil shale processes require the handling of large volumes of solids. Understanding the unit operations of key process components and their interaction is a major focus of our current research. Since the solid and gas retention times in our pilot retort are comparable to those in larger units, we can use this pilot plant to begin answering the many questions we have about handling bulk solids for a commercially sized plant. We envision three stages of operation prior to commercial demonstration.

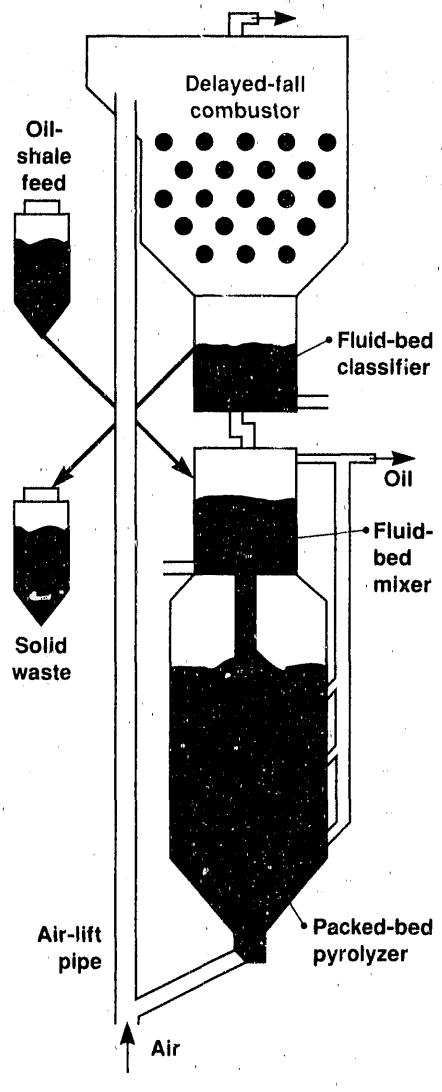


Figure 1. *Hot-recycled-solid retort. Raw and recycled shale are mixed in the fluid-bed mixer and sent to the packed-bed pyrolyzer for oil generation. The shale is then lifted pneumatically to the delayed-fall combustor, where residual carbon is burned to provide the process heat. Solid waste is discharged from the fluid-bed classifier.*

The first stage is our laboratory 4-tonne/day pilot plant (Figure 1). The major components include a fluid-bed mixer, to mix the raw and recycled shale, and a packed-bed pyrolyzer. The mixed shale is pyrolyzed for 3 min to generate oil. Shale leaving the packed bed is lifted to a delayed-fall combustor, where residual carbon is burned to provide the process heat. Solid waste is discharged from a fluid-bed classifier, which also serves as a pressure block that separates the reducing and oxidizing atmospheres. The whole oil is then condensed for subsequent analysis and characterization.

The second stage of the pilot program will be a 100-tonne/day HRS retort. This small-scale plant can be built at an industry-owned site in western Colorado at a capital cost of less than $18 million and can be in operation by 1994. At the third stage, a consortium of government and private industry could construct and operate a 1000-tonne/day pilot plant before the end of the century. Completion of the field program in 8 to 10 years would provide private industry with the technical knowledge to build a commercially sized, 12,000-tonne/day demonstration plant shortly after the end of the decade.

Contact: R. J. Cena (415) 422-7336.

Environmental Restoration and Waste Management

We have established an interdisciplinary program to evaluate hazardous waste problems at DOE installations and to develop the technologies to clean up these sites and manage their wastes. One method we are developing uses* in situ *microbial filters, which transform toxic organic compounds to nontoxic substances.

The Laboratory's interdisciplinary research and development program for environmental restoration and waste management was established in 1989 to improve methods for characterizing contaminated sites and remediating problem areas. We are also searching for ways to better manage the radioactive, hazardous, and mixed wastes that are produced and, where possible, to reduce waste accumulations. The program involves specialists from Biomedical and Environmental Sciences, Chemistry and Materials Sciences, Earth Sciences, Energy, Engineering, Environmental Protection, Hazards Control, Lasers, and Nuclear Chemistry. As part of this program, we are working with other DOE laboratories to develop integrated demonstration projects to test selected waste clean-up technologies. We also are working to establish a university consortium in the western U.S. to improve public education and research in these areas.

At many DOE sites, the subsurface is contaminated with hazardous or toxic organic compounds. At present, these compounds must be pumped to the surface to be treated. This process is slow and expensive, and often it is not very effective because it does not address directly the slow release of sorbed contaminants over time. However, we found that many toxic compounds can be transformed to nontoxic substances by *in situ* microorganisms. Although this process is slow, it can be much cheaper than the pump-and-treat remediation method. Also, bioremediation is better for the environment and human health because it treats the contamination directly rather than transferring it to an intermediate medium, such as activated charcoal, that requires its own separate stage of treatment.

To better understand how the microbial process operates and how we can best apply it, we developed a microbial filter project. Using LLNL expertise in biocatalysis, microbial ecology, aqueous geochemistry, and subsurface flow and transport, we prepared a systematic approach for treating chlorinated aliphatic compounds that are ubiquitous contaminants at DOE sites. First, we isolate indigenous bacteria and perform laboratory studies to determine metabolic pathways and optimal nutrient packages. We also study the aqueous geochemistry to evaluate the interaction of organic and inorganic compounds in the subsurface and to determine changes in solution chemistry caused by the hazardous waste and by the biotransformation process. Then with mathematical modeling, we integrate the transport, sorption, and biological processes to determine an optimum strategy for microbial remediation of the contamination. To validate the software package and test our approach, we will use large-scale, two-dimensional experiments that incorporate common media heterogeneities. When this stage of testing is completed, we will evaluate our method with pilot studies in the field.

Contact: J. Yow (415) 422-3521.

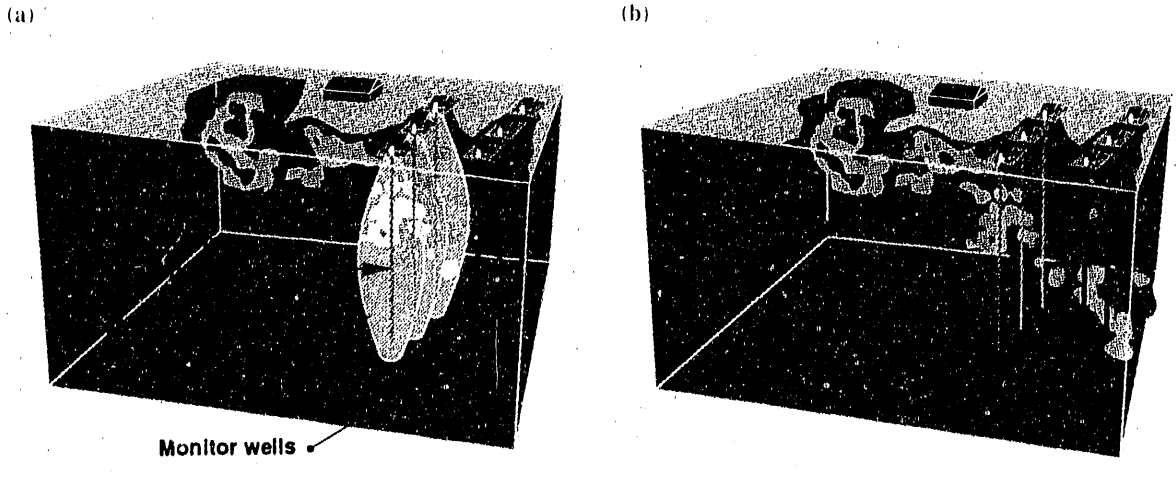


Figure 1.
(a) Microbial filter remediation process and (b) pump-and-treat method. The microbial filter treats the contamination directly rather than transferring it to an intermediate medium, such as activated charcoal, that requires another stage of treatment.

Discriminating between Nuclear Explosions and Earthquakes

We performed a detailed study to discriminate between nuclear explosions and earthquakes, using data from the Nevada Test Site. We also evaluated new pattern-recognition algorithms, such as artificial neural networks, which we would like to use to improve our ability to classify events.

One of the primary missions of the Seismic Verification Program at LLNL is to improve this nation's ability to monitor a region and verify compliance with a treaty limiting or banning nuclear tests. In our seismic research efforts, we are addressing the technical issues of detecting and locating seismic events, discriminating between earthquakes and explosions, and estimating the yield of nuclear explosions. Our emphasis is on monitoring an area to enforce provisions of a Low-Yield Threshold Test Ban Treaty or Comprehensive Test-Ban Treaty, both of which would include the use of in-country stations. Therefore, we must be able to discriminate earthquakes from underground nuclear explosions at small magnitudes (<4) and at regional distances (<2000 km).

The data set for our study consists of 233 explosions at the Nevada Test Site (NTS) and 130 earthquakes in the western U.S., all ranging from 2.5 to 6.5 in magnitude and recorded at four broadband seismic stations operated by LLNL.[1,2] The stations surround the NTS at distances between 200 and 400 km and are routinely used to obtain rapid estimates of explosion yields. Most of the discriminants that we evaluated are based on physical differences that are expected to occur between earthquakes and explosions. For example, earthquakes result from the sudden release of stored elastic energy along a fault surface. The shearing along the rupture surface releases a large amount of shear energy relative to compressional energy. Thus, on a seismic record of an earthquake, the shear phases (the S, L_g, Rayleigh, and Love waves) are expected to be larger than the compressional phases (the P and P_g waves). In contrast, a pure explosion source is a center of compression and, in theory, releases only P waves and Rayleigh waves. A typical seismogram for an explosion has much more compressional energy than the (late-arriving) shear energy.

Figure 1 compares the seismogram of an earthquake with that of an explosion. Although both events have a body-wave magnitude (m_b) of about 4.2, the surface-wave magnitude (M_s) for the earthquake is larger and occurs much later than that for the explosion. This difference is the basis of the $m_b - M_s$ discriminant: for an earthquake and explosion of similar m_b, the earthquake will generally have a greater M_s.

We evaluated 12 regional discriminants that appeared to have promising discrimination potential and found significant variability between them.[3] Figure 2 shows an example of the $m_b - M_s$ discriminant averaged for the four-station network. Some discriminants showed very good separation between the earthquakes and explosions, but we could not obtain measurements at small magnitudes. We also found that using only one discriminant to classify an event was much less accurate than combining discriminants. For events recorded at individual stations, we had a misclassification rate between 3 and 40% for the individual discriminants. However, when we averaged the results from our network of stations,

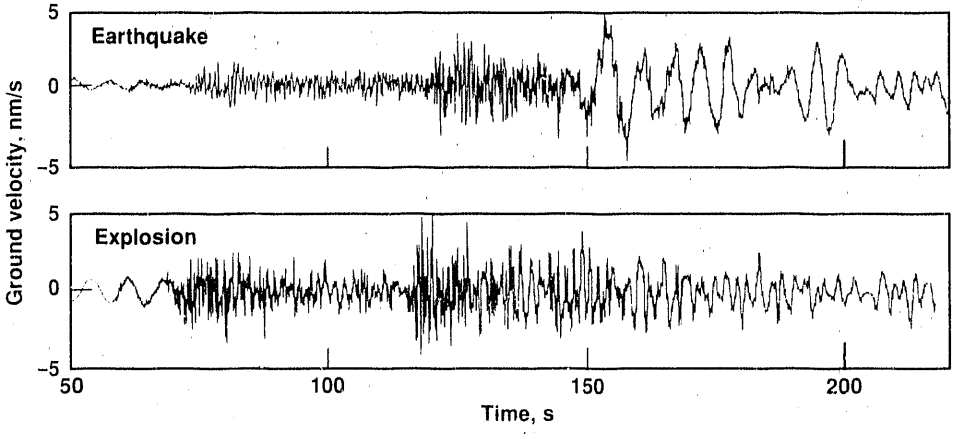


Figure 1. *Seismogram from an earthquake located near the NTS and a nuclear explosion. Both events had a body-wave magnitude of $m_b \approx 4.2$ and were recorded at the same station. The earthquake is characterized by large, late-arriving surface waves that are poorly developed for the explosion.*

the maximum misclassification rate dropped to 25%.

To reduce this rate further, we combined the discriminants using standard multivariate techniques. With this method, our misclassification rate using results from individual stations ranged from 3 to 10% for explosions and from 4 to 26% for earthquakes. When we combined the results for all four stations, the rate dropped to 0 to 2% for explosions and 3 to 4% for earthquakes. However, our misclassification rates are generally higher for $m_b < 4$ and for earthquakes rather than explosions.

We also tried to improve our misclassification rate by using improved discrimination algorithms, such as artificial neural networks (ANNs).[4] The ANNs consist of many nonlinear elements that operate in parallel and are arranged in patterns that mimic those of biological neural networks (Figure 3). Thus they are well-suited to classification problems. We tested an ANN on a set of distance-corrected P_n, P_g, and L_g spectra from 83 earthquakes that occurred in the western U.S. and 87 explosions at the NTS, both recorded at the four LLNL seismic stations. Using a majority voting scheme with the four-station seismic network, we were able to classify events correctly in more than 97% of the cases.

We found that the ANN and the multivariate discrimination method perform about the same, but the ANN has three advantages. (1) It can be adapted to fit more complex decision surfaces than the traditional techniques. (2) It provides numerical advantages for large data sets. (3) As new events are recorded and independently identified, we can input them to the ANN and update the network weights; in contrast, many difficult calculations must be performed to update a linear discrimination function.

From this evaluation of of seismic discriminants and discrimination algorithms, we have confidence that our results can be used to predict performance in treaty-verification monitoring situations.

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Contact: S. R. Taylor (415) 423-0616.

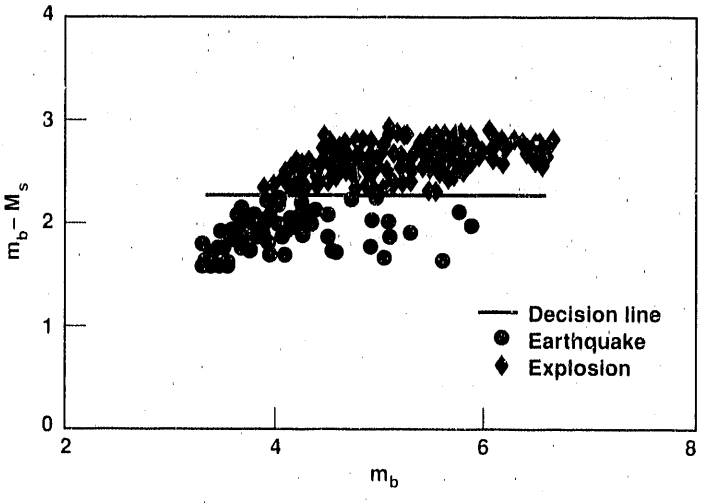


Figure 2. *Network averaged $m_b - M_s$ discriminant versus m_b, where m_b is the body-wave magnitude and M_s is the surface-wave magnitude. The decision line was calculated using a classification algorithm.*

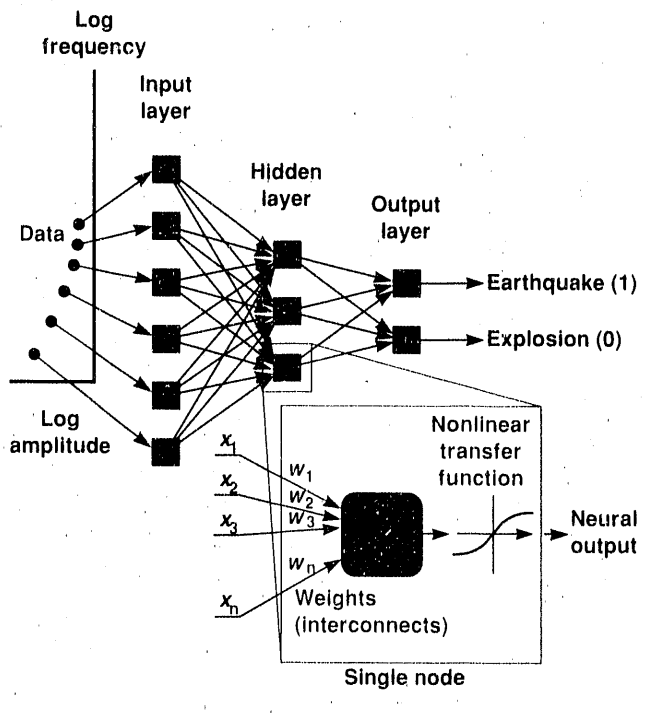


Figure 3. *Architecture of an artificial neural network. Seismic spectra are input to a three-layer network consisting of interconnected nodes. Each node weights and sums the input from each node in the overlying layer. Output is passed through a nonlinear transfer function, which simulates firing of biological synapses, and is input into each node in the next layer. The final output is a number between 0 and 1, where 0 = explosion, 1 = earthquake, and 0.5 = undecided.*

A Test of Newton's Inverse-Square Law of Gravity

We have tested Newton's law of gravitation by measuring gravity on a 465-m-high tower at the Nevada Test Site. Our measurements agree with the Newtonian extrapolation of the surface gravity field to within 1 part in 10^7. These results can be used to constrain modern theories of quantum gravity.

Gravity is the only fundamental force that we have been unable to describe quantum mechanically. Newton's inverse-square law of gravity states that all particles attract each other with a force inversely proportional to the square of their separation. This law has been tested at a laboratory scale and on a planetary scale. However, in recent studies at distances from 10 m to 10 km, evidence is given for a non-Newtonian force. These studies suggest that gravity changes with height up a tower or down a borehole in such a way that the "constant" of proportionality in the inverse-square law changes by 1% over those distances.

These results are exciting because grand unification theories suggest that undiscovered fundamental forces may break down Newton's law. According to such theories, new particles and forces must be added to the simple Newtonian prescription.

We are testing this possibility at the Nevada Test Site (NTS) using the Bare Reactor Experiment Nevada (BREN) tower. We chose this location to eliminate the limitations of previous experiments. For example, in subsurface borehole experiments, mass distributions beneath the holes may affect the results. Because the density distribution in the earth is unknown, borehole gravity is not a good way to test Newton's law. However, on a tower, a gravity survey can be conducted on the earth's surface, so knowledge of the mass distributions in the earth is not needed. Thus, in our experiment, we extrapolate ground measurements, using Newton's theory of the gravitational interaction, up to the points measured on the tower. If a discrepancy is found between the measurements and the predictions, then Newton's law fails.

A previous tower experiment suffered the effects of another limitation. In that study, the surface gravity field was not sampled adequately because the surrounding area was swampy. Our 465-m BREN tower is located in the desert, where surface gravity measurements are straightforward.

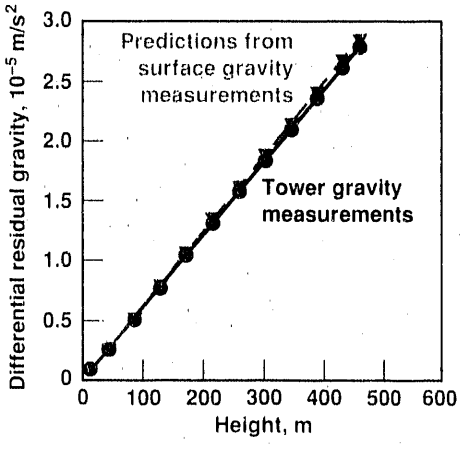


Figure 1. *Results of our first-phase experiment. The tower gravity measurements (circles) agree well with our predictions (triangles). A deviation from Newton's law of gravity would cause a discrepancy between these points and their curves.*

Our study is being conducted in two phases. In the first phase, completed this year, we designed a surface gravity survey to predict gravity measurements up the tower using the inverse-square law. We then measured gravity at 42 observation points on the tower and at 281 locations on the ground. To detect a 1% change in the constant in Newton's law, we must predict gravity at the top of the tower to 5 parts in 10^7. The first phase was designed to produce an uncertainty of 1 part in 10^7 at the top of the tower. The second phase, which is scheduled for 1990, will be a factor-of-three more accurate.

The first-phase results, with the gravity effect of an "average" earth subtracted, are shown in Figure 1. The tower gravity measurements agree well with the predictions obtained from surface gravity measurements. A deviation from Newton's law of gravity would cause a discrepancy between these points. Thus, on the basis of these results, we constrain any new forces to be less than one-fifth of the value previously reported.

Uncertainty about a fundamental physical law has provided a window to look for new phenomena that could lead to many approaches for grand unification theories. Our experiment has put tight constraints on non-Newtonian gravity effects. Thus, our certainty in the validity of Newton's law is increasing.

Contact: P. W. Kasameyer (415) 422-6487.

Numerical Simulation of Solute Transport in Porous Media

We are examining the effects of material heterogeneities on groundwater flow and transport processes as well as the chemical interactions that occur in such systems.

To analyze the movement and transformation of toxic or radioactive substances that have been released into subsurface soils and groundwaters, we are developing predictive models of the reactive and transport phenomena associated with liquid and gaseous chemicals in porous flow systems. Practical applications of this work include determining potential health risks from contaminated water wells or designing and evaluating techniques to clean groundwater environments. We report here on the application of several computational tools that may allow us to better understand several complex chemical and physical phenomena that occur in natural subsurface flow systems.

Subsurface materials can be extremely variable in terms of their type and spatial distribution. Our ability to fully characterize or simulate the detailed local hydraulic or chemical behavior in actual formations over large regions is limited. Therefore, in recent years, much research has been devoted to finding out how heterogeneities affect the movement of contaminants in the subsurface and how the more dominant transport behavior can be accurately predicted from simple, measurable medium characteristics.

We have initiated a set of computational experiments to study contaminant movements through large heterogeneous flow systems in porous media. In this approach, "synthetic" flow fields were developed corresponding to hypothetical, spatially variable hydraulic property distributions (see Figure 1). Solute transport was then simulated within these fields, followed by analyses of the ensuing hydraulic and dispersive behavior. The transport model can be applied to large, three-dimensional problems dealing with the motion of one or more dissolved chemical constituents through saturated or unsaturated groundwater systems. It is based on a random-walk particle method that can readily treat multidimensional flow and diffusive processes in a computationally efficient manner. Preliminary simulations with nonreactive tracers showed that noticeably distorted mass distributions developed (Figure 2). Quantitative measurements of plume displacements and spreading about its center of mass compared favorably with predictions of several theoretical models.

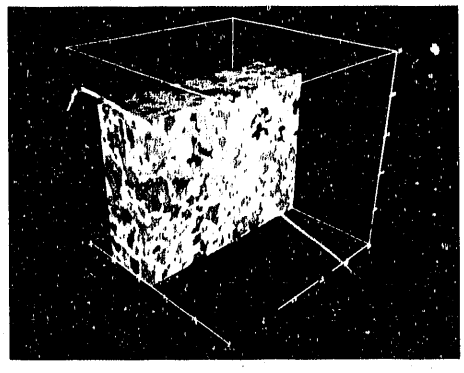
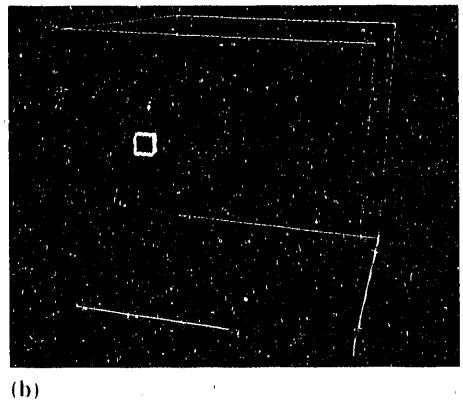


Figure 1. *Image of an artificially generated porous medium, showing highs (blue-green) and lows (yellow-red) of the hydraulic conductivity.*

(a)



(b)

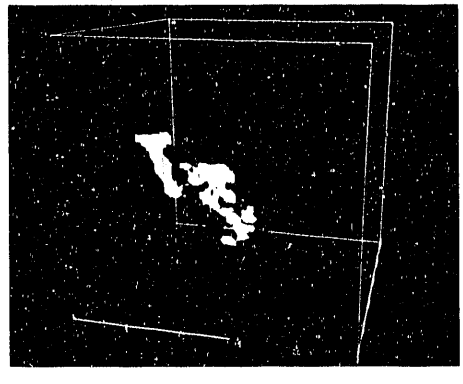


Figure 2. *Image of (a) a chemical plume at its initial location and (b) its contorted shape at a later time, showing highs (blue-green), and lows (yellow-red) in concentration.*

We are extending the capabilities of this model to treat chemical reactions that may occur among different dissolved chemical compounds or between the chemicals and the solid soil minerals. Numerical experiments may then be conducted to examine, for example, the capacity of heterogeneous soils to retard the movement of contaminants or the effectiveness of proposed in situ remediation techniques that are based on injecting bacteria or otherwise promoting bacterial growth to degrade the toxic compounds.

Contact: A. F. B. Tompson (415) 422-6348 or R. B. Knapp (415) 423-3328.

Biomedical and Environmental Science

Chromosome strands (chromatids) are being pulled apart as a cell prepares to divide. Much of our biomedical and environmental research involves work with chromosomes and the DNA they carry.

The mission of LLNL's Biomedical and Environmental Research Program is to understand the potential health and environmental consequences of the development and utilization of various energy sources. In particular, we are finding ways to identify and measure genetic damage as an indicator of human health effects. We are examining local- and global-scale environmental changes involving the atmosphere. We are also studying a variety of ecological effects resulting from energy production and usage; we are particularly concerned with groundwater as a transmission medium of ecological contaminants. We are also devising methods for making comprehensive assessments of the various risks involved.

Perhaps the most exciting area of current biological research is the human genome initiative—an international effort to characterize the genetic code of man. Many developments in science and technology have been required for this initiative in order to map, sequence, and interpret the information coded by the genome.

Just this July, the DOE named LLNL a Center for Human Genome Research. Together with the two other DOE centers, at the Los Alamos National Laboratory and at the Lawrence Berkeley Laboratory, we will participate in an international effort to construct a physical map of the DNA in all 24 human chromosomes. Such a map is expected to help identify and isolate genes involved in a multitude of human diseases with the goal of understanding the causes and finding treatments for many of them. We at LLNL have responsibility for mapping chromosome 19. This work is proceeding quite rapidly using Livermore-invented, newly automated equipment and techniques. We have been able

to order and overlap fragments for approximately 60% of this chromosome. The results are fascinating, and the medical community is already studying and applying this mapping information.

New genetic techniques are being used in many other projects as well. For example, several studies are using recombinant-DNA methods to create transgenic organisms as important new research tools. Also, we are continuing the vigorous application of DNA probes for *in situ* hybridization, including the "painting" or staining of chromosomes to greatly improve the ease and accuracy with which we can identify chromosome aberrations. We have also demonstrated the dramatically successful cloning of two human genes that are responsible for the repair of DNA damage.

We are continuing to make progress in our effort to gain a complete understanding of the biological effects of radiation on humans. In particular, we are using a novel method, combining Laboratory expertise in monoclonal antibodies with LLNL-developed high-speed cell sorting, to test human red blood cells for mutations. This work is being applied to survivors of the Hiroshima and Nagasaki atomic bombs and, more recently, to individuals exposed to radiation released in the Chernobyl nuclear reactor accident. This method shows considerable promise as a human radiation "biodosimeter." Also being carried out in connection with the A-bomb survivors is a marvelous example of Laboratory high technology being used to solve a chronic and difficult problem. The technology is accelerator mass spectrometry (AMS), the challenge is to measure specific radionuclides at extremely low concentrations, and the goal is to determine the amount of neutron activation in environmental samples from Japan. Extrapolation from the samples would give us greatly improved estimates of the corresponding neutron doses received by the A-bomb survivors.

AMS is also proving to be a very sensitive and versatile technique in other areas of biomedical and environmental research. For example, we recently described a three-order-of-magnitude improvement in the sensitivity of detection of DNA damage (adducts) using this technique.

Monoclonal antibodies continue to be of great interest to us, primarily as sophisticated and powerful reagents for biological and epidemiological studies. Antibodies from a single clone (i.e., monoclonal) can be created to target specific biological components (e.g., red blood cells carrying particular marker molecules or actively dividing breast cancer cells). We have made a concerted effort to transfer this technology to the commercial sector; a half-dozen or so LLNL-developed antibodies are now marketed as chemical or biochemical reagents. Recently, we combined our monoclonal-antibody capability with a conventional chemical-analysis method to generate new resolution and sensitivity in the analysis of toxic constituents of the human diet.

Stimulated by current DOE emphasis on environmental restoration and waste management, we have many applications for funding pending at the DOE for research into better methods for characterizing and ameliorating contamination problems. These methods are outgrowths of on-going Laboratory work in fiber-optic detection, microbial metabolism, enzyme applications in chemical engineering, and risk assessment. For example, we are applying these methods to the biodegradation of waste products from high-explosive testing at LLNL's Site 300.

Finally, in conjunction with the Physics Department, we are conducting important research in atmospheric sciences (see p. 83). The major emphasis of this work—global climate changes—stems from energy-related concerns about the accumulation of carbon dioxide in the atmosphere and the resultant global warming (the so-called greenhouse effect).

Contact: M. L. Mendelsohn (415) 422-5765.

A Human DNA Repair Gene with High Evolutionary Conservation

We have cloned a human repair gene required for the removal of DNA damage caused by sunlight. The protein product of this gene is more than 50% identical to a yeast protein. This similarity provides insight into the biochemical function of the human gene and suggests it has additional vital roles in DNA metabolism.

Human genetic material, DNA or deoxyribonucleic acid, contains approximately 100,000 genes, all the information that is needed for human growth and development. These genes and their protein products are responsible for determining cell functions and the body's structure. Damage to the DNA can arise from exposure to environmental chemicals and radiation as well as from spontaneous errors in DNA metabolism. Virtually all living cells have remarkably sophisticated biochemical machinery for repairing their genetic material. However, if DNA repair does not occur or if it is performed improperly, mutations occur. The result can be the initial step in cancer development, as demonstrated by the cancer-prone nature of several genetic diseases caused by repair deficiencies. If the mutations occur in the reproductive cells, a newly arising genetic defect can be passed on to the offspring (Figure 1).

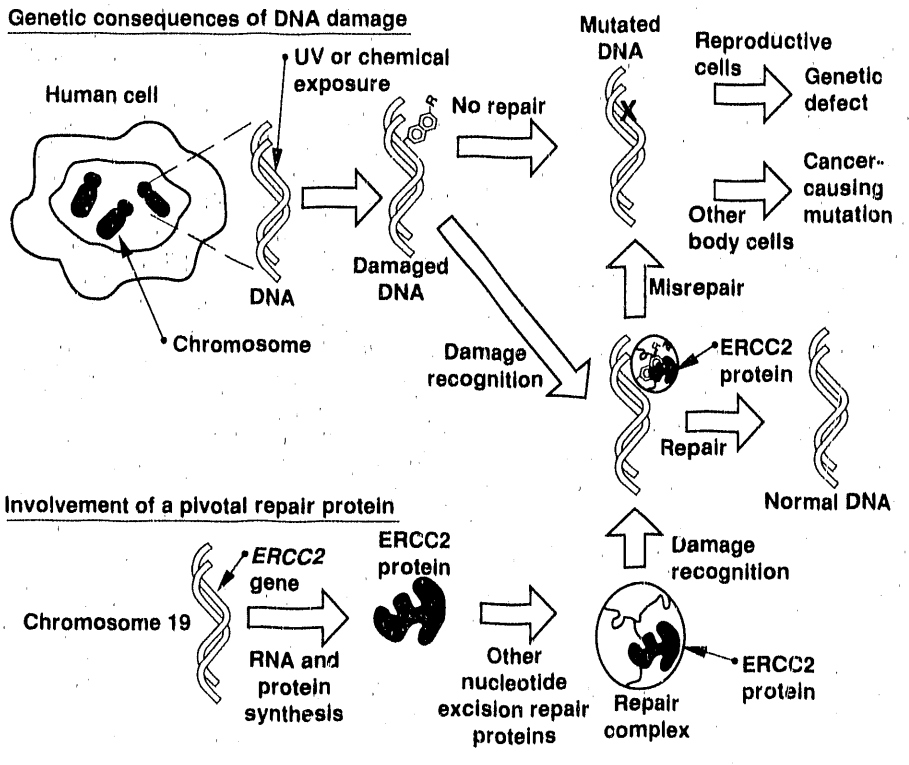


Figure 1. *The process of DNA repair and the role of ERCC2 protein in that process, as well as the potential consequences of misrepaired or unrepaired DNA damage.*

The nucleotide excision repair pathway is a major component of the DNA repair process and is responsible for the removal of DNA damage from ultraviolet (UV) radiation (found in sunlight) and from some chemicals, including many environmental pollutants. People with the genetic disorder xeroderma pigmentosum are unable to carry out this important repair process and are extremely sun-sensitive and prone to skin cancers.

Genetic analysis indicates that approximately seven to ten genes are necessary for this repair process. The protein products of these genes are believed to form a multiprotein complex (see Figure 1). In order to dissect this intricate repair process, we have isolated and characterized one of the human genes that codes for one of these various repair proteins. This gene is known as the *ERCC2* gene (excision repair cross complementing, meaning that correction occurs across species from human to hamster). The gene was isolated by molecular cloning techniques using repair-defective mutants of hamster cells that were previously isolated and characterized at LLNL. The defect in these hamster cells was corrected by introducing human DNA derived from the white

blood cells of volunteer donors. The *ERCC2* gene is the second mammalian DNA repair gene to be cloned.

Analysis of DNA base sequence revealed that *ERCC2* is the human counterpart of the yeast RAD3 (radiation sensitivity) nucleotide excision repair gene. Proteins are composed of a linear sequence of amino acids; the amino acid sequences of the proteins produced by *ERCC2* and *RAD3* are 52% identical and, allowing for chemically similar amino acids, 73% homologous. This similarity demonstrates a remarkable evolutionary conservation. That is, relatively few changes have occurred over a very long period of time, implying that this is an extremely important repair protein.

The RAD3 protein has recently been purified and determined to be a DNA unwinding enzyme, known as a helicase. Comparison of the amino acid sequence of a related group of DNA helicases revealed conserved regions, some with identified functional roles. The overall similarity of ERCC2 and RAD3 and the increased similarity (74% identity and 89% homology) within important functional domains indicate that ERCC2 will also be a DNA helicase. These results provide the first information about the specific biochemical function of any mammalian nucleotide excision repair gene.

In addition to its repair function, RAD3 also has a DNA replication function and an essential function. The essential function means that a functional RAD3 protein is necessary for cells to be able to grow and multiply, even in the absence of any DNA damage. Evidence from analysis of mutant cell frequencies obtained using mutagenic agents with different properties indicates that ERCC2 also has an essential function in mammalian cells in addition to its known role in DNA repair. Our results thus far indicate that the human DNA repair protein ERCC2 will, like RAD3 in yeast, have similar multifaceted roles in DNA metabolism.

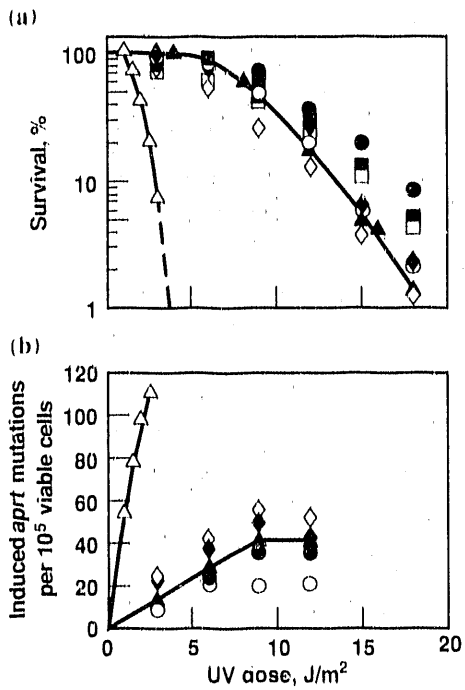


Figure 2. *(a) Level of cell survival after UV exposure in hamster mutant cells (open triangles), in normal cells (solid triangles), and in* ERCC2*-transformed mutant cells (remaining data points). (b) Level of mutations induced in a particular gene (the* aprt *gene) after UV exposure in hamster mutant cells (open triangles), normal cells (solid triangles), and* ERCC2*-transformed mutant cells (remaining data points).*

The ability of the human *ERCC2* gene to function in mutant hamster cells that are "transformed" with this gene was also assessed quantitatively. The transformed cells show normal hamster repair characteristics for UV-induced cell killing, UV-induced mutations, UV-induced DNA strand cutting associated with repair, and removal of specific UV-induced lesions from DNA (Figure 2). Thus, the human ERCC2 protein is able to function in a quantitatively efficient manner in the hamster repair-protein complex.

We are working to determine whether a defect in the *ERCC2* gene is responsible for the repair deficiency in any of the groups of xeroderma pigmentosum patients. As our studies continue and we begin to understand the basis of the multiple roles for *ERCC2* in DNA repair and replication, we will gain insight into those cellular processes that are vital for maintaining the integrity of genetic material. Such an understanding may give us further insight into the relationship between individual genetic variability and risk of cancer.

Contact: C. A. Weber (415) 423-8155 or L. H. Thompson (415) 422-5658.

Analysis of Trace Chemicals in Complex Mixtures by Liquid Chromotography/ Immunoassay

We have developed an assay method in which antibodies are used as chemically selective detectors to analyze families of structurally related chemicals. This method is often three orders of magnitude more sensitive than alternative techniques based on high-performance liquid chromatography/ultraviolet light absorbance detection.

We have developed a means of quantifying the amount of a particular trace chemical, or families of chemicals, in complex mixtures using liquid chromatography followed by immunoassay with specific monoclonal antibodies (LC/IA). Unknown chemicals are identified from the retention time of the analytes on the high-performance liquid chromatography (HPLC) column and from their specific binding to the panel of antibodies. Used in this way, the antibodies become chemically selective detectors for HPLC. LC/IA is thus a hybrid analytical procedure, such as gas chromatography/ mass spectroscopy (GC/MS) and HPLC/UV (ultraviolet light absorbance), that can be used to acquire very precise information about trace chemicals in complex mixtures. This technique has many potential applications, including monitoring human exposures to specific carcinogens or to specific DOE-related chemical wastes.

Carcinogen exposure often occurs in the context of a complex mixture of chemicals, such as the human diet. We have developed detection schemes for members of a family of cooking-produced carcinogens formed in meats, of which 2-amino-3,4-dimethylimidazo[4,5-f]quinoxaline (MeIQx) is one example. First, we developed monoclonal antibodies to MeIQx. Then, extracts of well-done cooked beef were chromatographically separated by HPLC, and the presence of MeIQx was detected by immunoassay with antibody AIA-2. The power of this technique is illustrated in Figure 1. MeIQx is one of several thousand chemicals present in the beef extract and is present at only one part per billion. In spite of its low level and the presence of many other chemicals, the immunoassay reveals only a single positive peak in fraction 16, which co-elutes with authentic MeIQx.

Although the illustration given here uses dietary exposure to carcinogens as the model, our LC/IA techniques can be applied to a wide range of occupational and environmental exposures to pollutant chemicals. With appropriate antibodies, similar LC/IA analysis could be used to look for evidence of human exposure to energy-related pollutants, analyze people for specific DOE-related hazardous waste exposures, and identify differences between people in their capacity to metabolize these chemicals.

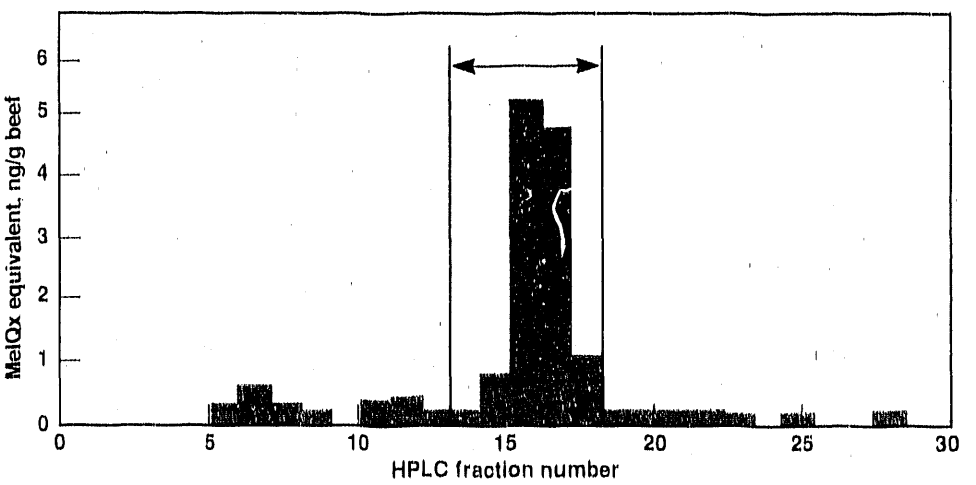


Figure 1. *Extract of fried well-done beef was separated by high-performance liquid chromatography, and each fraction was detected by immunoassay using our AIA-2 monoclonal antibody. The selectivity of this antibody is shown by the fact that although there are thousands of compounds present in the beef extract, only a single peak corresponding to the cooking-produced carcinogen MeIQx is observed.*

Contact: M. Vanderlaan (415) 422-5721.

DNA Probes from Human Chromosomes

We have developed a novel technique to isolate, clone, and amplify small DNA segments (called probes). The probes are very useful for mapping chromosome 19 and a disease gene, the myotonic dystrophy gene, located on that chromosome.

The human genome is the hereditary blueprint in each cell in our bodies, encoded in the DNA molecules. There are only four molecular building blocks in DNA, and it is the linear sequence of these building blocks that determines our hereditary properties. Because of the sheer size of this genetic information (approximately three billion building blocks) and the slowness of current sequencing techniques, scientists have only recently begun to decipher the messages hidden in our genes.

Before large-scale DNA-sequence analysis can begin, a road map of our genes is needed. Along with the Los Alamos and Berkeley laboratories, we are preparing such a map under a DOE initiative. LLNL's immediate goal is to prepare a high-resolution map of a small human chromosome, number 19. (Humans have 22 pairs of chromosomes and two sex chromosomes, two Xs in females or an X and a Y in males.)

Mapping requires efficient mapping tools, such as DNA probes. DNA probes are short molecules that have been isolated from much larger DNA molecules and then replicated in bulk quantity (amplified). Probes are usually obtained through laborious recombinant-DNA procedures. We have expanded a process called the "polymerase chain reaction" (PCR), which was initially developed by CETUS Corporation in Emeryville, to permit more rapid amplification of new probe molecules.

The selectivity of the PCR amplification process is defined by two primers. Primers are very short DNA molecules (about 20 building blocks long) that hybridize to the genome sequences flanking the probe fragment to be amplified (Figure 1). Primers can only be synthesized after the sequence has been determined, implying previous isolation of the probe fragment by molecular cloning techniques.

Because there are highly repetitive DNA sequences in the human genome, new DNA probes can be PCR-amplified without previous isolation of the sequence. One such sequence, called ALU, is dispersed throughout the genome, and there are many occurrences in the human genome where two ALUs are close by. PCR primers with a partial ALU sequence can initiate the amplification process even though the intervening DNA fragments have never before been isolated.

We have used ALU-PCR with bulk DNA from hybrid cell lines. Many well-characterized human-hamster hybrid cell lines now exist, each containing only defined minor portions of human chromosomes and a full set of hamster chromosomes. Because hamster chromosomes do not have ALUs, the ALU-PCR procedure produces amplifed DNA fragments specific for the human chromosomal regions present in the hybrid cell line. Thus we now have a tool that allows us to focus on regions of interest and obtain specific probe mixtures.

Our experiments have resulted in extensive collections of cloned probes for a small area from chromosome 19. This region contains a disease gene involved in myotonic dystrophy, a fairly frequently occurring form of muscular dystrophy. Although the gene is known to reside in this area of chromosome 19, its precise location and DNA sequence are unknown. It is likely that our probes will be very instrumental in the isolation of the disease gene, which could lead to a more rational therapy and better diagnostics. We are collaborating with research groups in the U.S., Canada, and Europe to isolate this myotonic dystrophy gene. This is only one application of DNA probes; they will play key roles in the mapping of more genes on chromosome 19 and in mapping the other human chromosomes.

Contact: P. J. de Jong (415) 423-8145.

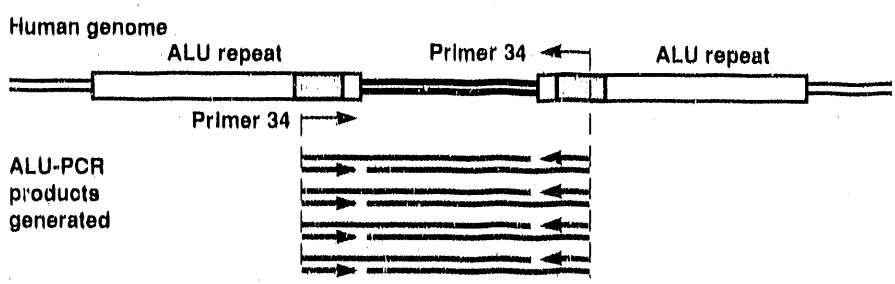


Figure 1. *PCR amplification requires two primers (arrow heads) to bind to closely spaced sites along the two strands of complementary DNA (solid black lines). The desired DNA region (heavy colored lines) can be amplified with two identical #34 primers. The gray areas in the ALU repeat units correspond to a region of the repeat that has no counterpart in hamster DNA.*

AMS Validation of Neutron Doses

As part of a joint effort between the U.S. and Japan, we are using accelerator mass spectrometry (AMS) to help reconstruct the neutron doses received by survivors of the Hiroshima and Nagasaki atomic bombs.

During the past decade, the U.S. and Japan have undertaken a substantial effort to revaluate the radiation doses received by survivors of the Hiroshima and Nagasaki atomic bombings.[1] This effort was largely prompted by calculations at LLNL that indicated serious problems with the old dosimetry, T65D.[2] As a result, a new dosimetry system, DS86, is now being applied to the atomic-bomb biomedical data and the assessment of radiation-induced cancer risk in man.

However, more recently, it has become apparent that DS86 may be flawed. A discrepancy has been observed between the neutron activation predicted from the new DS86 dosimetry system (which is based on calculations) and the activation actually measured using decay-counting methods. For Hiroshima, calculated thermal neutron activation (for cobalt and europium) appeared to be higher than measured near the bomb's epicenters and substantially lower than measured at distances beyond about 1 km. However, for both cities, the poor precision of decay-counting methods some 45 years after the bombs cannot provide a solid quantitative measure of this discrepancy.

For atomic-bomb samples, accelerator mass spectrometry (AMS) offers a much more precise method for measuring neutron activation than does decay counting. Decay counting is based on radioactive disintegrations of isotopes with short half-lives. However, because of the length of time since the atomic bombs, the isotopes most useful for decay counting have largely decayed away. AMS does not count radioactive disintegrations; rather, it counts individual atomic nuclei. Therefore, we can measure isotopes with longer half-lives and thus obtain more precise results despite the passage of time. In addition, AMS can be used to make measurements on a variety of mineral samples (including granite, tile and concrete) that are more available than the usual sample materials needed for decay counting.

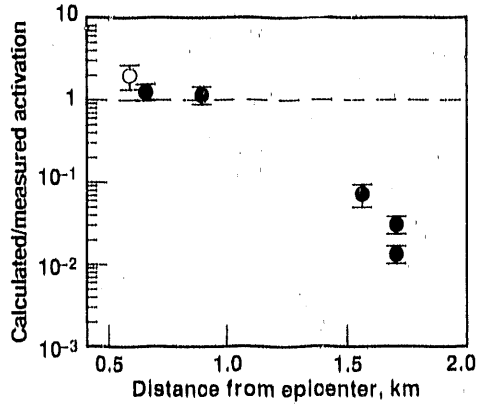


Figure 1. ***Ratios of calculated to measured neutron activation for chlorine in samples from Hiroshima plotted as a function of distance from the atomic-bomb explosion (epicenter). Calculations are for DS86 neutrons. Closed symbols are LLNL data of Straume et al.; the open symbol was obtained using data from Kato et al.[3]***

We have shown that AMS can be used to measure neutron activation in Hiroshima and Nagasaki accurately. AMS was used to measure the isotopes of chlorine in mineral samples from Hiroshima. Initial results using this approach are illustrated in Figure 1. Here, ratios of calculated to measured neutron activation are plotted. Note that the ratios should approximate unity (the dashed line); however, they depart seriously from expectations, especially at the farthest distances. Our results demonstrate that (1) AMS measurements are sufficiently precise to quantify thermal neutron activation accurately in samples at distances approaching 2000 m and (2) the AMS measurements clearly establish a problem with the DS86 calculations. During the next two years, we will use AMS to measure more samples in an effort to clarify the nature of the discrepancy between measured and DS86 calculated values.

References

1. W. C. Roesch, Ed., *DS86 Final Report, U.S.–Japan Joint Reassessment of Atomic Bomb Radiation Dosimetry in Hiroshima and Nagasaki*, Radiation Effects Research Foundation, Hiroshima, Japan (1987).
2. W. E. Loewe and E. Mendelsohn, *Revised Estimates of Dose at Hiroshima and Nagasaki, and Possible Consequences for Radiation-Induced Leukemia*, Lawrence Livermore National Laboratory, Rept. D-80-14 (1980).
3. K. Kato et al., *J. Rad., Res.* **29**, 261–266 (1988).

Contact: T. Straume (415) 422-5138.

Biodegradation of High-Explosive Wastes

Treatment methods for high-explosive (HE) wastes present in soil and water are needed to protect human health and the environment. We have developed a population of microorganisms that can degrade an HE compound to harmless byproducts.

Research and development activities involving high explosives (HE) at federal facilities, including Department of Energy laboratories, have resulted in the contamination of soils and groundwaters. Unfortunately, no technologies are currently in place that address the elimination of HE and its residues in environmental media. Bioremediation (the application of biodegradation technology to transform hazardous waste to harmless byproducts) is a promising strategy that that may well offer the versatility needed to treat HE and its residues. The goal of our research is to develop a biological system for the remediation of HE-contaminated groundwater and wastewater so that environmental quality can be preserved.

Our approach relies on the adaptation of a native population of microorganisms to transform HE compounds to innocuous byproducts (e.g., carbon dioxide and water). Microorganisms isolated from an HE-receiving waste pond were initially cultured in batch reactors that contained low concentrations of an HE compound, RDX, along with a variety of nutrient preparations (Figure 1). Glucose was also added to enhance co-metabolic processes. (Co-metabolism is the transformation of an unusable substance that occurs in the presence of a readily metabolized food source, such as glucose.) In this way, natural selection operated to stimulate the growth of a diverse microbial population with an enhanced metabolic capability for degrading RDX.

We have successfully demonstrated the degradation of RDX under aerobic conditions. The occurrence of RDX degradation under these conditions is significant because this process has not been previously reported. In addition, it does not lead to the formation of potentially carcinogenic byproducts (e.g., formaldehyde and hydrazines), which are known to arise from the anaerobic degradation of RDX.

We are now in the process of defining a strategy for treating waters contaminated with HE compounds (Figure 1). Bench-scale flow reactors are being used to define the optimum conditions for the continuous treatment of HE-contaminated water. The results of these studies will be used to design an upflow treatment system that will subsequently be tested in the field. By establishing a system for the biological degradation of RDX, we will be in a position to rapidly develop treatment strategies for other conventional explosives and for new explosives currently under development.

Reference

L. E. L. Etnier, "Water Quality Criteria for Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX)," *Regul. Toxicol. Pharmacol.* 9, 147 (1989).

Contact: J. P. Knezovich (415) 422-0925 or J. I. Daniels (415) 422-0910.

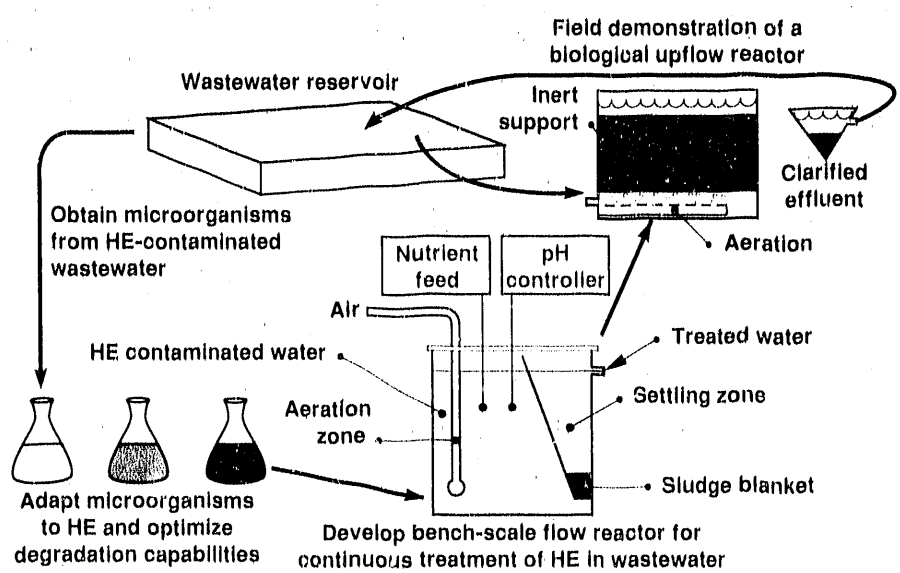
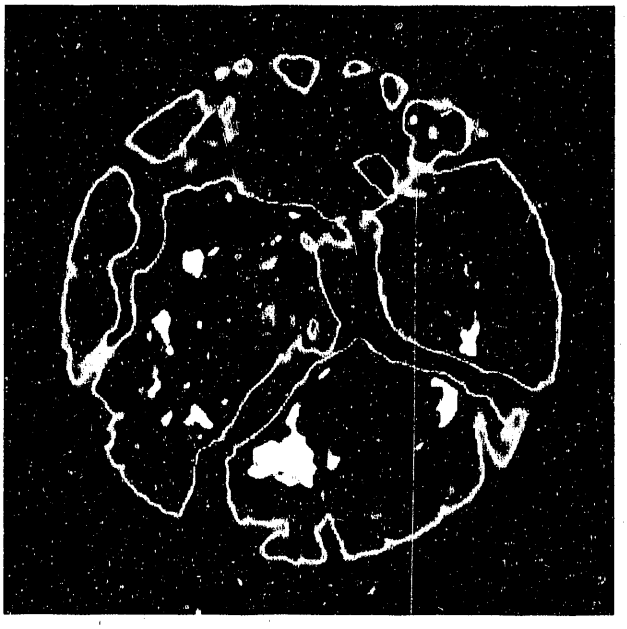


Figure 1. *Diagram of our strategy for developing and demonstrating a biological process for the transformation of high explosives (HE) and residues into innocuous byproducts (e.g., carbon dioxide and water).*

Engineering



Soil sample used to explore the use of computerized tomography to study surface crusting of soil, a major problem for farmers in the San Joaquin Valley. Nondestructive evaluation (NDE) is one of the eight Thrust Areas in Engineering, and computerized tomography is one of several NDE methods being developed.

The mission of Engineering at LLNL is, in the near term, to provide the expertise and capabilities necessary to support Laboratory programs and, for the longer term, to develop the base of knowledge required to anticipate and fulfill future Laboratory and national engineering needs. Engineering's presence as an effective team member in the Laboratory's major programs is evidenced by its contributions to so many of the programmatic successes described in this issue.

In order to anticipate future technological needs and to develop and introduce new technologies, we have established the Engineering Research and Development (ER&D) Program. We focus our efforts on identifying and then developing those key technologies that will "enable" future Laboratory projects. The ER&D Program is structured around eight Thrust Areas: computational electronics and electromagnetics, computational mechanics, diagnostics and microelectronics, fabrication technology, materials engineering and science, microwaves and pulsed power, nondestructive evaluation, and remote sensing, imaging and signal engineering. Thrust Area Leaders set the overall direction of the "thrust," ensure quality and progress in the activities, maintain links with Laboratory and outside experts, and facilitate collaboration and cross fertilization among diverse scientific and technical disciplines. The Thrust Areas are also tasked with identifying those engineering technologies needed to satisfy urgent or pending national needs, providing a stimulating environment that will continue to attract high-quality, research-oriented employees, and promoting collaboration with colleagues at universities (especially in the University of California system), other laboratories, and industry.

Although the projects described in the following articles represent only a small subset of the engineering accomplishments made during the

past year, they illustrate the breadth of our activities and the wealth of our engineering expertise. Engineering has made other significant achievements that we expect will soon become key elements in our technology base and find regular use in Laboratory programs, and will have great impact on current and future Laboratory and national needs.

One R&D area of particular importance is motivated by the demands of experimental scientists for diagnostic instruments and recording systems that can detect, transmit, and record large quantities of fast transient electronic signals with extremely high fidelity. Advances have been achieved in the area of high-bandwidth, high-data-rate systems for modulating optical signals, for faithfully transmitting these signals over large distances, and for recording the signals with new digitizers, streak cameras, and oscilloscopes. Specific projects include wideband (20-GHz) electro-optic modulators, high-speed gallium-arsenide CCD (charge-coupled device) digitizers, and wavelength-deflection streak cameras.

National needs for continuing improvements in nuclear safeguards and security have motivated R&D projects that span the scope of systems science and engineering. For example, we have developed advanced computer systems designed specifically for security monitoring and access control and have applied our systems research capabilities to nuclear safeguards evaluation. Drawing on our expertise in microelectronics design and fabrication, we have devised security measures to protect integrated circuits from unauthorized probing.

Our work on nondestructive evaluation has this year led to the introduction or significant improvement of a number of laboratory diagnostic instruments. The spectral range of a Laboratory-developed acoustic microscope has been extended to 1 GHz, thereby improving its resolution to the 5-μm range and providing a tenfold increase in the accuracy of nondestructive part inspections. We have also introduced the use of spectral analysis of Rayleigh wave scattering to characterize the distribution of surface flaw depths in various materials; this technique makes it possible to assess the level of damage in a material and will have a significant impact on quality assurance in materials fabrication.

In the realm of material science, we continue to make major strides, using advanced computer models and experimental techniques, to improve our understanding of the stress, creep, and failure mechanisms in composite materials. We have also developed and introduced into routine use several new tooling and composite machining techniques, including diamond-coated machine tool bits for improved finish and accuracy, elastomer mandrels for fabricating various tubular shapes, and new concepts for hybridizing composite forms. Each of these technological advances expands our capabilities to reliably fabricate composite parts with predictable properties and characteristics.

Engineers and computer scientists in Engineering continue to advance the state of the art in computer modeling for mechanics, electromagnetics, and electronics as well as in scientific databases and computer graphics. Of particular significance is the rapid development of scientific visualization capabilities; this has been a Laboratory-wide effort for a number of years and engineering personnel have been prominent participants. These new visualization tools and facilities allow scientists to interactively manipulate large quantities of data into more easily interpreted or viewed formats, thus making it possible for them to obtain a rapid and enhanced understanding of the data.

We have been very successful in fulfilling our mission to anticipate, develop, and providing the engineering technologies and personnel required by the Laboratory's programmatic endeavors. Drawing upon the expertise and facilities already established, we are confident that Engineering will continue to make outstanding and notable contributions in the years to come.

Contact: E. A. Lafranchi (415) 422-8355.

Algorithms to Improve Atmospheric Imaging

We have developed algorithms that remove the blurring effects of atmospheric turbulence from telescopic images.

The resolution of telescope images is a combination of the telescope's own resolving power and the limits imposed by viewing distant objects through the atmosphere. A telescope with a diameter greater than about 10 cm, used for visible imaging, is completely limited by the atmosphere. The resolution can be improved by recent advances in short-exposure-imaging technology and new computer postprocessing algorithms. We have taken significant steps to prove the feasibility of this method.

We are using novel imaging techniques that "freeze" the turbulence-induced atmospheric effects on the image by reducing exposure time. Each short-exposure interference pattern is called a speckle image because its appearance is analogous to speckle observed with coherent laser illumination. Procedures for extracting information from speckle-image sequences are called "speckle interferometry."

In 1988, we carried out a horizontal-path imaging experiment using a 0.5-m telescope and a charge-coupled device (CCD)-based speckle camera focused on a target transparency located 1.2 km away. We applied state-of-the-art image reconstruction algorithms to the speckle images based on analysis of various correlation functions of the ensemble of images. We obtained high-resolution images of a satellite transparency illuminated with light levels representative of low-earth-orbit (LEO) objects scaled to fit our horizontal path scenario. We also developed a numerical simulation of the technique and obtained similar results, verifying our understanding of the basic physics associated with the method.

In 1989, we concentrated on the imaging of fainter objects with a range of a few thousand kilometers in high-earth orbit (HEO). We had to develop a hybrid algorithm to obtain a satisfactory reconstruction. Our algorithm successfully dealt with the main problem—the additive detector noise characteristic of CCD electronic amplifiers—and we demonstrated high-resolution imaging of targets with luminosities representing HEO satellites. We applied our algorithm to data from the horizontal path imaging experiment, scaled to represent the imaging of a satellite at an altitude of 3000 km. Figure 1 shows an example of a reconstructed image from 1000 speckle frames collected with our CCD camera. A comparison of the relatively featureless, noisy speckle frame (b) with the outcome of the reconstruction process (c) shows the power of our algorithm; and a comparison of the final product (c) with the image obtainable by a perfect 0.5-m telescope with no atmospheric degradation (a) shows that we have indeed achieved diffraction-limited detail.

Our main goal for 1990 is to apply our algorithms to speckle images of actual satellites obtained with our CCD speckle camera mounted on the 1.6-m telescope at the Air Force Maui Optical Tracking Station. We hope to reconstruct images of LEO satellites out to 500 km and to explore new ways to improve our reconstruction algorithms. We are using least-squares methods for phase recovery and incorporating *a priori* information such as positivity and boundedness of the object. Our goal is to demonstrate imaging of objects out to geostationary orbits (38,000 km).

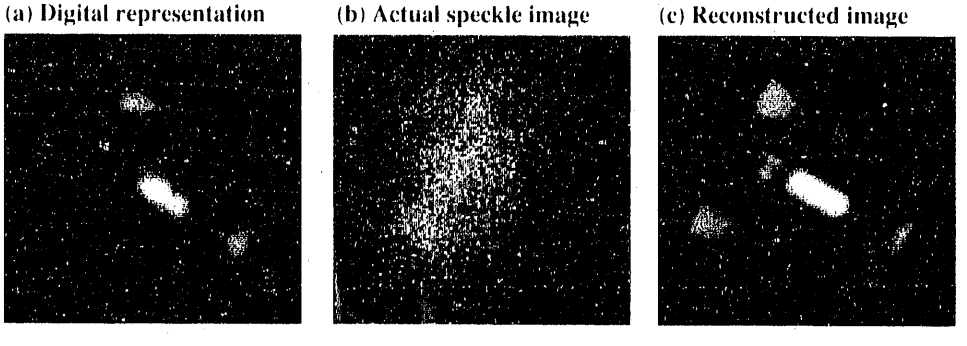


Figure 1. *(a) A digital representation of the diffraction-limited image obtainable with an optically perfect 0.5-m telescope and no atmospheric image degradation. (b) Actual speckle image of the target transparency, obtained at 1.2 km through the turbulent atmosphere, with a 0.5-m telescope and an exposure time of 5 ms. (c) Results of using our algorithm to process 1000 speckle images.*

Contact: T. W. Lawrence (415) 422-5322.

Development of a 20-GHz Integrated Optical Modulator

High-performance, lithium niobate, integrated optical modulators have been fielded in the fastest diagnostic system used to date in underground nuclear tests. These modulators have wide bandwidths (>20 GHz), low switching voltages (<10 V), and low optical insertion losses (<3 dB).

Many LLNL diagnostic applications require the transmission of a single analog signal from a remote radiation sensor. We have developed integrated optical systems in which the signal source is a semiconductor laser diode and the signal is transmitted over an optical fiber. The light signal is manipulated and controlled by a high-speed electro-optic modulator in much the same way that conventional integrated electronic circuits manipulate electrical signals. Our optical transmission systems use the integrated optics approach, combining the inherent high fidelity, bandwidth, and information capacity that characterize optical media. They offer the advantages of wide bandwidth, low loss, small size and weight, and immunity to electromagnetic interference.

For diagnostic applications in underground nuclear tests, the voltage output from a radiation detector is applied to a device located in a source laser's optical-fiber signal path. This device modulates the light signal external to the laser source in response to the applied voltage input, thus encoding the detector's electrical signal on the optical waveform produced by the laser. The resulting variations in laser light are recorded with a streak camera. A laser wavelength of 810 nm accommodates the streak camera's photocathode.

The key component in this system is the integrated optical modulator. We have concentrated on one particular type, the Mach-Zehnder interferometer, because of its wide bandwidth and low switching voltage. The Mach-Zehnder modulator (Figure 1) is an electro-optically tunable interferometer formed by photolithographic techniques similar to those used in semiconductor chip manufacture. First, optical waveguides are defined in the lithium niobate electro-optic crystal by the diffusion of titanium; then gold electrodes are deposited on the waveguides. The structure is designed so that the light splits at the input Y branch into two beams that propagate independently for a few millimeters and then recombine at the output Y branch. If no electric field is applied, the beams arrive at the output Y branch in phase and recombine without loss. If an electric field is applied, however, a path length difference is introduced between the two beams, and the combined beam does not propagate efficiently. Thus, the device operates as an electrically driven optical modulator.

The requirements for such devices include wide bandwidth, low switching voltage (the voltage required to change the light transmission through the device from 100% to 0%), and low optical insertion loss. There are tradeoffs in the complicated interplay among these three device parameters. We have been able to achieve a delicate balance between the waveguide and electrode parameters so that we can repeatedly and reliably fabricate wide bandwidth (>20 GHz), low switching voltage (<10 V), and low optical insertion loss (<3 dB) within a given device. We fielded such an integrated, optically based diagnostic system with a time response of <50 ps in an underground nuclear test and have obtained exceptionally high-quality data.

Contact: D. Lafaw (415) 423-4604 or M. Lowry (415) 423-2924.

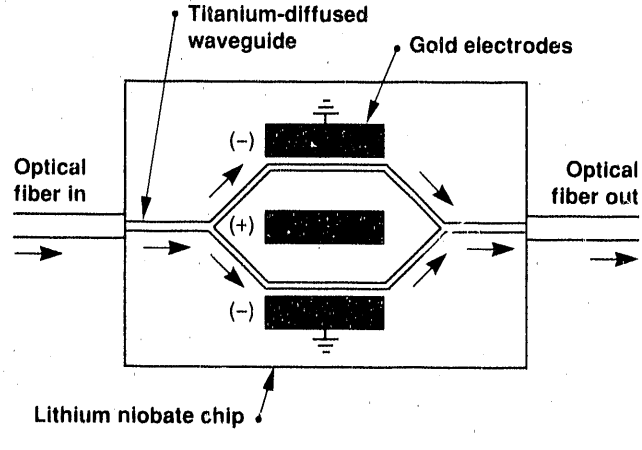


Figure 1. *Schematic diagram of a Mach-Zehnder integrated optical modulator. Fabricated of lithium niobate using photolithographic techniques, this device is essentially an electro-optically tunable interferometer.*

High-Power Microwave Generation

We are researching high-speed, high-voltage, laser-triggered photoconductive switching, assessing how this technology can be applied to high-power, narrow-pulse microwave generation, and collaborating with industry to demonstrate new system concepts.

High-power microwave weapons can be used to upset sensitive electronics in radars and other military targets. Narrow-pulse, high-power microwave sources are also being developed for advanced ultrawideband radars. Ultrawideband radars have several advantages over conventional radar technology including high-resolution range measurements and imaging, improved target discrimination and penetration (earth, walls, and foliage), and ultrashort-range capability.

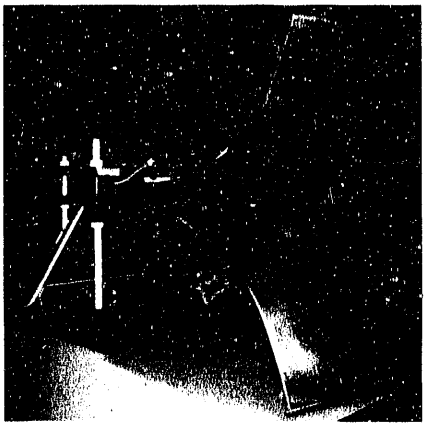
Photoconductivity—the modulation of the conductivity of a semiconductor material by light—is a uniquely important technology for high-speed, high-voltage switching. Using high-voltage, laser-triggered, photoconductive gallium arsenide (GaAs) switches, we have generated 35-kV pulses with risetimes as short as 135 ps. These switches can hold off electric fields greater than 100 kV/cm. We have developed a prototype high-power microwave generator using photoconductive switching technology with which we have generated 10-MW, nanosecond-pulse-length, 1.5-GHz microwaves. By increasing the power generated by each, and stacking many of these modules, we may be able to develop a compact high-power microwave generator capable of producing several gigawatts of peak power.

Solid-state photoconductive switches have many advantages over conventional gas and mechanical switches, including very fast switching, low trigger jitter, simple mechanical structure, optical isolation of the trigger, high thermal capacity and conductivity, and flexible geometry. Switching speed is virtually limited by the optical trigger speed, and picosecond switching has been achieved. Current densities as high as 2 MA/cm^2 have been reported in GaAs photoconductive switches. Combining high current density with hold-off voltages of more than 100 kV/cm makes photoconductive devices very attractive for fast, high-power switching.

We are conducting research on laser-triggered photoconductive switching in GaAs and applying this technology to the development of a compact, narrow-pulse, high-power microwave generator. The prototype is a GaAs-switched, mismatched Blumlein generator. The generator concept, shown in Figure 1, was jointly developed by researchers at LLNL, Rockwell International, and the University of Texas. It consists of a photoconductive-switched, 10-Ω parallel-plate Blumlein coupled to a 40-Ω parallel plate-transmission line and antenna. The impedance mismatch between the Blumlein and the transmission line generates a short burst of microwave energy. When these generators are stacked and switched in phase, they can produce gigawatt subnanosecond microwave pulses.

Several key technological issues remain. A wideband antenna is required that will efficiently focus and radiate short-pulse, wideband waveforms. Compact, efficient, high-repetition lasers are needed to trigger the photoconductive switches. Switch efficiency and life must be improved.

Contact: M. D. Pocha (415) 422-8664 or W. W. Hofer (415) 422-1636.



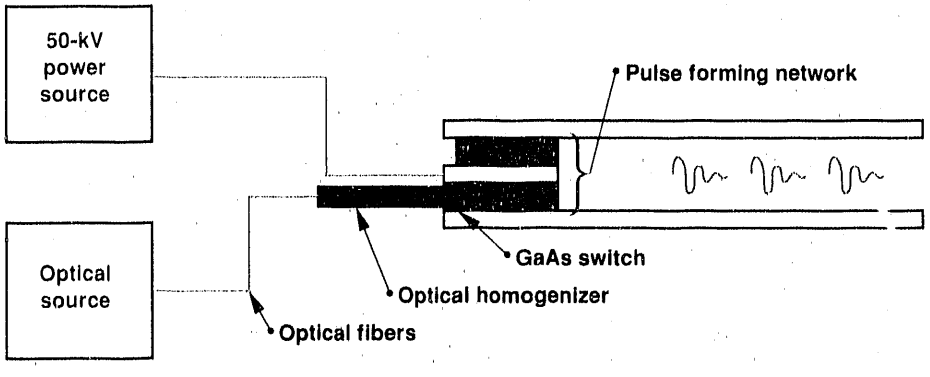


Figure 1. *Photograph and diagram of a prototype GaAs-switched, mismatched Blumlein high-power microwave generator.*

Predicting Thermal Loads that Cause Crack Growth and Failure

We have developed a postprocessor to use with the NIKE2D and TOPAZ2D codes to predict the fracture behavior of brittle solids; this work will improve our ability to use these materials for high-temperature and high-stress applications.

Thermal stresses associated with crack growth are a common cause of failure in glass, ceramics, and other brittle solids. To quantify how thermal stresses cause cracks to grow from existing defects, we implemented a J Integral postprocessor for use with the finite-element codes NIKE2D and TOPAZ2D. With the postprocessor, we can predict the thermal gradients and loads that will cause crack growth and failure in a component based on its critical J Integral value or energy-release rate.

We have thoroughly verified the postprocessor and have used it in conjunction with an experimental effort to measure critical energy-release rates for thermally stressed glass plates under two types of thermal gradients. We have also used this method of assessing the effects of thermal stresses on pre-existing flaws to study damage in the Nova laser's final-focusing lens and to predict the cracking in optical components exposed to high-energy x-ray fluences.

The J Integral has a contour integral term that takes the difference between the strain energy density and the traction vector multiplied by the displacement gradient in the direction of crack advance, and an area integral term that is the product of the mean stress multiplied by the temperature gradient. In combination, these terms yield the energy-release rate at the crack tip for both mechanical and thermal loading. For brittle materials, the resistance to crack growth is typically measured using critical stress-intensity factors, which are proportional to the square root of the energy-release rate or the J Integral value.

In implementing this formulation as a postprocessor, we calculate the temperature fields around a crack tip using the thermal finite-element code TOPAZ2D. We then use these temperatures as input to the finite-element code NIKE2D for calculating stresses and displacements. Using this information from the binary plotfiles, the postprocessor calculates the stress-intensity factors.

We verified the J Integral postprocessor by comparing its results to those from an analytical solution that uses a complex variable method to calculate energy-release rates at a crack tip in a heated rectangular plate with a steady-state temperature distribution. For three different meshes of varying coarseness and two paths within each mesh, the J Integral values were consistent and equal to the analytical solution to within 1%. This clearly demonstrates that the J Integral postprocessor is accurate and that its values are independent of the contour path of integration and the level of discretization in the finite-element mesh.

We applied our new thermal-stress capability to experiments in the thermal fracture of glass. Figure 1 shows a Mode II (in-plane crack sliding) thermal-fracture specimen, as well as some details of the heating and cooling system. It is evident that the J Integral postprocessor together with TOPAZ2D and NIKE2D will be of great help as we work to understand the fracture behavior of brittle solids and their inherent defects under mechanical and thermal loading. Such knowledge is essential if we are to widen the use of these materials for high-temperature and high-stress applications.

Contact: R. A. Riddle (415) 423-7541.

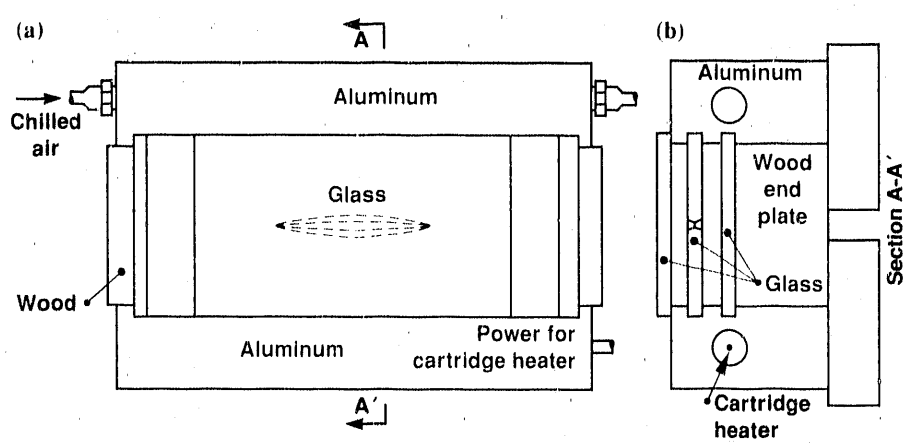


Figure 1. *Thermal-fracture specimen for measuring the critical Mode II stress-intensity factor: (a) in-plane view and (b) orthogonal view through section A-A′.*

Fiber Composite Materials for Extreme Environments

A new, multiaxial testing capability allows us to characterize the three-dimensional performance envelope of advanced fiber composite materials under the combined loading of axial load, torque, and internal pressure.

We are developing fiber composite materials for use in extremely challenging, three-dimensional loading environments such as warhead penetrator cases and advanced munition components. Advanced composite materials—typically graphite fibers embedded in an epoxy resin matrix—are especially useful because of their high strength, high stiffness, low density, and low atomic number. We are developing a three-dimensional failure criterion for use to improve the modeling and design of advanced composite structures that can withstand ever-increasing loading extremes.

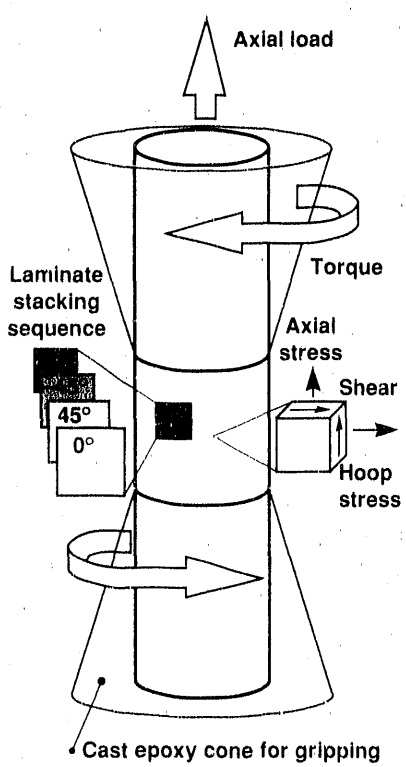


Figure 1. *Diagram of multiaxial test specimen.*

One of our goals (and a major difficulty) is to characterize the three-dimensional performance envelope of these materials. The performance of fiber composite materials is complex and highly dependent on the orientation of the fibers and the configuration of the laminates. The performance envelope is defined by the locus of various combinations of the three-dimensional stresses required to induced failure. Fiber composite materials possess many unique and independent failure modes that require us to generate the overall performance envelope or failure surface.

We have developed a multiaxial testing capability for composites that enable us to generate a significant portion of the performance envelope. The test specimen is a composite tube 5 cm (2 in.) in diameter with 15° cast epoxy end cones for gripping (Figure 1). This specimen is fitted into a computer-controlled hydraulic test machine that can simultaneously apply axial load, torque, and internal pressure. The combined loading reveals complex failure mechanisms and makes it possible to optimize the design of advanced composite materials for specific severe conditions.

An example of a two-dimensional performance envelope for an early-generation composite material is shown in Figure 2. Note that the limiting maximum shear stress increases by 25% when the test specimen is simultaneously loaded in tension to 80% of its maximum axial load-carrying capacity. Current-generation fibers now being tested show similar behavior at stress levels nearly three times greater. Visualizing the complex failure surfaces of these materials will greatly enhance our performance-modeling capabilities.

Contact: S. E. Groves (415) 422-1331.

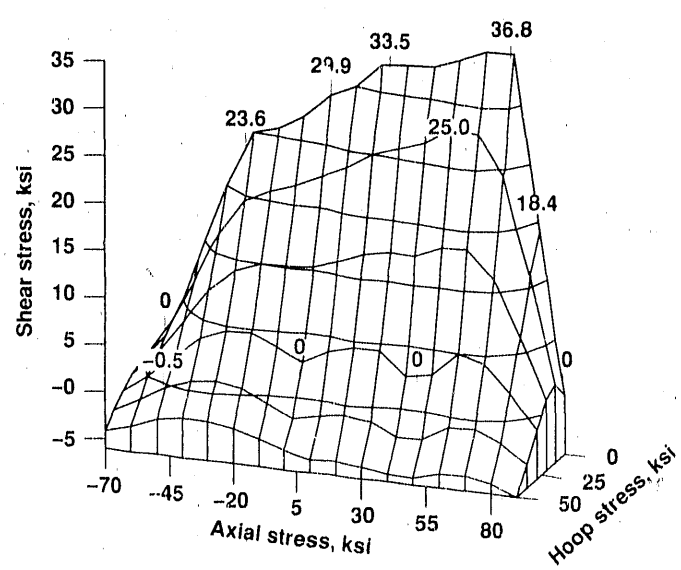


Figure 2. *Multiaxial failure surface for a [0/±45/90]s T300/F263 graphite/epoxy laminate determined using our multiaxial loading test system.*

Computer-Simulated Sheet-Metal Hydroforming

LLNL-developed finite-element codes allow engineers to simulate sheet-metal-forming operations. Run on supercomputers, three-dimensional analyses accurately predict sheet-metal responses to complex tooling geometries.

Until recently, tooling design has been a black art in which experienced technicians modify their punches and dies to produce sheet-metal parts that are free of tears and wrinkles and have enough strength to maintain their shape during service. Experience has been gained only through trial and error. Now, however, engineers can use our finite-element analysis tools to gain insight into the details of tooling design and greatly reduce the costly lead time required to form complex parts successfully.

Finite-element analysis is especially well suited to solving problems in sheet-metal forming since complex geometries can be treated with ease. For several years, we have performed interesting two-dimensional analyses, and the inherent symmetries of these problems make them amenable to experienced intuition. However, with the advent of modern supercomputers, three-dimensional modelings are now tractable. Three-dimensional analysis of sheet-metal forming problems is especially revealing and useful as deformations with multidimensional curvatures can defy the intuition of even the most experienced tooling designers.

To illustrate our capabilities, consider the part shown in Figure 1a, which was assigned a low manufacturing-feasibility index by experts at a DOE production facility. We used LLNL's analysis codes INGRID, DYNA3D, and TAURUS to develop the model shown in Figure 1b. In this example, we began with a flat sheet of aluminum and simulated the forming process, incorporating the tooling and lubricant conditions and the forming pressure histories. Comparison of Figures 1a and 1b clearly shows that our model is an accurate simulation of the part's geometry and stress distributions. The red stress contours, which indicate the locations where the model predicts part failures, correspond to the maximum stress the material can withstand.

A particularly important capability of our modeling approach is that it accurately represents the points of contact between the sheet metal and the tooling, which may be made and broken several times during the simulation. This is a capability in which LLNL codes excel, because our robust algorithms account for varying friction conditions as well as for the presence of corners and bodies that are in contact at multiple points. Another important feature in our codes is that we may choose not to calculate the stress to which the relatively rigid tooling parts are subjected. This allows us to represent complex tooling geometry in great detail without adding time-consuming stress calculations to the model.

Another innovation is our use of the explicit dynamics code DYNA3D to perform what has been considered an implicit quasi-static calculation. By advancing the punch at an artificially fast rate, we can reduce the previous limitation of small time-step sizes and use the explicit approach. We are now working to establish quantitative measures of the artificial dynamic effects that may be introduced in simulations of this kind.

Contact: B. N. Maker (415) 422-1385.

(a) (b)

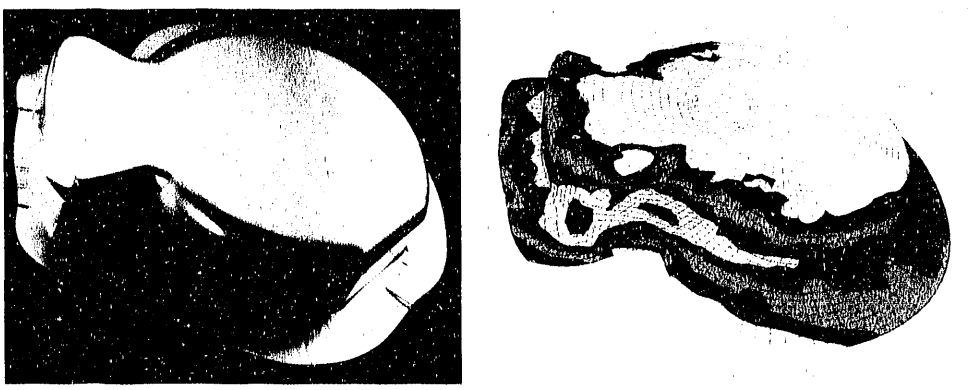
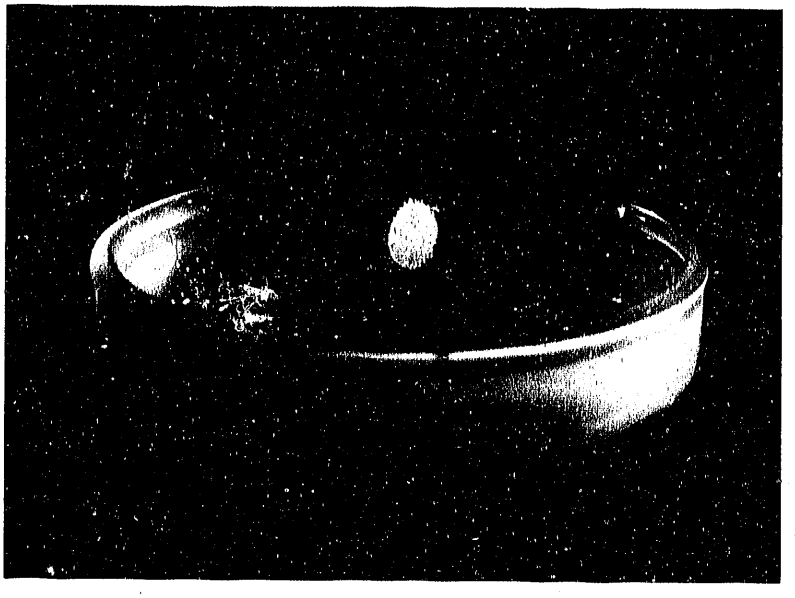


Figure 1. *Cover for a portion of the SRAM II missile (a) produced in the hydroform process and (b) simulated using finite-element analysis. In (b), the red contours, which show stresses that exceed the material's maximum (or ultimate) strength, correlate well with the failure locations in the actual part.*

Physics



Magnet levitated by a block of superconductor cooled to liquid-nitrogen temperatures. Some of our most exciting research involves theoretical and experimental studies of the properties of high-temperature superconductors.

The charter of the Physics Department is (1) to pursue research on the forefront of physics in areas that are important to current and future Laboratory programs, (2) to exploit unique facilities and expertise to initiate and carry out high-leverage scientific and technological projects, (3) to interact vigorously with outside academic and technical communities, and (4) to recruit and develop outstanding scientists and leaders for the Laboratory. The Department's traditional focus has been on long-term physics research that could have a significant impact on the Laboratory's nuclear weapons program. This effort has been concentrated in the disciplines of astrophysics, atomic physics, condensed matter physics, nuclear physics, and plasma physics, and in such computationally intensive topics as compressible hydrodynamics and transport theory.

Articles in this section highlight our recent achievements in the theory of superconductivity, in nuclear data modeling, and in PEGASYS (an experiment designed to study highly inelastic interactions of electrons and nuclei). Other particularly notable accomplishments were made this year in the atomic physics of heavy elements, in the study of highly distorted nuclei, and in modeling supernova explosions. The Physics Department also was instrumental in initiating a Laboratory-wide project to explore the suitability of massively parallel computing for simulating the physical conditions in nuclear weapons and fusion systems.

Our recent work in atomic physics has exploited the remarkable capabilities of the Electron Beam Ion Trap (EBIT), an instrument in which both the structural and dynamic properties of highly charged ions can be measured. The EBIT has sparked a revolution in atomic physics by making experimentally accessible virtually all ionic states of all elements in the periodic table. (The very highest charged states of the heaviest elements will become available with the SuperEBIT, which is under construction and very nearly complete.) During the past year, we used the EBIT to make a number of

"first" measurements of the energies of x-ray lines of highly charged ions and of such complex atomic reactions as dielectronic recombination. These measurements have provided benchmark data for our theoretical computer codes, which can now be used to generate needed atomic information for many ions of programmatic interest.

The conventional properties of nuclei are usually calculated using (Hartree-Fock) computer codes. By running these codes for highly distorted nuclei, the so-called "shape" isomers, we have delineated a family of nuclear excited states with megaelectron-volt energies and conceivably long lifetimes. If such states do exist in nature—not just in computer calculations—they could be used as energy storage states, with energies much greater than high explosives and with more stability than fissioning nuclei. We have begun both an intense effort to calculate the lifetimes of the shape isomers and an experimental program with other institutions to search for them. The experimental effort has produced very significant results; work at the Lawrence Berkeley Laboratory and measurements made at Argonne National Laboratory have provided definite evidence for the existence of such isomers.

Last year also saw the culmination of nearly 25 years of leadership in modeling supernova explosions. The first detailed theory of such events, worked out at LLNL in the early 1960s, involved the rapid implosion of a stellar core which emitted neutrinos that blew off the outer portion of the star. Many refinements of this scenario were subsequently made, and detailed numerical descriptions of the pre-supernova evolutions were incorporated into the model. With the fortuitous occurrence and detection, two years ago, of the SN 1987A supernova, we have been able to compare our calculational models with data from that event. This comparison has validated nearly all major features of our theory—an extraordinary triumph when one considers the extremely complex explosion physics associated with the supernova model.

An increasing fraction of Physics Department work has been directed toward projects funded outside the nuclear weapons and fusion communities. In large measure, this represents the successful transfer of expertise developed in those programs to other problems of national importance. Three articles here highlight some of this work: the innovative Brilliant Pebbles project, supported by the Strategic Defense Initiative Organization; the XMM or X-Ray Multimirror Mission, for which we are helping develop an x-ray spectrometer under NASA funding; and a long-term effort sponsored by the DOE's Office of Energy Research to analyze and understand the differences among various models of the atmospheric greenhouse effect. Our work in other climate-related projects is continuing to grow, and we have several substantial initiatives in modeling atmospheric chemistry, in developing coupled atmospheric-oceanic models, and in simulating the possible consequences of toxic gas releases.

The Physics Department is continuing to encourage and foster outside collaborations and interactions. The LLNL branch of the University of California's Institute for Geophysics and Planetary Physics has very successful and active programs in astrophysics, high-pressure physics, and seismology. We sponsor a number of advanced mathematical projects, such as neural network modeling in the Institute for Scientific Computing Research. Also this past year, we formally assumed responsibility for the Plasma Physics Research Institute. Our Center for Accelerator Mass Spectrometry has made several major technical achievements, including successful operation of the facility for carbon-14 measurement. During the coming months, we expect to demonstrate successful use of accelerator mass spectrometry for other radioisotopes, which will allow us to carry out innovative measurements for biomedical and environmental science applications.

Contact: C. B. Tarter (415) 422-4169.

Brilliant Pebbles

We are developing a strategic defense system that consists of many identical, sophisticated spacecraft in low earth orbit. These "Brilliant Pebbles" can detect and hunt down missiles over thousands of kilometers, once enabled by human command. The Brilliant Pebbles system can be implemented using existing American technology and at relatively low cost.

LLNL has been participating in the technology development of a strategic defense system which, in its simplest form, consists of nothing more than a set of identical, highly capable, small spacecraft deployed in low earth orbit. These spacecraft, known as "Brilliant Pebbles" because they are highly intelligent but sharply scaled-down "Smart Rocks," are in place to stop—through collisions at high velocities—advanced ballistic missiles and their components in flight. Each Brilliant Pebble is equipped with the functional analogs of brains, eyes, and legs (Figure 1), enabling it to detect and hunt down missiles over distances of thousands of kilometers without external aid, although subject to human command and control. These Pebbles, roughly one meter long and weighing roughly fifty kilograms, can be implemented with existing American technology for a deployed cost estimated at $1 million apiece, and fewer than 10,000 of them appear likely to offer a robust, stand-alone strategic defense capability.

A key element of the Brilliant Pebbles concept is the move from reliance on a small number of complex assets to the use of a larger number of simple assets. Because Brilliant Pebbles consists of many small, hardened, and inexpensive spacecraft, the system is intrinsically survivable, being far more expensive to attack successfully than to deploy. The low cost of each Pebble is due both to its use of readily available commercial technology and to the use of mass-production techniques in its manufacture.

Perhaps one of the most important virtues of the Brilliant Pebbles system is its intrinsic testability. Once enabled by the human commander, each Pebble is capable of performing its role in a defensive engagement—detection, tracking, assignment, and interception—without dependence on communication or any other defense assets. Because Pebbles do not interact during the course of an engagement, it is possible to test each spacecraft individually and have full confidence that a constellation of them will behave in the same fashion as predicted from the exhaustive testing of a single Pebble. No other system that depends on communication between many elements can make this claim.

Today's Brilliant Pebbles effort grew out of LLNL technology-base work that has been funded by the Strategic Defense Initiative Organization (SDIO) since 1985. The Brilliant Pebbles effort formally commenced in November 1987. After an intensive, independent technical review by the SDIO and the Department of Defense during the

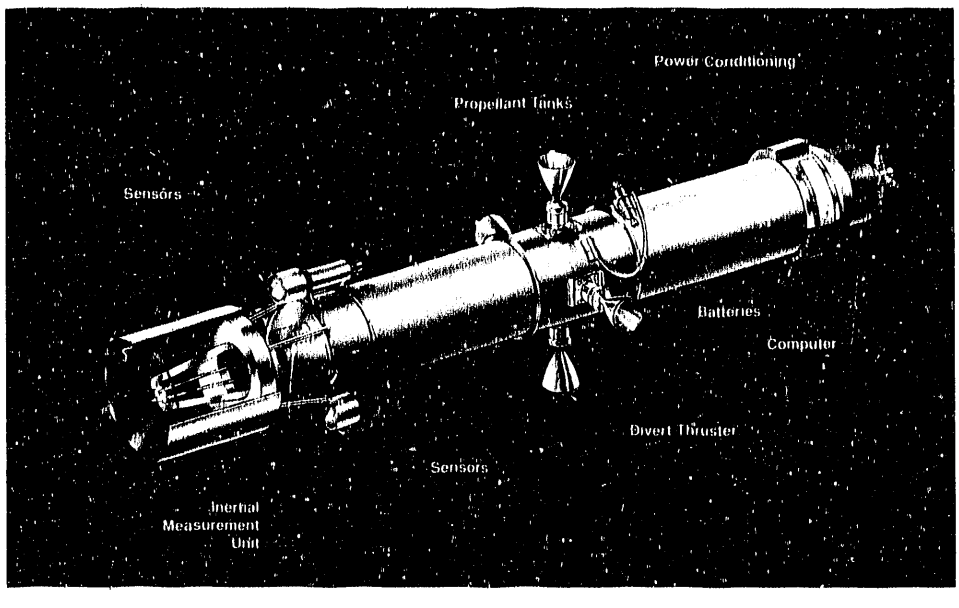


Figure 1. *The terminal stage of a Brilliant Pebble, known as a kinetic kill vehicle, carries its "brain" (a very-high-performance microprocessor-based computer system), its "eyes" (a collection of video cameras for tracking its target), and its "legs" (an agile rocket propulsion system that enables it to navigate to and intercept a maneuvering ballistic missile or postboost vehicle). Other components include an inertial measurement unit, used to help the Pebble navigate to its target, and batteries and a power converter, which provide electrical power to all the Pebble's subsystems.*

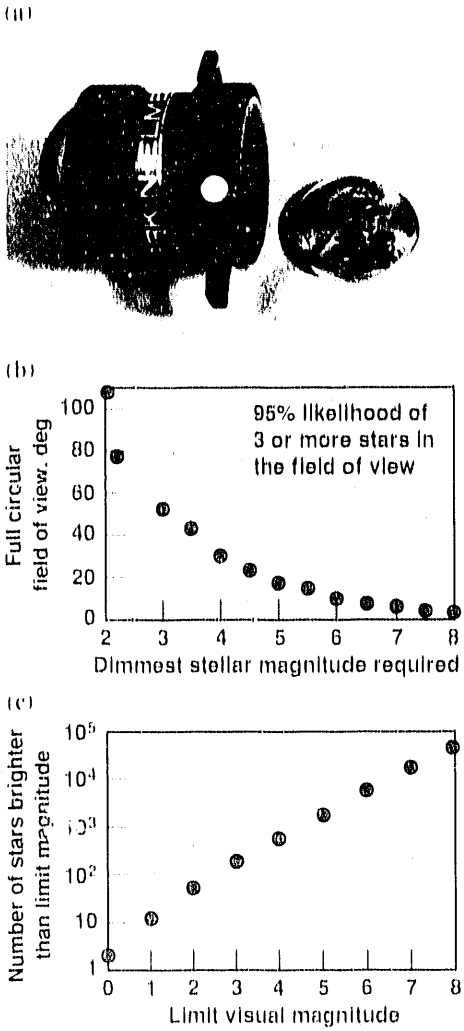


Figure 2. *The WFOV Star Tracker uses a miniature, all-concentric refractive lens (a) to give it a wide field of view (nearly 60 deg) and a large amount of light-gathering power, all in a very small package. With such a wide field of view (b), the Star Tracker can navigate using a catalog of only the brightest stars. The number of bright stars is small (c), so the software that matches stars against the catalog can run very quickly, producing results in a few hundredths of a second. The result is an instrument that can determine its position, with no a priori information, several orders of magnitude faster than was previously possible—fast enough to use the WFOV Star Tracker for real-time navigation of an agile spacecraft.*

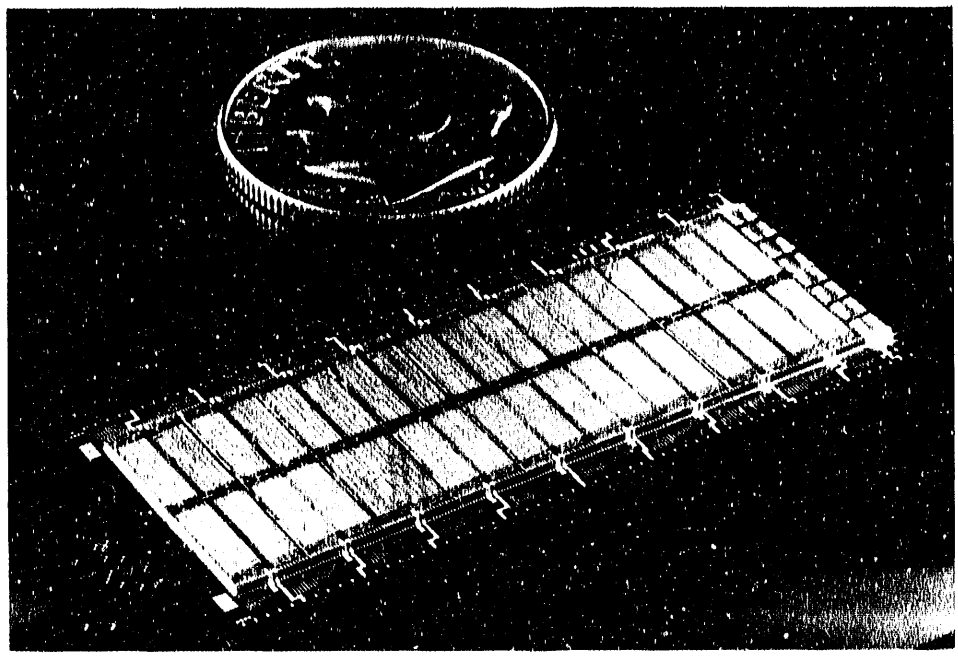


Figure 3. *Laser pantography allows extremely high packaging densities for integrated circuits. This photograph of a high-speed memory module for the Brilliant Pebble flight computer shows how 18 computer chips are placed shoulder-to-shoulder on a single silicon wafer, which is, in turn, part of a hermetic package. This module is less than one-tenth the size and weight of the conventionally packaged chips that it replaces.*

summer of 1989, the concept was adopted as the new baseline for the space-based segment of the Strategic Defense System.

Current efforts at LLNL are focused on the execution of a program of Brilliant Pebble flight tests in compliance with the Antiballistic Missile (ABM) Treaty; the first test is scheduled to begin in mid-1990. In addition, we are continuing the development of advanced supporting technologies. An example is the WFOV Star Tracker shown in Figure 2—an outgrowth of previously funded work in wide-field-of-view (WFOV) imaging systems.[1] This instrument, which weighs only a few ounces, allows a Pebble to navigate by using the stars as references in much the same way as ancient mariners did. Another example is laser pantography, a technology that allows extremely high-density wafer-scale packaging of integrated circuits.[2] Figure 3 shows a high-speed memory module, produced by laser pantography for the Brilliant Pebble flight computer.

References

1. "The Wide Field of View Camera," December 1988 issue of *Energy and Technology Review* (UCRL-52000-88-12), pp. 1–12.
2. "Laser Pantography," December 1985 issue of *Energy and Technology Review* (UCRL-52000-85-12), pp. 10–20.

Reflection Grating Array for an X-Ray Satellite

We have resolved fundamental scientific and engineering issues in designing and fabricating an x-ray reflection-grating array that will be part of a satellite spectrometer.

The x-ray spectrum of a cosmic source is its fingerprint, a collection of information unique to that source. This spectrum reveals information about such fundamental properties as the temperature, density, velocity, and composition of the region in which the spectrum originated. While the value of such spectra has long been known, they have been acquired for only a handful of cosmic sources. More progress has awaited the advent of instruments of higher sensitivity. The most powerful tool available for understanding these cosmic x-ray sources is the x-ray spectrometer.

Recognizing the need for high-sensitivity x-ray spectroscopy, the European Space Agency (ESA) has planned a space mission to be launched in the late 1990s, the X-Ray Multimirror Mission (XMM), which will deploy a satellite-based reflection-grating spectrometer (RGS). By detecting the x-ray spectra of thousands of cosmic sources, the RGS will vastly increase our understanding of many classes of objects that emit x rays, such as neutron stars, black holes, and quasars. LLNL and the University of California, Berkeley, are collaborating in designing, constructing, and calibrating the array of reflection gratings for the ESA under a contract from NASA.

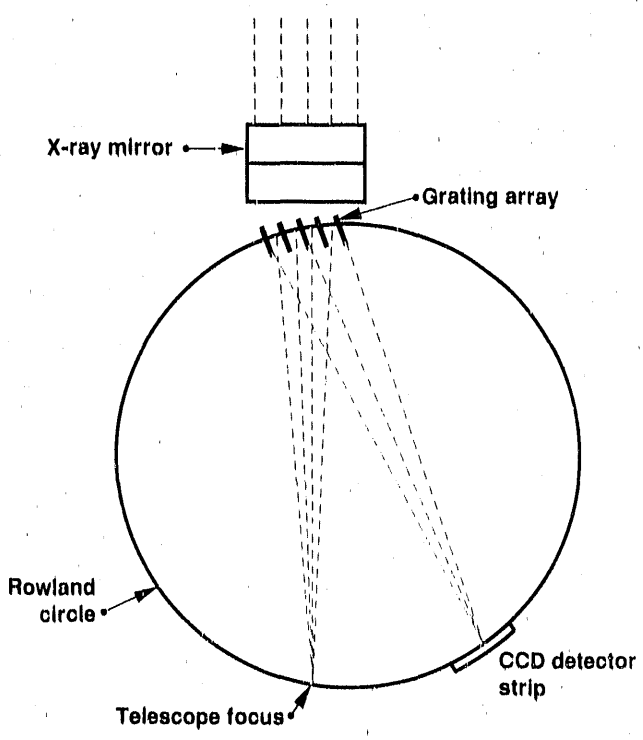


Figure 1. *Optical design of the reflection-grating spectrometer. The reflection gratings at the exit of the x-ray mirror are oriented at grazing incidence to the beam. The gratings intercept only a fraction of the beam; roughly half the light passes through the telescope focal plane. The intercepted rays are diffracted to a strip of charge-coupled devices (CCDs) that serve as the spectroscopic detector. To eliminate aberrations associated with the arraying geometry, the gratings, the telescope focus, and the CCD detector strip all lie on a large Rowland circle.*

The RGS sits at the focus of a large mirror (see Figure 1) that collects and focuses x rays onto the reflection gratings, thin (~1 mm) beryllium wafers coated with gold in which thousands of grooves have been etched. The gratings disperse the reflected x rays into their component energies exactly as a prism disperses light into its component colors. Once sorted by their energy, the x rays are detected by a charge-coupled device (CCD), an x-ray detector being built by our European collaborators.

A variety of technical issues must be resolved. About 600 reflection gratings sit in each of two boxes; to attain high resolutions they are aligned to accuracies of several arc seconds and must be flat to better than 1 μm over a 20 × 10-cm area. These requirements impose severe demands on materials and alignment techniques. To thoroughly characterize the gratings' behavior under x-ray illumination, we must construct a major facility for calibrating a huge number of gratings (up to several thousand) to ensure that only the highest performing need be selected for flight. Solution of all the technical problems requires close collaboration among LLNL experts in x-ray physics, precision engineering, and materials science.

LLNL astrophysicists, because of their expertise in x-ray spectroscopy and high-temperature plasmas, will also be heavily involved in analyzing data from the RGS. Work is under way to define and eventually to write much of the software needed for analyzing data.

Contact: C. Hailey (415) 422-4511.

The PEGASYS Project at SLAC

Construction of a facility for studying the behavior of quarks in nucleons and nuclei has been proposed for the Positron Electron Project storage ring at the Stanford Linear Accelerator Center.

Deep inelastic electron scattering provides the most detailed information about the constituents of the nucleon: quarks and gluons. However, early experiments observed only the scattered electron, and even today little is known about the fate of the struck quark and how it evolves into the jet of observable particles that is produced. Over the past three years, more than 60 physicists from institutions in the U.S., the Soviet Union, Israel, Poland, and Italy have collaborated to develop a proposal for a unique facility at the Positron Electron Project (PEP) storage ring at the Stanford Linear Accelerator Center (SLAC). The proposed facility is to be called the Positron Electron Project Gas Jet Spectrometer System, or PEGASYS (Figure 1). At this facility, we will use interactions between high-energy electrons and atomic nuclei to make detailed tests of quantum chromodynamics, which is our best theory of the strong interaction that binds quarks and gluons into observable particles such as nucleons and mesons.

Four design features will make the PEGASYS facility unsurpassed for studying the disintegration of the target nuclei by the electron beam:

- The PEP storage ring will produce a high-current, high-energy (15-GeV) electron beam.
- A large-aperture, high-resolution forward spectrometer will detect the scattered electron and the jet of particles produced in each collision.
- An extremely thin cryogenic gas-jet target (ng/cm^2) can be made to provide a wide range of target nuclei (for example, H_2, D_2, N_2, Ar, Xe).
- Additional detectors will detect the low-energy decay products (such as photons, nucleons, alpha particles, and heavy ions) of the target nucleus.

In the past year, the project received scientific approval from SLAC and passed a technical and budgetary review. The spokesman for the collaboration and the system manager for the magnet are both LLNL scientists. It is hoped that construction of PEGASYS will begin in 1992 and that the experimental program can begin in 1994.

One of the main experiments to be performed at PEGASYS will determine the inelastic quark-nucleon inelastic cross section and the distance over which quarks materialize into observable particles (hadrons). Determining these qualities will involve careful, systematic measurements of the attenuation of fast hadrons produced in deep inelastic scattering within nuclei of different radii. Another important experiment will be a search for a new particle that interacts only with charged leptons (electrons, muons, and tau particles). Such a particle would be identified from the properties of electrons and muons observed in the PEGASYS spectrometer. For masses between 10 MeV and a few GeV, PEGASYS will improve the limits on such objects by several orders of magnitude in coupling constant.

Contact: F. S. Dietrich (415) 422-4521 or K. A. van Bibber (415) 423-8949.

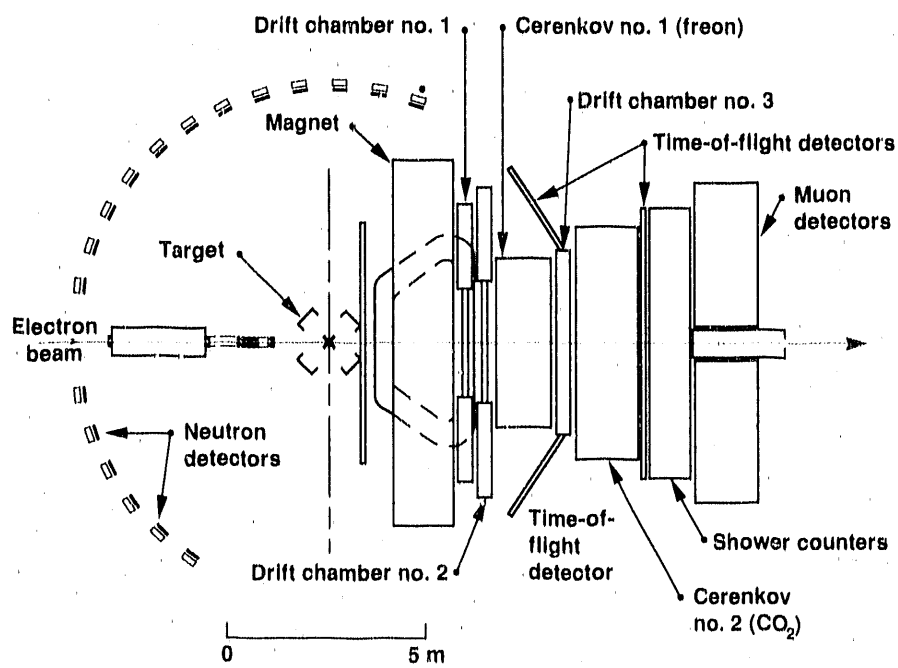


Figure 1. *Plan view of the PEGASYS facility. A beam of 15-GeV electrons enters from the left and scatters from nuclei on the target. The scattered electrons and most of the particles produced in the interaction with the target are detected in the spectrometer shown to the right of the target. Also shown is the array of detectors for measuring neutrons emitted by the struck nucleus. The types of particles produced and their momentum distributions will yield unique information on the behavior of quarks traveling through a nuclear medium.*

High-Temperature Superconductors: Novel Quantum Spin Liquids?

We suggest that high-temperature superconductivity may result from a novel quantum spin liquid in the CuO_2 layers, characterized by broken time-reversal symmetry and excitations with statistics intermediate between those of bosons and fermions. These conclusions follow from a model that we are attempting to justify from quantitative electronic structure calculations.

Electrons in the high-temperature (T_c) cuprate superconductors are both itinerant, as in common metals, and strongly interacting, as in localized atomic and molecular systems. This is in between existing theories, which stress one limit at the expense of the other. To understand this behavior, our strategy has been to eliminate all extraneous degrees of freedom in the model problem and retain only those low-energy excitations that might be relevant to the superconductivity. We have made considerable progress in solving such a model and in justifying its validity.

The insulating parents of the cuprate superconductors contain CuO_2 layers that are one electron short per formula unit of having full Cu(3d) and O(2p) shells. Our model allows these "holes," indicated by their spins, to occupy sites on the square lattice shown in Figure 1a. They are unable to move because strong repulsion inhibits two holes from occupying the same site. The metallic high-T_c cuprates are doped with extra holes (Figure 1b). Having already "paid the price" for double occupancy, such extra holes may move but, according to the Pauli principle, only to sites occupied by a hole of the opposite spin. We believe this constrained carrier motion lies at the heart of the high-T_c phenomenon.

The long-range up-down spin order (spin solid) in Figure 1a becomes disordered (spin liquid) at the observed dopant concentration, as in Figure 1b. We have previously argued that this spin-liquid state in the CuO_2 layers should be isomorphic to the fractional quantum Hall state, observed when certain semiconductor interfaces are placed in a strong magnetic field. The implications of this isomorphism are far reaching. Most dramatic is that a doped hole and its accompanying eddy currents in the spin background act like a particle halfway between boson and fermion character (a semion). We have shown that such half-fractional statistics necessarily imply superconductivity below some temperature.

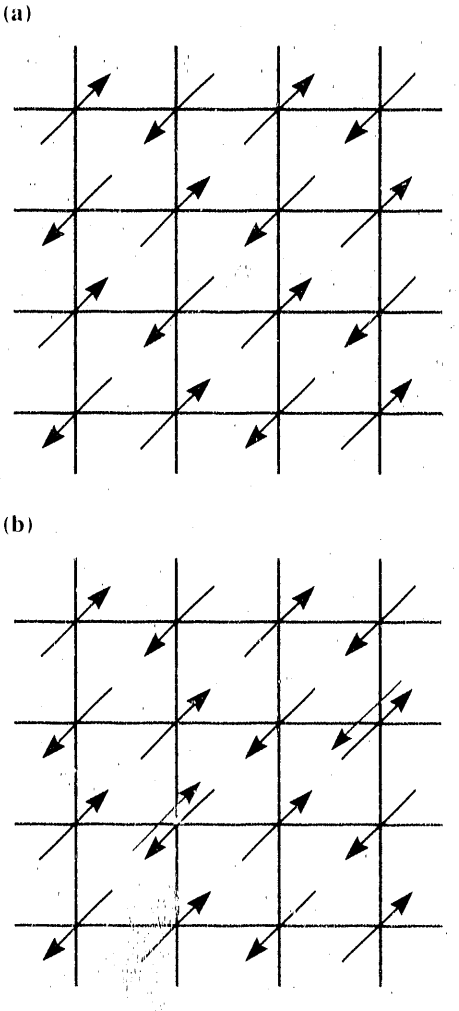


Figure 1. *Holes (spins indicated by arrows) in the CuO_2 layers of the high-T_c cuprates: (a) insulating parents, and (b) extra holes (colored arrows) responsible for superconductivity in the doped materials.*

Our work this year also supports the view that broken time-reversal symmetry must follow from the liquefaction of the spins. The above-mentioned eddy currents must then be either clockwise or counterclockwise in the ground state. This chiral nature of the spin liquid is a telling signature of the proposed state and is subject to experimental confirmation.

Figure 1 sketches the one-band Hubbard model, which incorporates only one type of state of mixed Cu(3d)-O(2p) character. Our effort is focused on an intermediate step—an extended Hubbard model—that admits all possible Cu(3d)-O(2p) hybrids. Although existing electronic structure techniques fail *in toto* for the itinerant yet strongly interacting states in the cuprates, we have shown how such methods can provide realistic, quantitative values of parameters defining extended Hubbard models for states exhibiting any degree of localization.

We have also generated such models for the insulating cuprate parent La_2CuO_4 and for the isostructural compounds La_2NiO_4, K_2CuF_4, and K_2NiF_4 and are solving them to demonstrate their quantitative validity against measured data for the insulating gap and magnetic character. Since only La_2CuO_4 can be doped to high-T_c superconductivity, we are seeking differences in the low-energy scale that will correlate with the presence or absence of superconductivity.

Contact: R. B. Laughlin (415) 422-7354, A. K. McMahan (415) 422-7198, or J. B. Grant (415) 423-4415.

Determining Why Climate Models Disagree

Climate models significantly disagree in their simulations of CO_2-induced climate change. We are attempting to identify the causes of these disagreements and to reduce the models' systematic errors.

Models of climate and climate change are built on the dynamical equations that govern the behavior of atmospheric wind, temperature, pressure, and moisture. These equations are supplemented by parameterizations of the heating caused by radiation and phase changes and by the turbulent fluxes of heat, moisture, and momentum. (Because such physical processes occur on scales that cannot be explicitly resolved by the model, they must be indirectly represented or "parameterized.") The models are normally solved in a global domain with between 2 and 20 levels in the vertical dimension and with either a spectral or finite-difference resolution of several hundred kilometers in the horizontal dimension. When integrated over several model years with realistic boundary conditions (which include the solar radiative flux, atmospheric composition, sea-surface temperature, and the earth's topography and albedo), such models yield a reasonably accurate simulation of the large-scale climate as presently observed. However, closer inspection reveals systematic errors in all variables, especially in those that are dependent on the parameterized convection and cloudiness.

We made a preliminary comparison of these models and found substantial differences in the climate simulated on regional and local scales (i.e., 1000 km) for both present and increased carbon dioxide (CO_2). As a result, predictions of the globally averaged surface warming to be expected when CO_2 concentrations double, as is anticipated in the next century, are uncertain by a substantial factor: they vary between about 2 and 4°C. It is not known whether this uncertainty is due to the models' formulation, resolution, or physical parameterizations, or whether it is a characteristic of such models (i.e., a reflection of their chaotic nature). We note, however, that the dozen or so climate models in current use have not been run under standard conditions or validated in a uniform way.

The purpose of LLNL's newly established Program for Climate Model Diagnosis and Intercomparison (PCMDI) is to determine the reasons for this uncertainty through a systematic program of comparative numerical experimentation, diagnosis, and intercomparison with a suite of representative climate models. In cooperation with the international modeling community, we have begun by examining the role of clouds in the earth's radiation budget. Preliminary results[1] reveal that the radiative effect of clouds on climate sensitivity varies by a factor of three among current models. Thus, a model's treatment of clouds is an important factor in its simulation of the possible climate changes due to increased CO_2.

A second critical factor in climate simulation is the horizontal resolution of the model. To examine this effect, we are cooperating with the European Centre for Medium Range Weather Forecasts in a series of extended integrations of their latest global model at four resolutions (Figure 1). The highest of these resolutions (the 1-deg grid) is about three times that used previously in climate simulation. By comparing the results from these calculations, we expect to be able to determine the dependence of a models' systematic errors on resolution and to test a variety of diagnostic, validation, and visualization programs.

Reference

1. R. D. Cess et al., *Science* **245**, 513 (1989).

Contact: W. L. Gates (415) 422-7642.

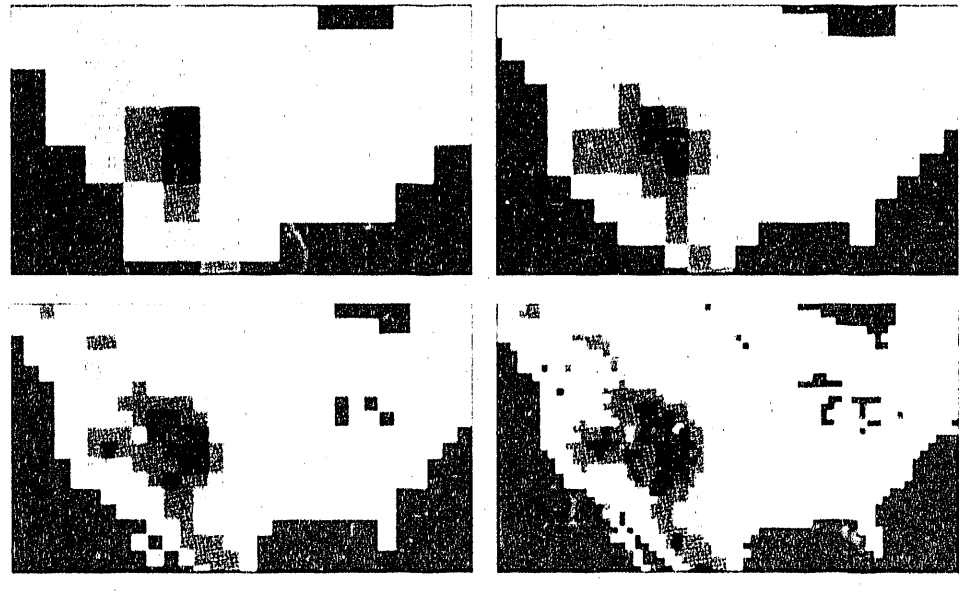


Figure 1. *The surface elevation and outline of North America at resolutions of 5-, 3-, 2-, and 1-deg latitude and longitude (color gradations are at 350-m intervals).*

Advanced Modeling of Thermonuclear Reaction Cross Sections

We have developed a unique computational modeling capability that enables us to calculate cross sections for thermonuclear reactions starting from the interaction between individual nucleons.

In order to model complex phenomena ranging from astrophysics to the design of fusion reactors and nuclear weapons, we need to know how the light charged particles—protons, deuterons, tritons, helium-3 nuclei, and helium-4 nuclei or alpha particles—interact with themselves and other light nuclei (atomic weight ≤ 16) at low energies. For these kinds of processes (called thermonuclear reactions), there is a need for more information on reaction cross sections than can be currently measured (the reaction cross section is a measure of the likelihood that the reaction—e.g., fusion—will occur). To address these needs, we have developed a unique computational modeling capability that allows us to calculate these cross sections starting from the nuclear force that acts between individual nucleons in the nucleus of atoms (the nucleon-nucleon interaction).

Two motives are driving this modeling effort. First, we want to improve the nuclear-reaction cross section data on which more macroscopic calculations of complex phenomena are based. Second, we want to further our understanding of the nuclear force by using the existing experimental nuclear-reaction database to test and constrain our model for the nucleon-nucleon interaction—the starting point for our cross-section modeling. This, in turn, provides the necessary feedback on how well we can calculate unmeasured or even unmeasurable cross sections. Furthermore, it gives us confidence in the accuracy of the calculated cross sections we produce for the macroscopic calculations of more complex phenomena (e.g., the design of fusion reactors).

In our modeling process, we must calculate wavefunctions for the states of the nuclei of interest. These nuclear structure calculations require a knowledge of the nucleon-nucleon interaction and a set (model space) of possible arrangements (configurations) of the nucleons in the nucleus. The nature of our cross-section modeling often requires that the structure calculations be performed with a large number of configurations (i.e., large model spaces). Previous nucleon-nucleon interactions that worked in small model spaces often fail in these large spaces because of various basic shortcomings, such as incorrect saturation properties.

We are developing a nucleon-nucleon interaction for use in large model spaces that has multiple components of different finite ranges and includes certain essential features such as density dependence and nonlocality. The assumed forms for our basis wavefunctions and the radial behavior of the individual components of the interaction allow us to obtain analytic, closed-form expressions for key macroscopic properties (e.g., binding energy per nucleon, saturation condition, incompressibility) of finite nuclei and infinite nuclear matter. We then use the known values for some of these macroscopic properties to determine the parameters of our interaction.

Three particularly important features of this nucleon-nucleon interaction are:

(1) We obtain the proper saturation behavior for an entire range of nuclei, including the nuclei of interest.

(2) The nonlocality can have the effect of providing a natural truncation of the model space by reducing some of the coupling between the simple and more complicated configurations.

(3) When taken in the short-range limit, the interaction reduces to the form of an interaction widely used in other nuclear physics calculations that do not depend on having a finite-range interaction.

Once we determine the form for the nucleon-nucleon interaction, we use the nuclear shell model code CRUNCHER[1] to perform the large-basis structure calculations. To understand how the nuclear structure determines the reaction cross sections, consider one of the most important thermonuclear reactions. When a low-energy deuteron (d) interacts with a triton (t), the compound nucleus ^{5}He is formed.

This compound nucleus can then decay back to a deuteron and a triton (elastic scattering), or a nuclear reaction can take place yielding a neutron (n), an alpha particle (α), and 17.59 MeV of additional energy. For the given incident energy of the deuteron, the probability of forming the compound nucleus depends on how much the ^{5}He nucleus at the corresponding excitation energy "looks like" a deuteron and a triton coupled together; that is, it depends on the wavefunctions (nuclear structure) of the deuteron, the triton, and the ^{5}He nucleus. Correspondingly, the way in which the compound nucleus decays is determined by how much the ^{5}He nucleus "looks like" a deuteron and a triton coupled together as compared with how much it "looks like" a neutron and an alpha particle coupled together. The quantification of "looks like" is called a spectroscopic amplitude.

Unique to the CRUNCHER code is the generalized formulation of multinucleon spectroscopic amplitudes that are required to describe typical thermonuclear reactions, such as:

$$(d + t) \rightarrow (n + \alpha + 17.59 \text{ MeV})$$

or

$$(d + {}^3He) \rightarrow (p + \alpha + 18.35 \text{ MeV}) .$$

Reaction cross sections are then obtained from the spectroscopic amplitude information by employing a multilevel, multichannel R-matrix reaction formalism.[2] We have already done considerable work using the R-matrix to describe experimental nuclear data by simply adjusting the parameters of the formalism. Using our new method, we can predict these parameters by the nuclear structure calculations and by the underlying nucleon-nucleon interaction.

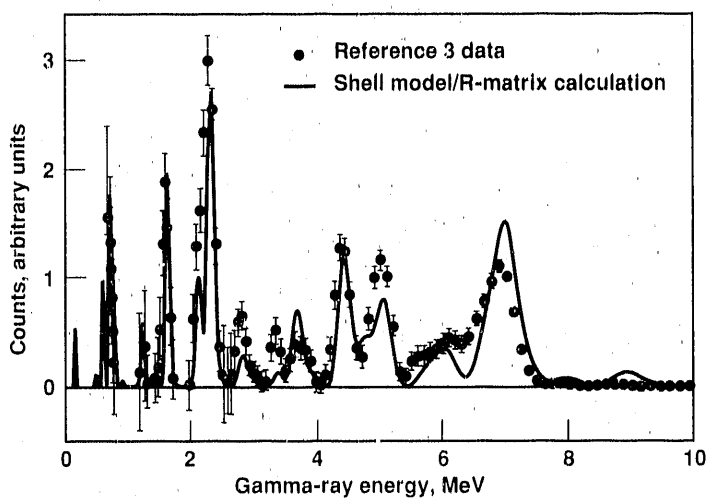


Figure 1. *Calculated and measured gamma-ray spectra for the $^{14}N(n,x\gamma)$ reaction at a laboratory angle of 125° for incident neutrons with energies between 10 and 12 MeV. This result represents our most complex calculation to date.*

Our modeling is not restricted only to thermonuclear reactions. In Figure 1, we compare a measured gamma-ray spectrum[3] with the result of one of our most complex calculations in which the gamma-ray yields from 32 individual gamma-producing reactions have been combined. As can be seen, our calculation is in excellent agreement with the experimental data, particularly considering the fundamental nature of these calculations.

We are continuing to develop our nucleon-nucleon interaction to accurately describe such well-known thermonuclear reactions as (d + t) and (d + ^{3}He). We will then be able to use this interaction to calculate the cross sections for other reactions, such as (d + ^{6}Li), that are important for fusion applications but for which limited experimental measurements exist.

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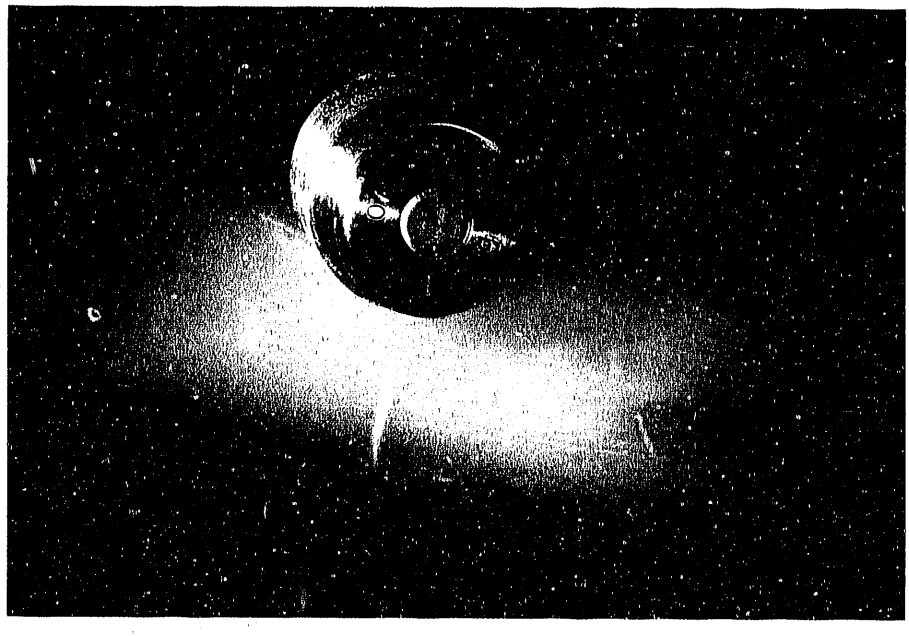
Contact: D. A. Resler (415) 423-0451 or R. M. White (415) 422-9668.

Chemistry and Materials Science



This block of "frozen smoke," actually a silica aerogel foam, can support 1600 times its own weight.

The Chemistry and Materials Science (C&MS) Department is responsible for providing the Laboratory with expert knowledge about the science and engineering of various materials and their properties, especially their synthesis, reactions, and characterization by chemical and physical means. We are particularly interested in advanced materials—substances that are distinguished by their usefulness under extreme conditions of temperature, pressure, density, and/or hostile environment. For example, we are studying certain mixed oxides that become superconducting at (relatively) high temperatures. Another fascinating advanced material is "frozen smoke," actually a silica aerogel foam. This new material has a vanishingly small density of 5 mg/cm^3 (one two-hundredth the density of water or slightly more than four times the density of air) but an unusually high relative mechanical strength—this 5-mg/cm^3 silica aerogel foam can support 1600 times its own weight.

Metallurgy is also an important research area in the C&MS Department. The behavior of metals under high deformation and of metals that have been deformed very rapidly are topics of particular interest. The properties of thin films of metals are under scrutiny; their mechanical strength or electronic behavior may be very different from that of the bulk metal. Theoretical studies are an important part of our metallurgy effort. A new method to calculate phase diagrams from first principles—that is, without fitting to empirical data—is described in this section.

The ability to analyze and characterize the composition of samples of materials is a key strength of C&MS. Two achievements are highlighted in following articles. In the first, x-rays from a synchrotron are used to follow the course of a solid combustion reaction; Bragg

scattering spectra, obtained sequentially in milliseconds, make it possible for us to follow the changing crystal structure as the reaction proceeds. In the second, computer software has been developed that can recognize patterns of mass spectra from unknown petroleum samples to determine their origin. We also have exciting projects in scanning tunneling microscopy, laser spectroscopy, laser-ionization mass spectroscopy, and magnetic resonance for characterizing samples as functions of time, space, element, topography, and other parameters of interest.

The properties of interfaces are critical to understanding bonding and adhesion between materials. We are investigating the behavior and properties of surfaces and interfaces both experimentally and theoretically. These studies must be done at the microscopic level and must address the phenomena at the level of atoms and molecules. A new theoretical approach that makes possible a first-principles description of the density of electronic states at a surface is one of the highlights of our work in this area.

Much of the work done by C&MS supports LLNL's weapons programs. For example, we have developed an ultrahigh-strength adhesive for a special beryllia bond and have perfected the associated application procedures. When properly applied, bond strengths of this epoxy are as high as 55 MPa (8000 psi). In another weapons-support project, we are evaluating a stainless-steel/stainless-uranium joint that replaces an expensive welding procedure and may allow the expensive stainless-uranium parts to be reused.

C&MS has traditionally been home to the Laboratory's research effort in high explosives and energetic materials. In one current research and development project, we are attempting to synthesize new compounds that have a high energy content but are less sensitive to shock and are otherwise less susceptible to inadvertent detonation. A spectroscopic study of the detonation process in a high-pressure cell has provided new insights into the sensitivity of such energetic materials. Theoretical studies of the complex chemical reactions that constitute the explosion process are in progress.

Other kinds of chemical synthesis are also of interest. For example, we are developing new, low-Z (atomic-number) polymers for inertial-confinement fusion (ICF) applications. In still other projects, we are making advances in the synthesis of new organometallic compounds or biomimetic compounds that can catalyze the oxidation of methane.

In a special C&MS project, we are attempting to polarize the nuclear spins of the deuteron and triton in the deuterium-tritium molecule. Such a configuration is expected to increase the fusion cross section substantially and thus would lead to a more cost-effective ICF system. Significant progress has been made in this very difficult process. The C&MS Department is also involved in a variety of other energy-related projects in fossil fuels, oil recovery from shale, and improved methods of petroleum exploration.

Contact: C. Gatrousis (415) 423-2851 or T. T. Sugihara (415) 423-8351.

The Chemistry and Physics of Modified Superconductors

We have been exploring a low-temperature process using bromine gas for converting initially insulating $YBa_2Cu_3O_6$ to a material that is superconducting at 90 K. In addition, our new technique for detwinning $YBa_2Cu_3O_7$ single crystals allows Raman analysis of the electron-phonon interaction along different crystal directions. We have also determined that these twin boundaries maintain (desired) high critical currents.

The goal of our research in superconductivity at relatively high transition temperatures, T_c, has been to elucidate the basic mechanisms that underlie the superconductivity of this class of materials. Over the past year, we have begun to use the expertise developed in our basic research to address the important issues involved in developing the new superconductors into commercial products. Our approach has been to create high-quality samples that have been modified in specific ways to investigate such effects as charge transfer, vortex pinning sites, and the electron-phonon interaction. In many cases, these studies involve the growth of large single-crystal samples, and are done in collaboration with the Physics Department at the University of California, Davis.

While all high-T_c superconductors are oxides, the role of oxygen in the $YBa_2Cu_3O_{7-d}$ system is especially crucial. Part of the function of the oxygen in $YBa_2Cu_3O_{7-d}$ superconductors is to dope holes onto particular CuO planes where the superconductivity occurs. When no excess holes are present, there are no mobile holes or electrons to carry a current, and the material is an insulator (not a conductor).

To study the role of charge transfer, we have successfully substituted bromine into initially insulating $YBa_2Cu_3O_6$ powder and obtained a material that is superconducting at 90 K. The bromination process differs significantly from oxygenation in that it can be carried out at low temperatures (260°C) and in only a few minutes. By contrast, oxygen treatments require temperatures of ~500°C for 8 to 12 hours. Figure 1 shows the relationship between the processing conditions and the fraction of the material that is superconducting. This processing temperature (<300°C) makes it possible, for the first time, to consider integrating high-T_c materials into conventional electronics-processing applications.

We have begun studying the properties of the resulting compound $YBa_2Cu_3O_6Br$ to determine its crystal structure, microscopic phase purity, thermal stability, oxygen content, and superconducting properties. The x-ray deficient data suggest that although the bromine may be displacing some oxygen atoms from lattice sites, the bromine is itself in interstitial or intercalated positions. We have also demonstrated that the bromination process is effective in improving the properties of oxygen-deficient thin films, a discovery with important potential electronics applications.

In a separate study, we have developed a simple uniaxial compression technique to detwin $YBa_2Cu_3O_7$ single crystals. It is well known that twins in $YBa_2Cu_3O_7$ are formed when samples are cooled from high temperatures to room temperature, and a shear deformation occurs during the phase transformation from the tetragonal to

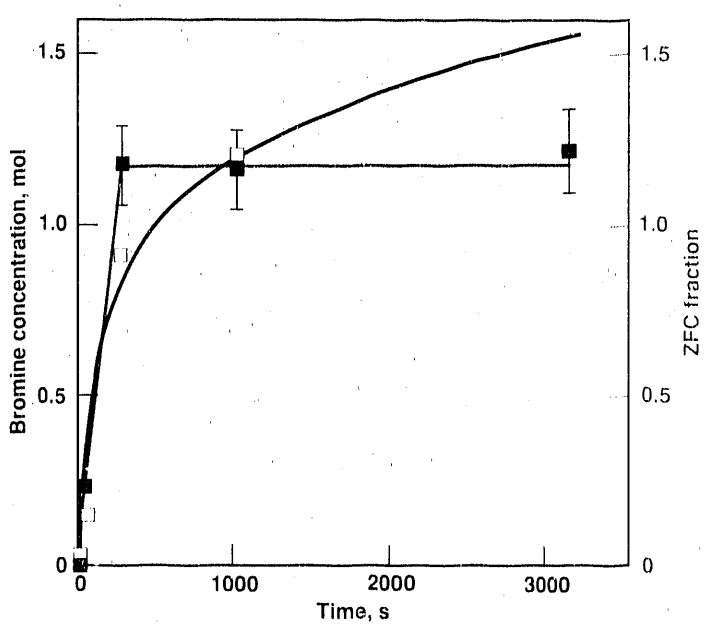


Figure 1. *Meissner fraction and weight gain vs bromine exposure time at 260°C. Bromine concentration follows a logarithmic dependence, indicating a diffusion-limited process. The plateau in the magnetization data (zero field cooling, or ZFC) indicates the optimal concentration for bromine under these conditions.*

the orthorhombic structure. This deformation causes the crystal to grow with an intertwining of the *a* and *b* axes in the basal plane, making it impossible to distinguish between these two axes. Therefore, to study the anisotropic properties of the crystals along the three directions, *a*, *b*, and *c*, we must first detwin the material.

$YBa_2Cu_3O_7$ single crystals used in this study were grown by a modified self-flux technique. Magnetization measurements on these crystals (Figure 2) show a transition temperature of 93 K with a transition width <1 K, indicating a very-high-quality sample. Crystals with at least one pair of parallel plane facets were chosen as candidates for detwinning, which we perform by applying uniaxial compression.

The critical current density, which measures the amount of current a superconductor can carry before it returns to the normal resistive stage, was measured on these same crystals before and after the detwinning treatment. By comparing critical current densities for the twinned and detwinned samples, we can determine how effectively twins impede the motion of magnetic flux vortices, an important mechanism for causing resistive losses in a superconductor. In collaboration with Argonne National Laboratory, we measured the critical current density along the *c* axis in the twinned and detwinned states and determined that the twin boundaries contribute a substantial fraction of the observed critical currents.

$YBa_2Cu_3O_7$ has been studied extensively by Raman spectroscopy, but with single crystals containing high densities of twins that

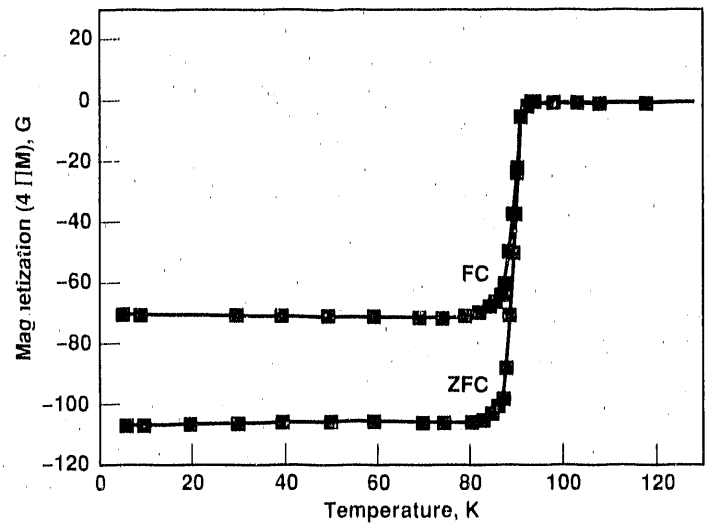


Figure 2. *Curves for the Meissner effect, or field cooling (FC), and shielding effect, or zero field cooling (ZFC), obtained for a typical twin-free crystal in a field of 20Oe parallel to the crystal's c axis. The transition temperature for this sample is 93 K, and the transition width of <1 K indicates a very-high-quality sample.*

interchange the *a* and *b* directions. Along the *b* direction are the oxygen atoms that form the Cu(1)–O(1) chains. There are no equivalent oxygen atoms along the *a* direction and hence no Cu(1)–O(1) chains in this direction. In collaboration with Sandia National Laboratory, we used the detwinned crystals to do a complete mapping of all the phonon modes.

Previously unreported features are seen in the spectra obtained with the incident laser beam propagating along the Cu(2)–O(2)&(3) planes. In particular, the degree of antiresonance (penetration of the Raman line below the background) of the 116-cm^{-1} phonon (a barium-atom vibration along the *c* axis) is much greater for polarization along the Cu(1)–O(1) chains than for polarization perpendicular to the Cu(1)–O(1) chains. Significantly, no antiresonant behavior is observed for this barium vibration in the spectra with light polarized along the *c* axis despite intense scattering from an electronic continuum.

The observed antiresonance is important because it is a characteristic signature of the interaction of a discrete phonon with the electronic continuum. In traditional superconductors, it is the electron-phonon interaction that underlies the pairing of the electrons and therefore the superconductivity. This type of Raman information, which can relate the strength of the electron-phonon interaction to the important crystal directions, is crucial to our attempts at understanding the role that the electron-phonon interaction still plays in the high-T_c oxide superconductors.

Contact: M. J. Fluss (415) 423-6665 or H. B. Radousky (415) 422-4478.

Fingerprinting Petroleum Problems

New gas chromatographic-mass spectrometric software makes it possible to match the chemical fingerprints of complex mixtures of organic compounds.

Monitoring the environment for chemical contaminations is a prime concern of both government and industry. One particularly pressing problem is to identify leaking underground fuel storage tanks and to clean up the contaminated area. In the U.S. alone, more than 3.5 million underground storage tanks are in use, most of them 30- to 40-year-old gasoline tanks. Approximately 75,000 to 100,000 of these have rusted and are leaking fuel into the surrounding soil and groundwater, and another 350,000 or more will begin leaking in the next five years. Often the contamination is discovered a sizable distance from its source, and the urgent need has been to trace the leak to its exact source—the particular underground tank—as quickly as possible.

Computer-guided gas chromatography-mass spectrometry (GC-MS) can routinely be used to perform trace analyses of environmental hydrocarbon contamination. Ultralow detection levels can now be achieved, and organic compounds in a sample can be characterized easily and exactly. However, seldom have the GC-MS data been used to pinpoint the exact source of the contamination. We have developed new software that enables us to do just that; we can now "fingerprint" contaminant organic compounds and apply statistical and pattern-recognition methods to identify the source of the contamination.

Our approach is to collect both the unknown fuel from the contamination site as well as samples of authentic fuels from known storage tanks in the area. Capillary gas-chromatographic columns, each containing one of the samples to be analyzed, are interfaced directly to GC-MS instrumentation. From the GC-MS data, we can choose mass-chromatogram plots that correspond to fragment ions that are indicative of unique fuel components (Figure 1). Mass-chromatogram plots are used to highlight the major and minor components in the sample; often, the minor compounds are the most diagnostic.

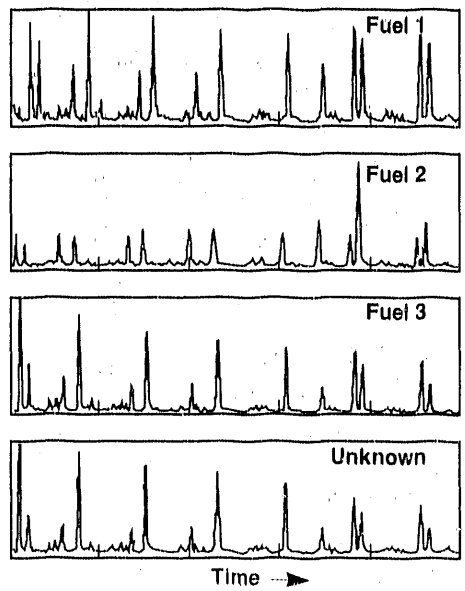


Figure 1. *Mass chromatogram plots comparing a fragment ion (m/z = 57) in three authentic fuels and an unknown fuel.*

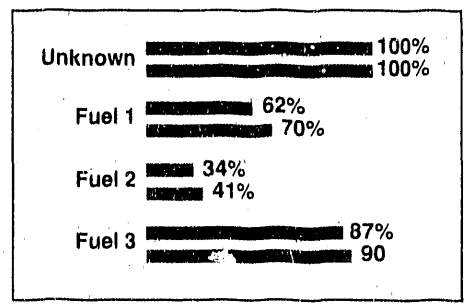


Figure 2. *Summarized data, unweighted (green) and weighted (gray), from many mass chromatogram comparisons identify the sample most similar to the unknown.*

The key to this approach is the new software we have developed for comparing computer-generated mass-chromatogram plots. By applying statistical and automated pattern-recognition methods to weight the contribution of each mass chromatogram, we directly compare the chemical fingerprints of the unknown fuel to those of the authentic fuels. The automated pattern-recognition software allows us to identify the authentic fuel that is most like the unknown fuel and to conclude with reasonable confidence that its tank is the source of contamination (Figure 2).

We have applied our GC-MS fingerprinting technique to many gasoline and petroleum fuel contamination sites, and every underground tank that we identified as suspect was proven indeed to be leaking. From these studies, we have elaborated our analytical techniques and have further improved the automated GC-MS software to the point that ultratrace (part-per-billion) analyses can be performed simultaneously on a large suite of chemicals to generate a fingerprint. This capability to analyze all compounds simultaneously at part-per-billion levels will find use in a wide variety of environmental samples and in many applications where trace-level chemical comparisons are needed, such as quality control in pharmaceuticals, the food and beverage industries, and the forensic sciences.

Contact: B. Andresen (415) 422-0903.

Chemical Dynamics of Solid-Combustion Reactions

We are using intense synchrotron x-radiation to follow the phase transformation of fast, high-temperature, solid-combustion reactions in real time down to 50 ms or less.

The solid-combustion process is used to synthesize diverse materials including ceramics, intermetallics, and composites. Much heat (>50 kJ/mol) is released during these solid-state reactions. Once they are initiated with an external source, these high-temperature synthesis reactions become self-sustained and propagate to completion within seconds. They consist usually of a starting powder compact of at least one solid reactant and are characterized by a fast-moving combustion wavefront (1–100 mm/s) and a high self-generated temperature (1000–4000 K). Conventional techniques allow us to measure wave velocities and temperature profiles as a function of time and sample position and to examine product phase(s) and microstructure; however, because of high temperatures and combustion rates, they do not allow *in-situ* real-time investigation of the combustion wavefront. Further development of solid combustion as a method to process and synthesize materials will depend heavily on directly monitoring the phase transformation and understanding the chemical kinetics of these complex reactions.

Using high-intensity synchrotron radiation, we conducted a series of proof-of-principle, time-resolved, x-ray diffraction experiments (at the Brookhaven National Synchrotron Light Source) to follow the phase transformation in several solid-combustion systems. To record the time-resolved diffraction patterns from the reacting specimen situated in a specially designed reaction-chamber diffractometer, we used a position-sensitive photodiode array able to record a full scan of 1024 pixels in 4 ms. A thermocouple embedded in the sample just upstream of the x-ray diffraction area triggered data collection. The diffraction peaks within a 6° window of 2θ space were recorded by computer at a set scan time and total scan time.

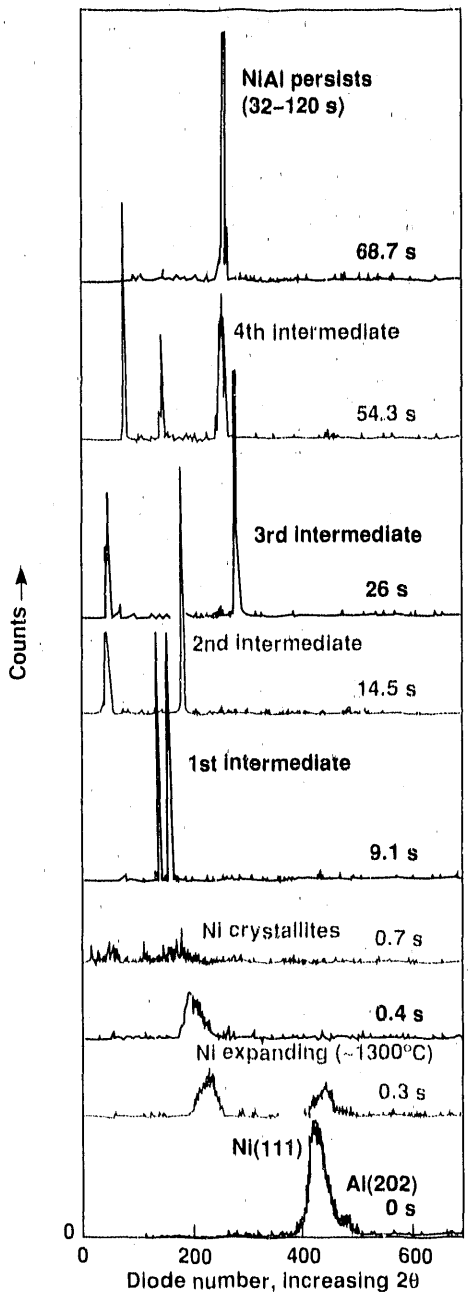


Figure 1. *Time-resolved x-ray diffraction scans of the Ni + Al reaction, showing critical phase changes of the reactants: appearance and disappearance of a series of apparent "reaction intermediates" before the final NiAl product is formed.*

Figure 1 shows the high-speed, time-resolved diffraction data for the Ni + Al reaction at ~1500°C. The detector was triggered at 0 s, and lattice expansion of the Ni reactant occurred on heating. The disappearance of the Ni peak was followed immediately by four apparent sets of diffraction peaks in the intervals 2.0–11.7 s, 13.5–17.5 s, 20–30 s, and 49.2–68.7 s. Some time later, these lines disappeared, as is characteristic of those of reaction intermediates. Finally, the NiAl product (110) peak appeared and lasted for the duration of the diffraction scans. With a focused beam and a higher x-ray flux, we achieved a 10-ms resolution with this system.

We have opened a new route to study the chemical dynamics and phase transformation of reactive systems *in situ* at high temperature and under other external perturbations (e.g., pressure, unidirectional stress, shock) in the millisecond domain. With increased photon fluxes (10^{12}–10^{16} photons/s) from third-generation synchrotron sources such as those of the Advanced Light Source at the Lawrence Berkeley Laboratory and the Advanced Photon Source at Argonne National Laboratory, submillisecond resolution is possible, and dynamic events in materials can be investigated in the microsecond regime.

Contact: J. Wong (415) 423-6385.

Electronic Structures of Surfaces

We have devised a method of calculating the electronic structure of surfaces, interfaces, and dislocations in metals.

The Laboratory spends much effort attempting to understand and exploit the properties of materials. Crucial to this effort is understanding the behavior of the electrons in the material, the "glue" that holds substances together. These electrons move about in very complicated ways, and cataloging their behavior is by no means simple. We can nevertheless obtain a great deal of information if we know the energetics of the electrons; in particular, if we know how many electrons per unit volume can, in principle, be found in a small range about a given energy. The function containing this information is called the density-of-states (DOS) function.

Many methods have been developed to evaluate the DOS function, ranging from numerical techniques to fully first-principles quantum-mechanical procedures. To deal with the characteristic complexity of real systems, DOS calculations usually employ sets of simplifying assumptions. One common assumption is that the material possesses perfect periodicity—that is, what happens in a small region of the material (such as a cell) is exactly what happens throughout the system. Although methods based on such assumptions often reveal much useful information, they cannot be used on systems with broken periodicity, such as surfaces and grain boundaries. Yet these systems are often of paramount scientific and technological importance. Clearly then, we need methods for studying the DOS functions of systems with reduced symmetry within a first-principles formalism.

We have developed just such a method, one employing the concept of semi-infinite periodicity and the property of removal invariance. A system that repeats periodically along a given direction is said to possess semi-infinite periodicity; since removing a finite number of repeating units from the free end of such a system does not change its properties, it also thus displays removal invariance. Exploiting these two concepts, our techniques enable us to obtain the DOS function for systems of reduced symmetry, such as internal interfaces, stacking faults, and grain boundaries, which might otherwise defy a truly first-principles treatment. The method used to carry out calculations is based on a formulation of multiple scattering theory in real space and was originally developed from laboratory observations.

Figure 1 shows the DOS curves for pure elemental copper and for a tilt grain boundary in copper. The two curves show similarities and differences. The similarities, such as the two peaks at higher energies, reveal which bulk symmetries are retained by the grain boundary. The differences have to do with that part of the symmetry that is lost. We can also extract other information (for example, about the energetics of the system) from such calculations. At present, we are working to calculate the DOS functions for other reduced symmetry systems, such as dislocations, and are refining our computer codes.

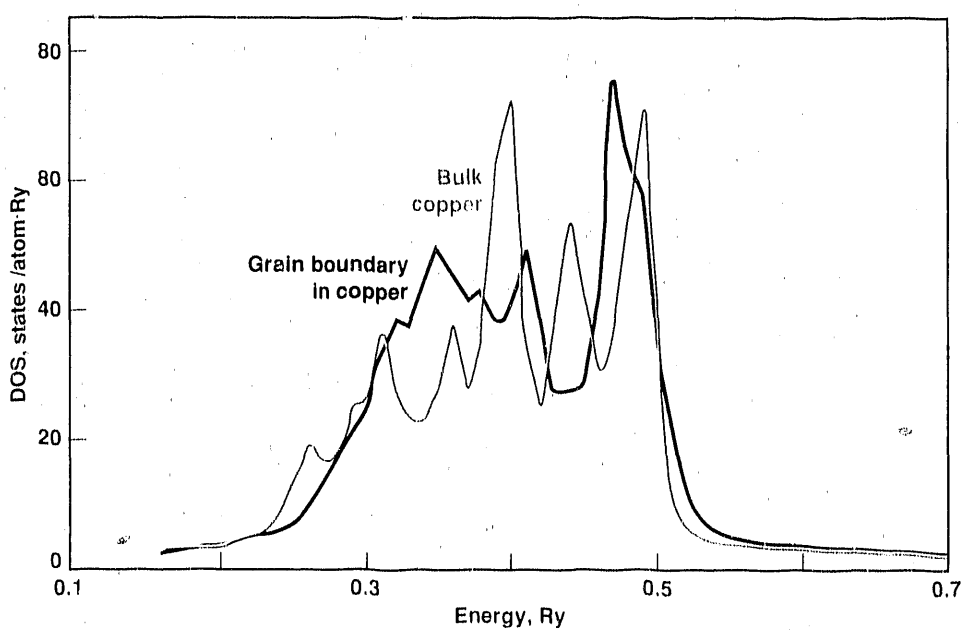


Figure 1. *DOS curves as a function of energy for bulk copper and a grain boundary in copper.*

Contact: A. Gonis (415) 422-7150.

From Electronic Structure to Phase Formation in Alloys

The study of ordering mechanisms in substitutional alloys is of great theoretical and technological value in the field of alloy phase formation. Our work demonstrates the validity and predictive power of the advanced methodology we have recently developed.

Addressing the problem of phase stability in substitutional alloys requires that we first ask what crystalline structure and atomic configuration an alloy system will probably exhibit at a given temperature and concentration. Usually the answer is summarized in a phase diagram that shows, in a temperature-vs-concentration representation, the domains of stability of the phases that develop on various crystalline structures. This information constitutes the basic road map for the alloy designer during the processing and control of new high-performance materials.

Our approach is to perform *ab initio* calculations of phase diagrams and then deduce relevant physical properties. Thus, starting from the simple knowledge of the total number of electrons of the alloy species, our calculations combine accurate quantum-mechanical and statistical thermodynamic determinations of the contributions to the total free energies that build up a phase diagram. The alloys studied so far include Pd-V, Pd-Rh, Ti-Cr, Ti-V, Cu-Zn, Ni-Ti, and Ni-Al, all of which present interesting physical properties. By studying the interplay between electronic properties, crystalline structure, and configurational order in alloys, we have acquired a better understanding of phase formation in alloys at a microscopic level.

For example, we performed first-principles calculations of electronic band structure and statistical simulations for Cu-Zn and produced remarkable results. We determined an order-disorder temperature of the CsCl type of order occurring on the body-centered cubic structure near $Cu_{50}Zn_{50}$ that was only 50 K higher than the experimental value. We also calculated an extremely small antiphase boundary energy in the Cu_3Au type of order, on the face-centered cubic structure, near Cu_3Zn, which is indicative of the possible existence of long-period superstructures around this composition (as recently suggested experimentally). Finally, the theoretical phase diagram closely matches the experimental one, with the signature of a structural transformation at low temperature, around $Cu_{50}Zn_{50}$, as observed experimentally.

To test the predictive capability of our theoretical tools, we recently performed a detailed analysis of the possible ordered states that can exist in alloys based on complex crystalline structures, such as A15, known otherwise for its superconductive properties. Besides the well-known ordered configuration of the composition A_3B, we predicted two new states, called X and Y in Figure 1, and have studied their stability properties. We have made phase-diagram computations and have initiated an experimental program to substantiate such findings.

Thus, in studying phase-stability properties, including order-disorder phenomena and structural transformations, we have acquired an in-depth knowledge at a fundamental level. Our use of a first-principles approach has yielded new concepts and predictions that support the experimental effort to design and process new classes of advanced materials.

Contact: P. Turchi (415) 422-9925.

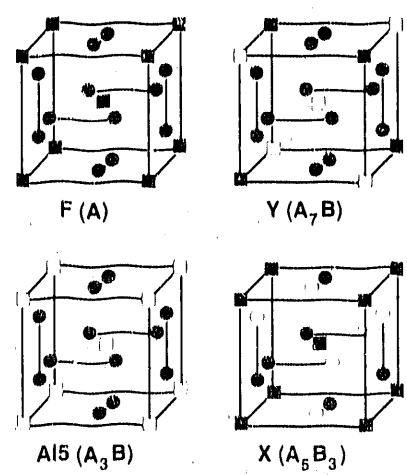
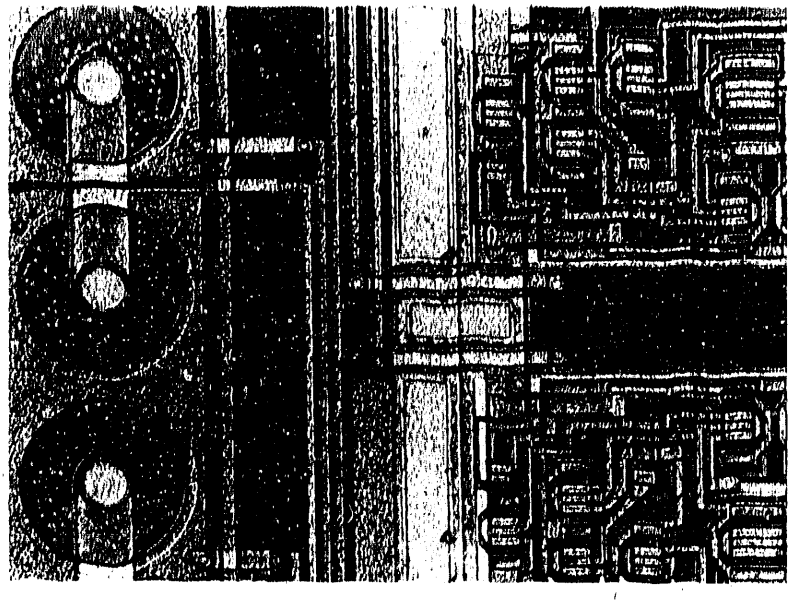


Figure 1. *Ordered configurations based on the A15 crystalline structure as deduced from theory. The solid squares and circles refer to the occupancy of the inequivalent sites by the A species; the open squares and circles refer to occupancy by the B species. The composition of each configuration is given in parentheses.*

Computations



Massively parallel computing and distributed computing, ever-increasing demands for archival storage, and the need for rapid visualization of scientific data are but a few of the challenges being addressed by the Computation Directorate.

The Computation Directorate is dedicated to providing high-quality computing services to the Laboratory, the Department of Energy, and other organizations as approved by the DOE. The Directorate works to assure that their computing requirements are effectively and efficiently served. This mission is particularly challenging since the computing field is changing rapidly on many fronts. The advent of massively parallel computing architectures, the new technologies for distributed computing, the increasing need to control software production costs, the insatiable demands for archival storage, and the need for data visualization of high-speed computing results are but a few of the challenges that are currently facing the computer industry.

The articles in this section illustrate the diversity of Computation's involvement. In addition to these highlights, the Computation Directorate has made notable accomplishments in new methods for solving linear and nonlinear problems, in software to control the Laboratory's isotope separation processes, and in computer-linked security enhancements for the LLNL site.

Much of the numerical modeling done for Laboratory problems requires the solution of very-large-scale systems of linear and nonlinear equations, and the solution of such systems demands the use of powerful iterative methods. For linear systems, the Computing and Mathematics Research Division (CMRD) developed a class of adaptive polynomial preconditioned conjugate gradient methods that are easy to implement and well-suited to vector and/or parallel computer architectures. The effectiveness of these new techniques was demonstrated in numerical

experiments on several architectures for problems arising in numerical modeling of groundwater flow, Stokes flow, elasticity, and constrained optimization. For nonlinear problems, CMRD developed Newton-like iteration methods, where the linear systems are solved only approximately by an iterative method. Methods for symmetric and nonsymmetric systems were combined with global convergence strategies to enhance their robustness. The convergence of the combined methods was analyzed, and the effectiveness of this approach was demonstrated on several problems, including a two-dimensional multi-frequency bidirectional laser oscillator model with up to 38,000 unknowns. Solution of such extremely large, nonsymmetric nonlinear systems has only just now become feasible with the development of these new techniques.

The Application Development Department (ADD) within the Computation Directorate provides software development expertise in areas such as physical simulation and modeling, real-time data acquisition and control, database management, graphics, and communications. This past year, the Laser Program Support organization within ADD completed a major milestone in the development of the supervisory control systems for the Isotope Separation and Materials Processing Program. A generalized control system was developed to perform the supervisory control functions for both the special isotope separation (SIS) and uranium atomic vapor lasers isotope separation (U-AVLIS) processes. The control system determines the interaction of all hardware on the two systems and issues commands to each front-end processor that controls a piece of hardware. The design of one control system for both the AIS and SIS processes substantially reduced the overall software development effort.

Also this year, the Safeguards and Security Enhancements Group within ADD completed the software development for three major new Laboratory security systems: CAIN II, SILAS, and Console. The CAIN II system controls access to portions of the Laboratory; in the numerous access booths, dispersed across the site, an individual's badge is checked against a personal identification number and other information. SILAS controls access to the secure vaults around the Laboratory. The Console system is the interface through which the Protective Service Officers monitor and control Laboratory security; communications with offices and facilities around the Laboratory are a major part of the Console system. These three systems are in daily use at LLNL. In addition, the Department of Energy has adopted the CAIN II system as a Department-wide standard, and at least one Department of Defense installation has requested that the CAIN II system be implemented at their facility.

Contact: R. R. Borchers (415) 422-9870 or J. E. Ranelletti (415) 422-3782.

Archival Storage System

Our software provides data-storage systems with automatic file migration between disks and tapes, and is particularly suitable for distributed environments. It has been licensed for commercial development and distribution.

Supercomputers have created the need for greatly expanded archival storage. We have developed new storage system software to meet this need and have licensed it to General Atomics (a San Diego firm). Under the licensing agreement, General Atomics will distribute and support the system under the name UniTree, paying the Laboratory a royalty for each system sold. Both the Laboratory and General Atomics will continue to develop the system and will share enhancements.

Through Unix-style directories, UniTree provides file and storage management with automatic file migration between storage media. UniTree keeps the most active files on magnetic disks, and automatically migrates less active files (identified by a formula including file size and time since last use) to magnetic tapes. The requester of a file need not know its location. As files are accessed, they are brought back from magnetic tape, if necessary, and sent to the user requesting them.

The LLNL system, controlled by an Amdahl 5868 mainframe, manages over six million files containing roughly seven terabytes of user data. Fifty gigabytes of new data are stored each week. The archive is stored on 40,000 magnetic tape cartridges, 30,000 of which are kept in the automated library (Figure 1). (The remainder, the least active files, are kept in a vault and must be manually remounted.) About 400,000 files are stored in a 180-gigabyte magnetic disk cache. Since most file requests access a small percentage of the archive (depending on user access patterns), the disk cache, representing less than 3% of the online storage capacity, serves over 80% of user requests. Since few requests require that tapes be mounted, the average time to access a file is reduced.

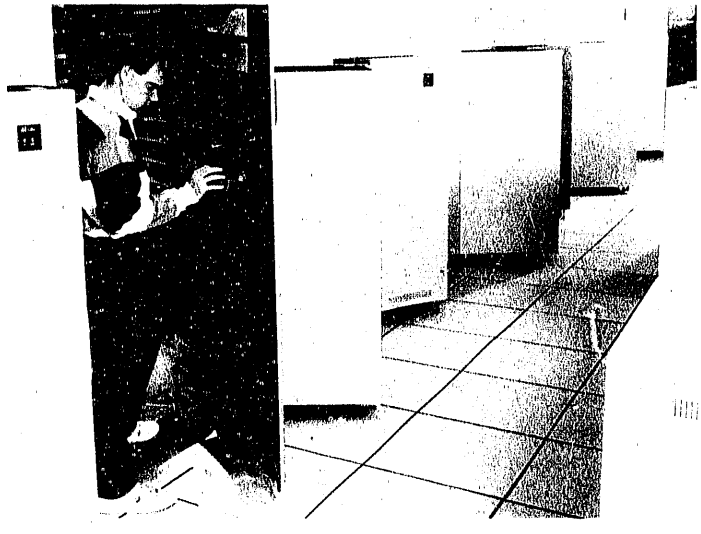


Figure 1. *The automated library, built by Storage Technology Corporation. Each of its five units holds 6000 magnetic tape cartridges and houses four tape drives. During periods of heavy load, the system moves cartridges automatically between units to reach available drives.*

The primary advantage of the new storage system is its software architecture, which emphasizes portability and modularity. An example of portability is that, although the LLNL system runs on Amdahl hardware, General Atomics will deliver the first UniTree systems on Digital Equipment Corporation machines. The modularity of UniTree allows it to be adapted more easily than previous systems to manage a variety of storage devices and to serve different networks and environments.

UniTree is particularly suitable for distributed environments, in which several independent machines cooperate to process user requests. It separates control and data streams so that control messages can take slow-speed paths and data can travel at high speed without interfering with each other. UniTree thus supports third-party file transfers in which data flow from source to sink (that is, in either direction between devices or between computers and devices) without moving through the process requesting the transfer. To separate requester-oriented naming mechanisms from the file identifiers (used by the disk and tape managers), name servers map between the two; these servers can be modified for different environments without changing disk and tape software. This feature also allows files and directories to migrate independently.

Contact: S. Coleman (415) 422-4323.

Adaptive Methods for Fluid Dynamics in Three Dimensions

Our adaptive numerical methods for modeling time-dependent, three-dimensional fluid flow combine high-resolution discretization techniques with local adaptive mesh refinement to focus computational effort where it is required.

Computational fluid dynamics plays a central role in numerical simulations arising in many LLNL and DOE mission areas, such as weapons design, weapons effects, fusion, and energy production. Such computations have typically assumed physical symmetry to reduce the dimensionality of the computation. However, there is an increasing need to perform calculations in three spatial dimensions. A common feature of three-dimensional (3D) flows is the appearance of small-scale, localized phenomena; one routinely encounters features such as jets, vortex rings, and mixing layers, whose characteristic length scales are small relative to the global dimensions of the problem, but whose dynamics play an important role in the overall physics. Adequate resolution of these phenomena using conventional spatial discretizations would require computational effort far in excess of the most optimistic projections for near-term growth in computational capabilities. To overcome this obstacle we are developing adaptive methods that will focus computational effort where it is most needed, significantly decreasing the computational resources required for modeling 3D flow phenomena.

As a first step in this development we have designed and implemented a 3D adaptive mesh refinement algorithm for Cartesian grids. This algorithm combines a high-resolution numerical integration scheme with local adaptive mesh refinement in which the finite difference mesh dynamically changes as a function of space, time, and data to maintain a fixed level of accuracy in the calculation. As our basic integration scheme, we are using a second-order variant of Godunov's method; it is a conservative finite-difference scheme that incorporates nonlinear wave-propagation properties of the flow to provide both high accuracy and robustness for strong shock waves.

The adaptive mesh refinement strategy employs a hierarchical grid structure composed of grids of varying resolution. The grid hierarchy is constructed from an initial coarse grid that uses an error-estimation procedure to identify cells having unacceptable errors. These cells are then clustered into grids that are subdivided to form finer cells where more resolution is required. This procedure is applied recursively until the desired accuracy is achieved or a maximum level of grid nesting is reached. The result is an extremely flexible method: the total number of mesh points in the calculation changes automatically as a function of time to concentrate computational effort in regions of greatest fluid-dynamical interest.

Figure 1 shows computational results obtained using the new method to model the collapse of an ellipsoidal cloud of Freon when hit by a shock wave. This calculation used two levels of refinement by a factor of four in each direction. Achieving comparable resolution with a single-grid computation would have required over one thousand hours on a Cray supercomputer; the use of adaptive mesh refinement reduced that time by a factor of ten.

Contact: J. Bell (415) 422-7105.

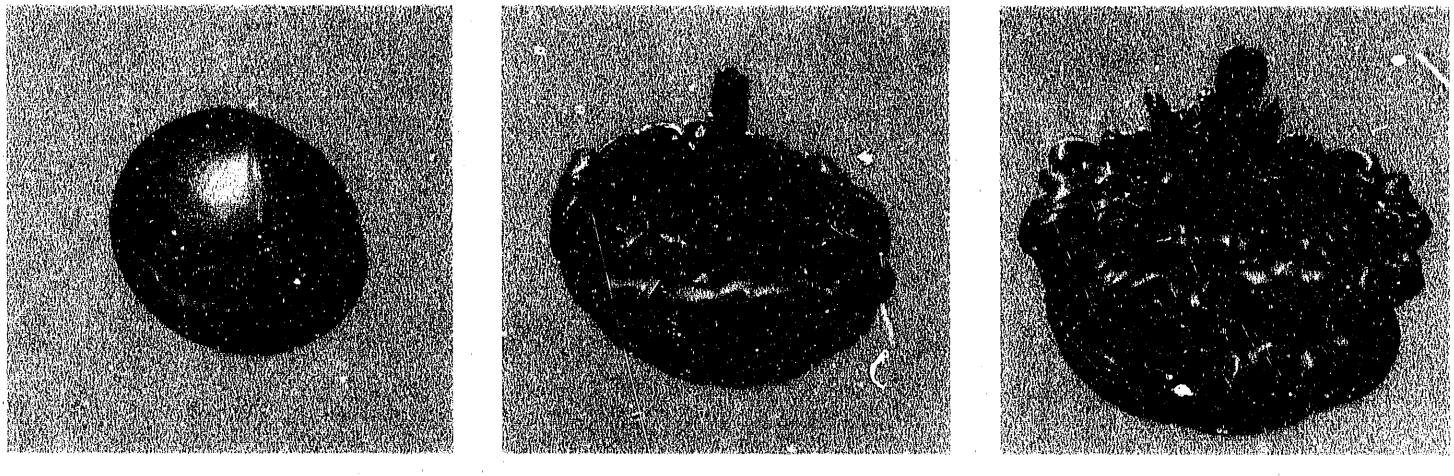


Figure 1. *Time sequence illustrating dynamics of shock-induced cloud collapse computed using adaptive mesh refinement. Images show the location of cloud material.*

TERPSICHORE: A New Plasma Physics Code

Our code TERPSICHORE solves large-scale physics computations on multiprocessor computers at record speeds.

Two lively areas of research, plasma physics and parallel processing, have been brought into convergence in the physics code TERPSICHORE (named for the Greek muse), and each area has been advanced as a result. The code advances plasma physics because, going beyond previous two-dimensional calculations, it is the first calculation of the magneto-hydrodynamic (MHD) stability of realistic three-dimensional plasma equilibria. TERPSICHORE (which won the Cray Research 1989 Gigaflop competition for the fastest scientific application code) advances computer science by being one of the first application codes to exploit many of the parallel computing features of large-memory supercomputers. Our algorithms not only exploit parallel vector architectures but do so using the latest vendor-supplied software for automatic multitasking and for optimized matrix manipulations.

TERPSICHORE was developed as part of an international collaboration between LLNL and L'Ecole Polytechnique in Lausanne, Switzerland.

In the study of realistic fusion devices, it is critical to be able to calculate the stability properties of three-dimensional plasma configurations. The motions of an unstable thermonuclear plasma can damage the chamber walls and cause the plasma to extinguish itself. We are hopeful that TERPSICHORE will be as successful in three dimensions as its predecessors were in two.

For input, TERPSICHORE takes data specifying an equilibrium configuration of a generally toroidal plasma. Many of the quantities of the analysis are represented by double finite Fourier series specified on each of several nested toroidal flux surfaces. TERPSICHORE begins the calculation by reconstructing the equilibrium solution, which it next maps to a different set of spatial coordinates that are optimum for the stability analysis. From the energy principle, a set of Euler-Lagrange equations is derived and appropriately discretized to form a linear matrix eigenvalue problem.

After developing the efficient parallelized matrix solvers PAMS and PAMERA to solve the eigensystem at gigaflop speeds (10^9 floating point operations per second), we learned that when used in TERPSICHORE, these solvers typically did less than 5% of the arithmetic work. The reconstruction, mapping, and matrix-generation phases took the other 95% of the work, nearly all of which (99%) was in the evaluation of myriads of flux tube integrals. Consequently, we developed the multiple flux tube integrals (MULFI) technique, in which multitasked groups of matrix-matrix products (using the extremely fast Cray Research routine MXM) rapidly evaluate these integrals. Tests showed that MULFI executes at about 1.7 and 2.0 gigaflops on the Cray-2 and Cray-Y/MP supercomputers, respectively.

Figure 1 shows the three-dimensional structure of an unstable plasma computed for the Helias Stellarator, a toroidal device being designed at the Max Planck Institute; the colors map the perturbed plasma pressure. This calculation was done at a record speed of 1.71 gigaflops on the Cray-Y/MP at Cray Research headquarters, in Mendota Heights, Minnesota. TERPSICHORE is now in routine use in the magnetic fusion effort, where, for example, it is contributing to the study of the race-track tokamak, a previously intractable problem.

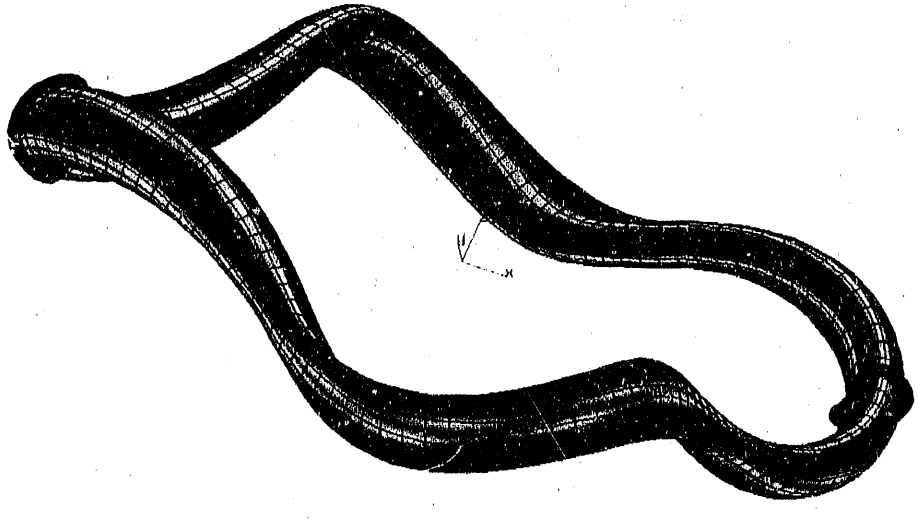


Figure 1. *Display of the most unstable magnetic flux surface of the Helias Stellarator configuration. We use colors to map the perturbed plasma pressure. Yellow-red indicates a raised pressure; blue-purple indicates a depression; green maps an unperturbed pressure. The unstable motion of the plasma would correspond to these pressure variations.*

Contact: D. Anderson (415) 422-9818.

The SISAL Language Project

Our parallel-processing application language is competitive on single processors and effectively exploits multiprocessors; it is being given a user interface that minimizes learning requirements.

Programming parallel computers in conventional languages such as Fortran has proven arduous and error prone. A solution is to develop programming languages that promote the construction of correct parallel programs by isolating the application programmer from the complexities of parallel processing. SISAL (for Streams and Iterations in a Single-Assignment Language) is an applicative language that makes it as easy to write parallel programs as it is to write sequential programs. However, applicative programs may spend large amounts of time and resources copying data and managing memory. To reduce these costs, we developed sophisticated compilers and runtime systems to support SISAL programs on commercial parallel computers. SISAL programs now run as fast as Fortran programs on single processors and achieve substantial speedup on multiple processors. We compared the two languages by running the Livermore Loops on the Sequent Balance. The Livermore Loops are a set of 24 kernels typical of the codes run at the Laboratory. The Sequent Balance is a shared-memory, multiple instruction-multiple data (MIMD) machine that uses as many as 32 processors.

Table 1 gives the Fortran and SISAL execution rates in thousands of floating point operations per second (kflops); Table 2 gives the execution times for three large scientific programs. The results show that the single processor performances of Fortran and SISAL are equivalent, and that SISAL can effectively exploit the multiple resources of the Sequent Balance. Since only half the Livermore Loops are parallel, one can expect at most a two-to-one speedup on multiple processors. The SISAL code runs on any number of processors without the need of rewriting or recompiling; only a single command line needs to be changed. To run the Fortran code on more than one processor requires extensive rewriting.

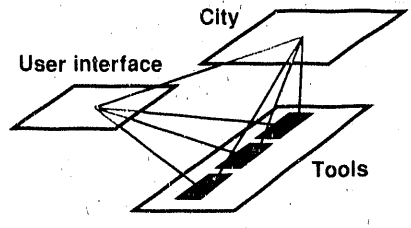


Figure 1. *SisalCity is an easy-to-use, robust integrated programming environment. Users can invoke any tool directly through the interface. If a tool must communicate with others, it is invoked through the City, which provides communication between tools as necessary.*

Although SISAL simplifies parallel programming, users still expect the support of a robust set of integrated programming tools. To meet this expectation, we are developing a programming environment for SISAL, called SisalCity, that helps users design, develop, debug, and analyze SISAL programs. Figure 1 shows the three components of the environment. The user interface comprises a set of configurable windows, complete with buttons that invoke predefined commands and popup menus. The City, when instructed, activates the tools (independent processes) and provides communication between them. The City has buttons for each tool, a number of utility buttons, a command window, and a window for error messages. The tools include an editor, a compiler, a debugger, a simulator capable of simulating the execution of SISAL programs on a variety of parallel architectures, a graph display routine, and tools to collect, analyze, and display execution data.

Contact: J. Feo (415) 422-6389.

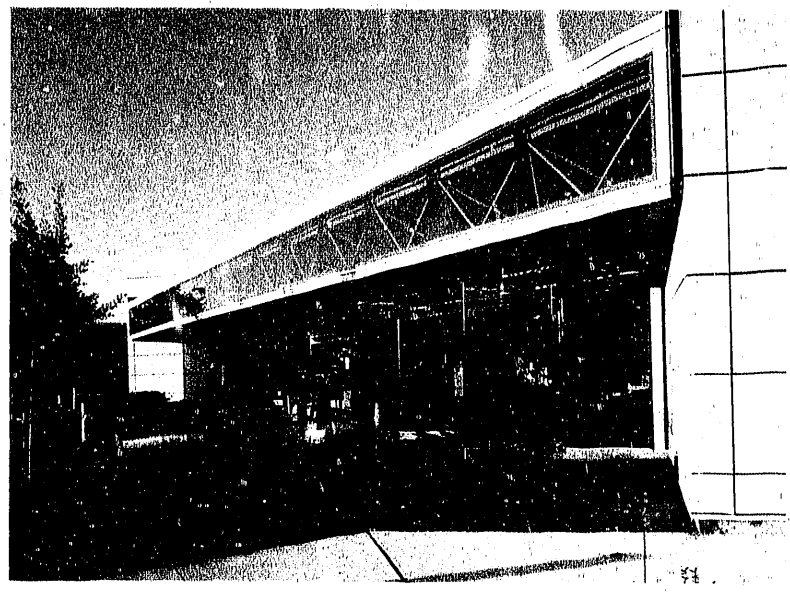
Table 1. **The performance of the Livermore Loops (in kflops).**

	Fortran	SISAL (1 processor)	SISAL (5 processors)
Minimum	12	15	15
Maximum	88	90	393
Average	55	48	140
Harmonic	45	44	75

Table 2. **Execution times of three large scientific programs.**

Program	Fortran	SISAL (1 processor)	SISAL (10 processors)
Gauss-Jordan elimination (100 × 100 array)	55.00 s	57.70 s	9.54 s
Numeric simulation of elution profiles	30.63 h	31.00 h	3.45 h
Simple (100 × 100 array)	3081.28 s	3099.32 s	422.04 s

Laboratory Administration



The Administration and Operations Directorate provides the infrastructure for the city-size Laboratory site and population. New medical facilities were brought into full operation this year and now offer an expanded clinical program for Laboratory employees.

The Laboratory's administrative activities are wide-ranging. LLNL is like a small city, complete with emergency services, sewage and waste disposal requirements, and the personal and professional needs of its 8200 employees. A number of administrative activities are carried out under the aegis of the Director's Office, including education, community relations and affirmative action, technology transfer, and the Environmental, Safety, and Health (ES&H) Council. The Laboratory's arms-control efforts are focused through the Center for Technical Studies on Security, Energy, and Arms Control.

The Administration and Operations (A&O) Directorate provides institutional services that are the foundation for the activities of the Laboratory's programmatic and support organizations. A&O is made up of Hazards Control, Plant Engineering, Health Services, Human Resources, Information Services, Quality Assurance, Environmental Protection, Safeguards and Security, and Business Operations Organizations. Staffing for these organizations represents about one-third of the LLNL workforce.

The prime focus of A&O efforts this year has been to support the Director's and the DOE's policy that ES&H be the Laboratory's number-one priority. As the Director has stated: "We must achieve the required organizational strength and technical competence in ES&H while preserving the historic culture in our extraordinarily successful Laboratory programs."

In support of this priority, important achievements were made this year by A&O's organizations. For example, Hazards Control expanded its safety audits and training programs, and made significant advances in improving testing methods for firefighter equipment. Plant Engineering completed several major Laboratory

facilities and provided major support to correct compliance violations and for site cleanup. Quality Assurance helped Laboratory programs meet their quality assurance objectives by conducting quality assurance appraisals and assisting support organizations, such as Mechanical Engineering and Electronics Engineering, to prepare quality assurance plans.

Health Services developed a progressive occupational health program and brought the Laboratory's new medical facilities into full operation with an expanded clinical program.

Environmental Protection implemented groundwater treatment systems to decontaminate water containing low levels of volatile organic chemicals (VOCs) to nondetectable levels. Risk analyses of existing groundwater indicate a very small maximum risk of an additional two-in-ten-million chance of developing cancer over a 70-year lifetime exposure to VOCs in groundwater should someone use it as a water source. However, no one is using this water. Since we are treating and decontaminating the VOC-containing groundwater, the actual risks will be even lower. A new LLNL sewer monitoring system with an alarm connection to the City of Livermore Water Treatment Plant was also installed this year.

In addition to the ES&H activities, numerous other achievements have been made in the A&O Directorate. Human Resources implemented a number of new programs, including an employee educational program on AIDS and a new substance abuse policy. The Laboratory instituted a substance abuse program in May 1989 to protect the health and safety of LLNL employees and to ensure the Laboratory's ability to meet its national security responsibilities. The program provides for a drug-free workplace and establishes the corrective actions that will be taken against those involved with illegal substances onsite. It also identifies the Laboratory's Employee Assistance Program as an effective support resource for those seeking recovery from substance abuse.

Safeguards and Security continued a major program to upgrade the Laboratory's layered security systems as part of the Phase-Two Safeguards and Security Enhancements (SSE-2). Layered security is the concept in which the level of security increases as one moves from the Laboratory perimeter toward the location of the most sensitive security assets. At the center is the Superblock, which contains the Plutonium Facility and storage of special nuclear material. Work is nearly complete on a new physical protection system around the Superblock, with a double-fenced isolation zone, alarms, observation towers, and secure pedestrian and vehicle portals. In conjunction with Sandia National Laboratories, Safeguards and Security developed a new safeguards effectiveness evaluation tool; this Analytic System and Software for Evaluating Safeguards and Security provides a comprehensive approach for evaluating the effectiveness of theft-protection measures for special nuclear material.

Facilities, equipment, and software for Information Services were upgraded this year. Installation of the onsite digital telephone system was completed. This new system incorporates the latest telecommunication standard—Integrated Service Digital Network—and will help to control future telecommunication costs.

Business Operations implemented an online informational system, called the Institutional Supplemental Labor Information System (ISLIS), to help meet the supplemental labor needs of the Laboratory.

Although A&O's functions and accomplishments may not be as visible as those of the major programs, they are crucial to the Laboratory's operation—A&O provides the infrastructure for the city-size Laboratory site and population. LLNL's ability to conduct state-of-the-art research depends on the quality of its administration and operational functions. The A&O Directorate will continue to support the Laboratory's programmatic and support organizations and to improve the institutional services to meet the challenges of the future.

Contact: P. E. Coyle, III (415) 423-7788, D. K. Fisher (415) 422-3343, or G. W. Campbell (415) 422-5217.

LLNL and Education

Improving the quality of science education is the goal of a number of innovative LLNL programs that seek to increase the public's scientific literacy and boost the number of students pursuing careers in science and engineering.

The National Science Foundation predicts that by the year 2006 there will be a shortage in the U.S. of nearly 700,000 scientists and engineers. In addition, many issues facing local communities and the general public are increasingly technical and complex. If the U.S. is to exploit science and technology wisely and maintain global leadership in technology, the general citizenry's understanding of science must be enhanced and new sources of scientific talent for the workforce must be tapped.

However, there appears to be a decline in the scientific literacy of the general public, perhaps because of the increasing complexity of modern technology and perhaps because of inadequacies in science education. In many sectors of the population, particularly among people of color and women, science has not been a career of choice. In addition, the current high-school dropout rate for hispanic and black students offers little promise for an increase in enrollment in college science programs without the infusion of new ideas and programs to stimulate interest in academic achievement.

To address this problem, the DOE has enjoined the national laboratories to work with their local communities and the nation's schools to design programs that will stimulate interest in technology and science. Energy Secretary James D. Watkins stated that "a partnership with education is now part of the mission of the national laboratories. ... Our scientists are going to go out and teach." LLNL is an active participant in local science education and supports a number of innovative programs at the Livermore site, in the local community, and around the nation. Many of these programs were developed long before the DOE directive was issued.

The Science Education Center was opened nearly a decade ago. At the time, it was the first such center at any DOE institution, and it has since become the model for similar facilities at other laboratories. In May 1990, the Center was awarded a grant of $142,000 from the National Science Foundation to finance educational programs for the coming year (part of a $622,000 grant made to the national laboratories for their educational programs). The grant will be used to support the Summer Technology Institute for teachers, which has been offered for the past several summers. This year, some 70 teachers from the San Joaquin Valley and the Bay Area will participate in the institute. During the summer of 1990, LLNL scientists and technicians will instruct teachers in basic science, computers, global issues, and multimedia. The teachers will develop new science and technology curricula for use in their classroom. Nearly 400 teachers will participate in workshops this summer.

Since 1968, LLNL has welcomed faculty and students of the Associated Western Universities (AWU) to the Laboratory for two-month summer programs. AWU (a consortium of 37 universities funded primarily by the DOE) awards fellowships for participation in research programs at DOE-associated laboratories. In 1989, LLNL hosted nearly 50 participants—students, graduate students, high-school teachers, and college faculty—in two summer sessions. Participants work with Laboratory scientists on projects of mutual interest ranging from biomedical research to state-of-the-art computing.

Each summer, the Computation Directorate holds the High School Supercomputer Honors Program. Funded by the DOE, this program brings together high-school students from across the nation and several foreign countries. During their two-week stay, they tour the site, attend lectures, and work with one of the Laboratory's Cray superconductors.

The goal of the American Indian Program is to increase the number of American Indian students pursuing careers in science and engineering. We are assisting the Navajo Community College in Tsaile, Arizona, in upgrading its science program; we are also conducting science workshops for elementary

Figure 1. *In February 1990, the Science and Engineering Alliance was signed by LLNL and four historically black universities.*

school teachers from the Navajo reservation. Central to this program is the relationship between LLNL and the American Indian Science and Engineering Society (AISES). Each spring, LLNL sponsors visits by AISES students to the Laboratory. Between 1983 and 1989, 82 AISES students visited LLNL: 22 have graduated from high school and are working, 34 are attending college, and 8 are in graduate school. This success rate appears to be improving; in April 1990, 14 AISES students visited LLNL and, at this writing, 13 either have graduated or are still in school.

The LLNL Historically Black Colleges and Universities Program is part of the DOE's effort to implement a White House initiative to advance the development of human potential in historically black colleges and universities and to strengthen their ability to provide high-quality education. Our program includes agreements to conduct collaborative research with several such institutions. The most recent agreement was signed February 21, 1990, with the Science and Engineering Alliance, a consortium of Alabama A&M University, Jackson State University, Prairie View A&M University, and Southern University and A&M College (Figure 1). We will collaborate with the Alliance on major research projects of mutual interest and will make available tothe Alliance LLNL's state-of-the-art scientific equipment and computer services on an as-available basis. We will also assist the Alliance in upgrading their science curriculum and in furthering the professional development of their science and engineering faculty.

The LESSON (LLNL Elementary Science Study of Nature) Program is 20 years old. During 1989, LLNL staff members presented 6200 hours of instruction to 137 teachers.

Figure 3. *The LESSON Program and the Bay Area Science and Technology Consortium enable students in public schools to "do" science, not just read about it.*

LESSON was initiated by LLNL employees who observed that students from urban schools with high minority enrollments were not receiving adequate science instruction and that many teachers felt uncomfortable teaching science. The LESSON Program includes a teacher's manual that contains 43 classroom science lesson plans covering physics, electricity and magnetism, biology, and chemistry, and take-home experiments for the students. Each lesson requires only low-cost readily available equipment (Figure 2). For example, in one experiment, water that has been contaminated with dirt, ink, oil, and perfume is purified using coffee filters, household bleach, and charcoal from tropical fish stores.

Another program initiated this year is the Bay Area Science and Technology Consortium and involves LLNL, Sandia National Laboratories, Livermore, Lawrence Berkeley Laboratory, and the Stanford Linear Accelerator Center, together with the California State Department of Education, UC Berkeley, and the Lawrence Hall of Science. The goal of this consortium is to enhance science and math instruction in all the Bay Area public schools. The initial focus will be on the Oakland public schools; it is one of many large, particularly troubled school districts in the nation. The consortium will train teachers in science at the various laboratories, loan equipment and computers to the schools, and send their own scientists into the classrooms to teach.

We are deeply committed to using LLNL expertise to help solve the nation's problem of inadequate science education. Our efforts are proving successful as evidenced by the constant stream of requests for science workshops and presentations, for copies of our LESSON manual, and for additional collaborative agreements from universities.

Contact: LLNL Science Education Program (415) 423-3177.

LLNL and Community Relations

The Laboratory supports a wide range of formal outreach efforts, with many other community-related activities being undertaken by LLNL departments and groups of Laboratory employees.

While the research done at LLNL is directed primarily to national-level concerns, we recognize that the Laboratory has an impact on the surrounding community. We make every attempt to ensure that the Laboratory's overall impact on its neighbors is positive and that any negative impacts are minimized. We also attempt to involve and inform the surrounding community about LLNL activities as much as is possible given the constraints under which we must operate. The Laboratory is committed to being a responsive and responsible member of the Livermore, Tri-Valley, Central Valley, and Bay Area communities.

The Public Affairs Office is responsible for official LLNL communications. In 1989, the Office received some 9500 calls for information from local and national news media, published nearly 200 news releases, and held more than 430 press conferences and visits. The Public Affairs Office also manages the Visitors Center. Last year, the Center played host to some 23,500 people and arranged tours of the Livermore site for 1271 people.

The Public Affairs Office also oversees the Technical Volunteers Program. This program has a register of more than 200 employees willing to lend their expertise to government and nonprofit service organizations to promote science education and to help find solutions to various technical problems. An adjunct to this program is the Speakers Bureau, with some 230 employees ready to speak to schools, service organizations, and private industry on subjects ranging from fusion to earthquake safety.

Figure 1. *LLNL employees collecting donations to help victims of the October 17, 1989, earthquake.*

A number of other public relations activities are carried out by various Laboratory groups and employees, both as LLNL-affiliated ventures and as private undertakings. Money raised by the annual HOME (Helping Others More Effectively) campaign is distributed to area social agencies; this year, Laboratory employees contributed $345,890 to the HOME campaign. LLNL employees also responded very generously following the October 17th earthquake. In the two weeks after the quake, $63,500 in cash and $80,000 in goods were collected for the Salvation Army's earthquake relief fund (Figure 1).

Engineering's Christmas Card Fund was started informally more than a decade ago. Directorate employees are asked to consider making donations, in lieu of spending money on Christmas cards for fellow workers, to purchase food gift certificates for local low-income families and house-bound seniors.

On a personal level is the Lunch Bunch, a group of LLNL employees who work during their lunch hours on projects to help local convalescent homes and shelters. Their activities have included organizing canned food drives, holiday decorating and parties, and in-house visits.

In May 1990, results were released of a survey about the public's view of the Laboratory. The study, directed by the Public Affairs Office and conducted by the Charlton Research Company, found that, in general, people in the local communities view LLNL positively as a place where intelligent scientists and engineers make valuable contributions on both the national and local level. The survey found that the closer people lived to the Laboratory, the more they knew about its activities and thus the more positive they felt toward LLNL.

This survey reaffirmed that good communication with the community is essential and indicated several areas that would benefit from increased efforts. One is getting timely, accurate information to Laboratory employees. This will benefit both the employees and the local public as the survey revealed that LLNL and its employees are viewed as important sources of information. Another involves reaching beyond the daily press and broadening our connections with major scientific and technical publications and with the broadcast media. Still another is increasing the activities that help integrate LLNL with the surrounding communities.

The survey also indicated that the communities want help in education. This is a principal mission of the Laboratory and a prime opportunity to increase community interest in science education and foster a better understanding of LLNL, its people, and its mission.

The issues facing communities today are increasingly technical and complex. At LLNL, we are applying our scientific and technical expertise to help solve community problems and assist schools with science education programs, in addition to aiding the community with money, time, and effort.

Contact: Public Affairs (415) 422-4599.

Technology Transfer: LLNL Partnerships with Industry

LLNL is rapidly expanding the transfer of Laboratory-developed technologies to industry; this year has seen an increase in the number and types of agreements with industrial partners and in the income received from these agreements.

The commercial potential of LLNL's research is being actively promoted especially in such areas as biotechnology, computers, energy, and materials science. The mission of the Technology Transfer Initiatives Program is to exploit the LLNL technologies that will bring new products and processes to market, thereby helping U.S. industry increase its competitive edge and creating new jobs for American workers. The growth in transfer agreements and licensing income is shown in Figure 1.

LLNL is a national scientific, technical, and engineering resource. Our interactions with scientific and technical colleagues in universities and industry have set the stage for technology transfer in fields in which we are leaders. In addition to the natural process of technology transfer by the movement of people to industry, we use three primary mechanisms to promote the commercial exploitation of Laboratory research: preferential licensing of intellectual property, cooperative research and development agreements, and fully sponsored projects. A few highlights of this year's accomplishments follow.

- The Livermore interactive network communication system (LINCS), a Unix-based archival storage system to manage the storage and retrieval of large files, was licensed to General Atomics, which plans to market the software under the name "UniTree."
- Under a cooperative research and development agreement, a major U.S. biotechnology firm will fund research and development over three years to produce DNA probes as commercial products using the fluorescence hybridization technique developed at LLNL. These DNA probes will be used for research into and clinical diagnostic products for cancer detection, hereditary disease detection, and prenatal testing.
- Under a license and collaborative agreement, with no funds exchanged, SyStemix, Inc., will provide personnel to prepare upgraded software for the newest version of LLNL's high-speed fluorescence-activated cell sorter and to replicate the cell sorter for SyStemix's use and at its cost. Rights to the new software will remain with the Department of Energy and LLNL, and SyStemix will have the newest cell sorter for its use in biological sample preparation and research.
- In the petroleum geochemistry project, LLNL has exchanged software with three U.S. petroleum service companies to enhance their competitiveness and our research capabilities. A separate research agreement to conduct experiments and develop computer models and analytical tools for locating oil deposits is being extended through December 1992 to a dozen companies.
- The California competitive technology program has granted funds to LLNL to enable Laboratory researchers to work with an industrial partner to develop a new three-dimensional x-ray computed-tomography system. The new system, called Konoscope, is designed for industrial applications for nondestructively examining the interior of objects.
- LLNL has joined with three industrial participants—North Star Steel (steel production), Ladish Co., Inc. (steel fabrication), and Caterpillar, Inc. (end user)—in a joint commercialization project. This project is part of the DOE Steel Initiative Program to develop the technology and establish the feasibility of large-scale processing and high-tonnage production and use of a new ultrahigh-carbon steel with superplastic properties.

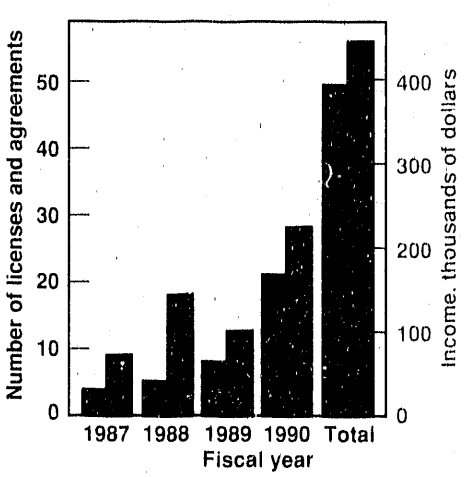


Figure 1. *Growth in LLNL partnerships with industry in both the number of license and collaborative agreements and licensing income received. (Figures for fiscal year 1990 are projected.)*

We expect significant growth in our relations with industry in fiscal year 1991, particularly in areas such as advanced laser applications, x-ray lithography, advanced high-speed cell sorting, and the detection of environmental contaminants with monoclonal antibodies.

Contact: G. T. Longerbeam (415) 423-7293 or C. F. Miller (415) 423-3082.

Challenging Times Require Innovative ES&H Solutions

Environmental protection, safety, and health (ES&H) have top priority at LLNL, and state-of-the-art Laboratory technologies are being applied to solve ES&H problems at LLNL, other DOE facilities, and throughout the country.

A fundamental challenge facing LLNL is to excel in environmental, safety, and health (ES&H) performance while enhancing the excellence in the Laboratory's programs. This includes complying with ES&H laws, which must be carried out in close mutual cooperation with the Department of Energy and the federal, state, and local governments. The Laboratory must also manage its operations in a manner that reduces ES&H risks to levels as low as reasonably achievable and openly communicate our activities to LLNL employees.

LLNL has always had an excellent safety record and the year past continued this trend. Continuing efforts in emergency preparedness and safety training have paid dividends. In 1989, there were no significant safety incidents at LLNL and there were fewer injuries than in previous years. Injuries due to overexertion remain the largest category, but cumulative trauma injuries are becoming more numerous, particularly those associated with repetitive motion such as computer keyboard work. Electric shock incidents were down this year, we hope as a result of increased safety awareness and training. LLNL's motor vehicle accident rate continued a four-year downward trend, and the dollar loss per miles driven was well below the DOE average.

Meeting the ES&H challenge in the 1990s requires that LLNL operate as an ES&H "center of excellence":

- Conducting ES&H operations to meet the spirit and the letter of the laws.
- Integrating ES&H expertise in programmatic operations.
- Providing ES&H expertise to help solve DOE-complex problems.
- Applying LLNL technology to help solve global ES&H issues.

We are taking state-of-the-art LLNL technology and applying it to solve ES&H problems at LLNL, other DOE facilities, and throughout the country. These activities are already well under way. The Laboratory is committed to minimizing the amount of waste produced, and to reducing its environmental discharges to levels as low as reasonably achievable.

In 1989, LLNL enhanced its commitment to ES&H as top priority. This has required a "cultural shift" as attention and funding is being directed to necessary changes in facilities and operations. A series of internal and external audits and appraisals, begun in the summer of 1989, has identified a number of issues that must be addressed. The Director has established a Waste Minimization Steering Committee to create programmatic waste-minimization plans and has formed an ES&H Council under Deputy Laboratory Director Duane Sewell to oversee all Laboratory ES&H activities. LLNL programs are now establishing ES&H assurance offices to implement self-correction processes.

The DOE Tiger Team Assessment, which took place in April 1990, found no basis to cease or curtail any ongoing LLNL operations. The inspectors recognized that the Laboratory's health and safety organizations are staffed by highly competent professionals. They found particular strengths in criticality safety, medical services, laser safety, and emergency response. Areas needing improvement involve quality assurance, independent oversight, control verification, and formality in documentation. Action plans have been developed to address these ES&H concerns and their root causes, and changes and corrections are already being made.

Environmental protection issues are also being vigorously addressed. Treatment and cleanup of the contaminated groundwater under the Livermore site has begun. Dozens of monitoring wells and treatment wells have been drilled (Figure 1), more than seven million gallons of groundwater has been treated, and recent sampling indicates that the westward movement of the contamination has been retarded. In the southern part of the Laboratory near Building 403, 5000 gallons of gasoline have already been cleaned up—a significant portion of a 17,000-gallon leak from underground Navy storage tanks that occurred in the 1970s.

Impacts on the Livermore Water Reclamation Plant as a result of any accidental LLNL discharges to the city sanitary sewer will be minimized

when the Laboratory's sewer diversion system becomes operational later this year. In addition, the effluent control upgrades for the Tritium Facility will reduce stack emissions from the facility by 90%.

Numerous upgrades were made to our hazardous waste management facilities. Although the existing storage facilities were in compliance with current regulations, we made these upgrades so that the Laboratory would meet the permit requirements of the State of California and the Environmental Protection Agency for the storage of hazardous and mixed waste.

An effort was begun this year in advanced research for hazardous waste management and environmental remediation. This interdisciplinary program was established to respond to the DOE's needs for characterizing and remediating contaminated sites and addressing key waste-management and minimization problems. The effort is focusing on four areas: minimizing waste accumulations, assessing waste streams, developing integrated demonstrations of waste cleanup technology, and innovative cleanup strategies. LLNL hydrogeologists are using unique drilling and sampling techniques, developed at LLNL for the Livermore site groundwater cleanup, to aid similar groundwater cleanup efforts at the Savannah River site. We are also forming a western U.S. university consortium to facilitate research and public education in these important areas.

On the health and safety front, the Laboratory's Occupational Health Program has been significantly enhanced with the addition of the decontamination and triage facility in the new medical building. In addition, the information generated from LLNL's unique melanoma screening program, which has been in place for nearly five years, will assist in the design of protocols for more rigorous screening of individuals at risk. A unique urine bioassay has been developed and implemented to evaluate employee exposure to metals and metallic compounds. In support of the Laboratory's commitment to a drug- and alcohol-free workplace, the Employee Assistance Program has been expanded to provide help for employees with substance-abuse problems.

ES&H work is being done not only under the aegis of the Laboratory's ES&H Council but also as part of every program's activities. A number of these efforts are highlighted in this issue of *Energy and Technology Review*. For example, the application of weapons technology to ES&H problems is discussed on p. 20; an underground microbial filter to halt groundwater pollution transport is described on p. 55; work to simulate solute transport, which has direct application to ES&H, is described on p. 59; a new biodegradation method for high-explosive compounds is explained on p. 67; an analytical method for pinpointing pollution sources is discussed on p. 90; and work being done to clean up contaminated groundwater under the Livermore site is described on p. 110.

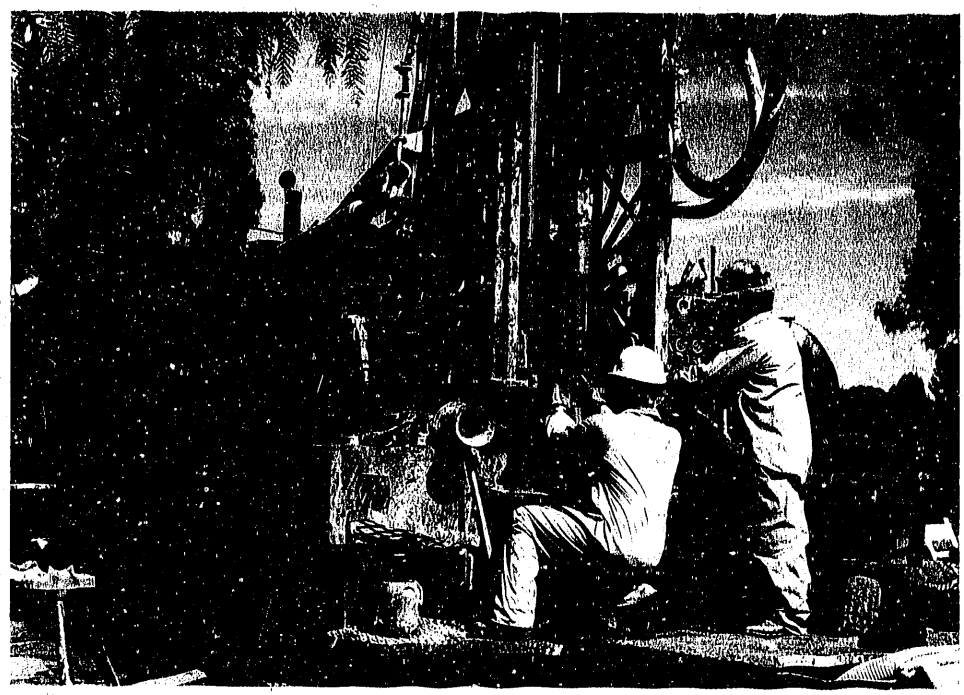


Figure 1. ***Workers drilling one of the numerous well used for monitoring, treatment, or sampling of the groundwater under the LLNL site.***

Contact: R. C. Ragaini (415) 423-8875.

Center for Technical Studies on Security, Energy, and Arms Control

The Laboratory is pursuing research in issues of national security. The Center for Technical Studies on Security, Energy, and Arms Control was founded to encourage this work, to make available Laboratory expertise to outside scholars and scientists, and to create a rich and mutually beneficial environment for the free exchange of ideas in these important areas.

The Center for Technical Studies on Security, Energy, and Arms Control was established at LLNL in November 1988 with the goal of providing visiting interns, scholars from universities and other institutions, as well as Laboratory scientists with the opportunity to use the knowledge and experience of ongoing LLNL programs in studies of international stability and security. Under the aegis of the Center, visiting scholars and specialists conduct research and interact with the LLNL scientists in a mutually beneficial exchange of knowledge and ideas.

Specifically, the Center supports critical studies of significant national issues by Laboratory personnel, hosts visiting scientists and scholars on sabbaticals, fellowships, or professional leave, and supports post-doctoral interns. The Center also conducts seminars, symposia, and workshops in collaboration with other institutions. An integral element of the Center's program is the publishing and dissemination of Center-sponsored work; this year, a publication series was initiated, and six papers have been published or are in press to date.

During 1989, the Center sponsored 25 seminars by outstanding scientists and thought-leaders from the national-security and arms-control community (Figure 1). Among the guest speakers were Sir Rudolf Peierls, Professor of Physics Emeritus, Oxford University and the University of Washington; Andrew Marshal, Director of Net Assessment, Department of Defense; and Ambassador Edward L. Rowny, Special Advisor to the President and Secretary of State for Arms Control Matters.

In May 1989, in collaboration with the California Seminar on International Security and Foreign Policy and the University of California's Institute of Global Conflict and Cooperation, the Center sponsored a symposium on the problem of ballistic missile proliferation. The symposium examined the relationship between the proliferation of nuclear and chemical technologies and the proliferation of ballistic missiles as well as possible policy initiatives and research strategies to deal with the threat posed by missile proliferation.

Figure 1. *Seminar sponsored by the Center for Technical Studies of Security, Energy, and Arms Control, held on April 24, 1990, featured Dr. Peter Zimmerman discussing arms-control monitoring with unclassified satellite imagery.*

The Center, together with the Laboratory's Defense Programs, sponsors an intern program in Arms Control and National and International Security Affairs. In the last three years, two pre-doctoral interns (from the Massachussetts Institute of Technology and the University of Maryland) and two post-doctoral interns (from the University of California, Berkeley, and Brown University) have participated. They spent from two months to two years at the Laboratory studying the vulnerabilities of U.S. space assets and possible technical and policy remedies for these vulnerabilities, arms-control projects relating to the Strategic Defense Initiative and nuclear weapons, force options for NATO, the use of lasers for various military operations, and rail-garrison basing of ballistic missiles.

In this era of rapid and unpredictable political change, especially in the Soviet Union and Eastern Europe, the Center provides a very valuable forum for the exchange of ideas and experience about national security and arms control. Visiting specialists, interns, and LLNL scientists all gain from the interaction, and the ultimate beneficiaries are the U.S. and the entire global community.

Contact: M. D. Nordyke (415) 423-7654.

Measuring the Size Distribution of Radon Decay Products

Diffusion battery samplers can measure the size distribution of radon decay products (progeny) in air. We are using these devices to size-fractionate the progeny activity in order to study their attachment rates to aerosols.

Radon and its decay products confined indoors are major contributors to the incidence of lung cancer. The radon progeny, ^{218}Po, ^{214}Pb, ^{214}Bi, and ^{214}Po, form by the decay of radon gas after it has infiltrated buildings from the soil. The progeny, with half-lives up to 30 min, are reactive and highly mobile indoors. They can react with pollutants or other gas species in the air to form clusters of molecules; they can deposit on surfaces and walls and become attached to aerosols already in the environment. The progeny are described as unattached while they exist in their free or clustered state and attached after they have deposited on aerosols. The estimated inhalation dosage and the location of progeny deposition in the respiratory system are strongly affected by the size distribution of the particles containing the activity.

The size distributions of progeny activity can be measured by diffusion batteries. Conventional diffusion batteries, which can typically classify aerosols from 5 to 300 nm in diameter, have long been used to size atmospheric aerosols. However, the distribution of free radon progeny lies below this range. In recent years, research applications measuring the diffusion coefficient of free progeny have used the graded-screen diffusion battery, which consists of several single screens having coarser mesh than conventional batteries. In ours (see Figure 1), the screens, 16 to 500 in mesh size, are stacked in a commercial 25-mm-diam filter holder. At a sampling flow rate of 4 liter/min, the first (coarsest) screen collects most of the smallest particles (0.2 nm) and the last (finest) screen collects most of the largest particles (30 nm diam).

Figure 1. *A six-stage graded-screen diffusion battery, fabricated for our research, used to measure the size distribution of free radon progeny.*

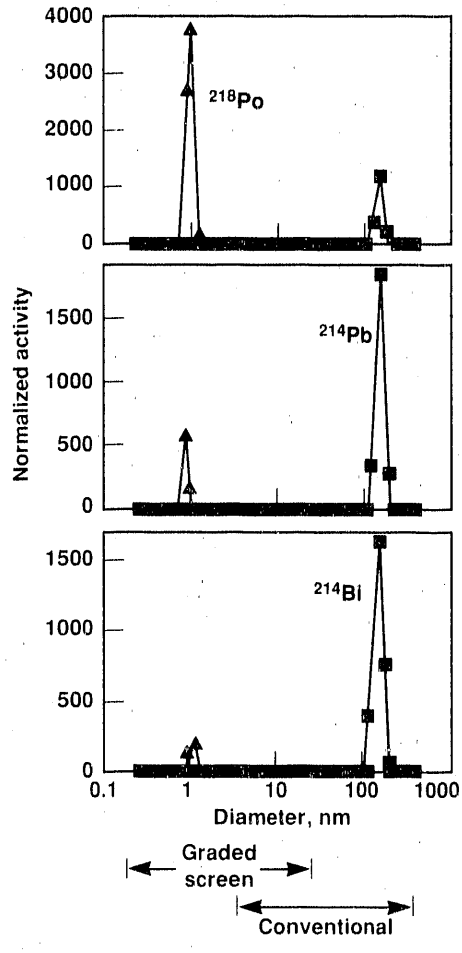


Figure 2. *Progeny size distributions in the presence of a 173-nm monodisperse aerosol. The triangles represent the graded-screen battery and free fraction; the squares represent the conventional battery and attached fraction.*

Activity collected on the screens is measured simultaneously by alpha and gamma spectroscopy. Activity deposited on the back of the screens is measured in a separate counting accumulation period. Size distributions are obtained by data inversion of the Fredholm integral equation of the first kind.

Figure 2 shows activity distributions for an experiment with radon gas mixed with an aerosol. The aerosol consisted of 173-nm-diam monodisperse polystyrene latex particles. The activity mode seen at 1 nm diameter in each distribution corresponds to the free daughter activity. The corresponding diffusion coefficient is ~0.05 cm^2/s. The mode at the larger size is the activity that has attached to the aerosol particles. The greatest abundance in the aerosol occurs for the third daughter in the decay chain, ^{214}Bi. We are routinely using several of the graded-screen batteries to characterize the behavior of free radon progeny and to separate the free and attached progeny activity.

Contact: A. Biermann (415) 422-8017.

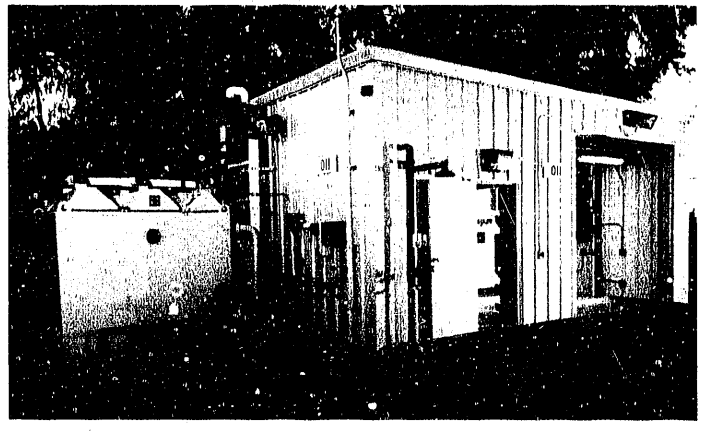
Groundwater Treatment at the Laboratory

The first of several treatment systems has been installed onsite and is removing and treating groundwater contaminated with volatile organic compounds in order to stop the westward movement of these contaminants.

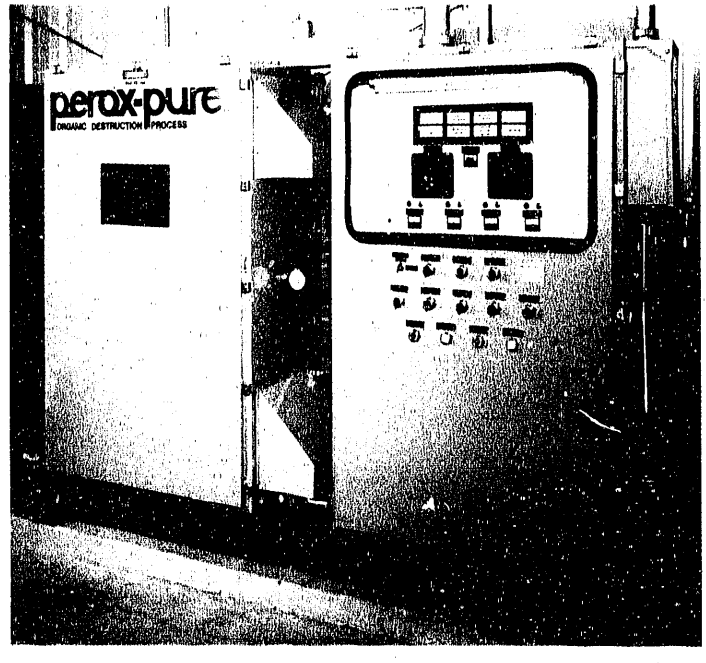
The Laboratory continues to make progress in cleaning up the volatile organic compounds (VOCs) that have contaminated the site since it was occupied by the U.S. Navy during World War II and the early postwar years. This year, we installed Treatment Facility A (Figure 1), the first of several groundwater treatment systems, in the southwest corner of the LLNL site. This is the area from which a groundwater plume containing VOCs appears to have been migrating at a rate of about 30 m/y. The contaminants are in very small amounts and present no exposure risks to LLNL employees or Livermore residents because they are trapped in soil and groundwater at sufficient depths and because there are no wells in use within the plume or its path. Treatment Facility A is operating 24 hours a day. As Figure 2 shows, groundwater is pumped through a commercially available ultraviolet-light/hydrogen peroxide (UV/H_2O_2) unit and an aeration tank with a carbon-adsorption system, designed and built by LLNL.

Figure 1. *(a) The new Treatment Facility A on the Livermore site and (b) the commercially available treatment unit inside.*

(a)



(b)



The facility treated some seven million gallons of groundwater this past year. At an average concentration of 200 ppb in the water processed to date, approximately 5.5 kg, or about 4 liters, of VOCs have been removed from the groundwater and destroyed. Samples taken from offsite monitoring wells to the west of the Laboratory indicate that the westward movement of VOCs in the groundwater has been retarded.

The UV/H_2O_2 treatment unit efficiently destroys perchloroethylene (PCE) and trichloroethylene (TCE). These compounds have a double carbon-carbon bond that is readily broken or oxidized by the hydroxyl radical created by the dissociation of H_2O_2 under the influence of UV radiation. However, analyses of treated water from the UV/H_2O_2 unit revealed that their single carbon-carbon bonded compounds were not completely destroyed (see Table 1). Because the haloalkanes (single bonds) are less readily destroyed than the alkenes (double bonds), we could not meet the water quality requirements of our discharge permit, which limits treated discharge water to <5 ppb total VOCs (a lower

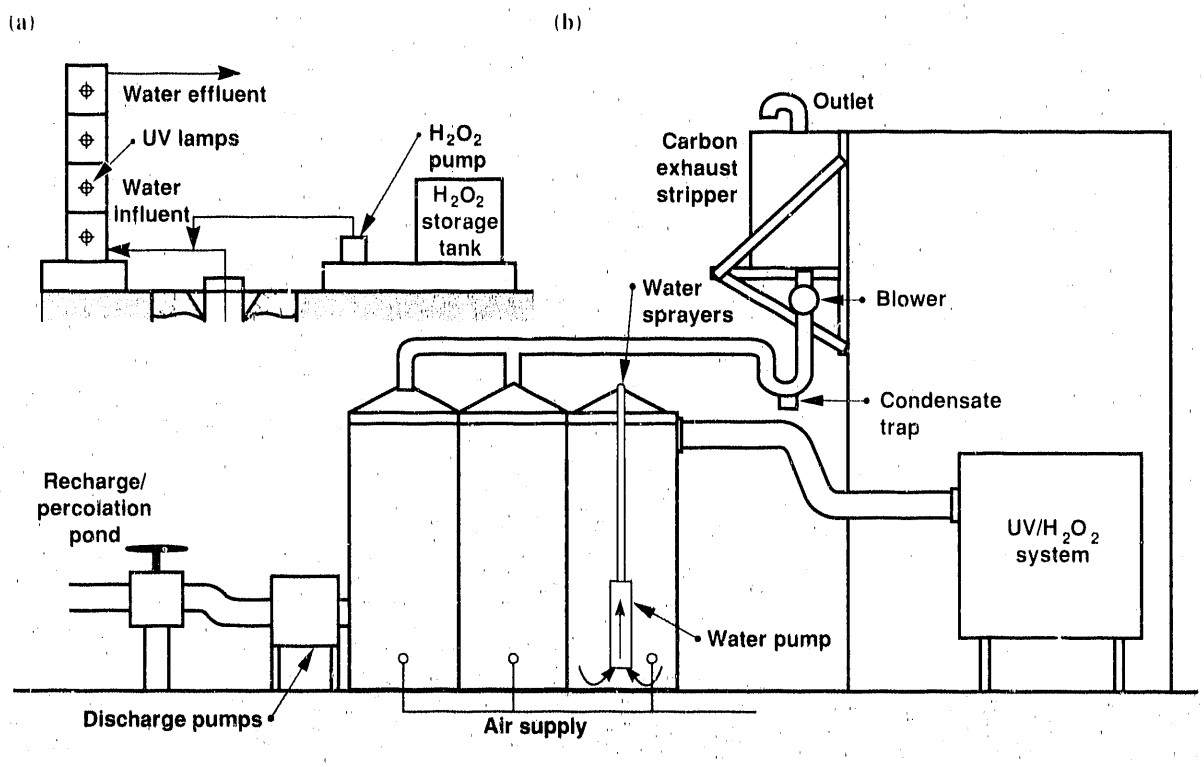


Figure 2. *(a) The UV/H_2O_2 treatment system and (b) the LLNL-designed and built effluent-polishing system. Contaminated water, pumped from the extraction well, is mixed with a 50% solution of H_2O_2; it flows past UV lamps that break down the contaminants. Water effluent is then discharged from the chamber. The effluent-polishing system uses a baffled spraying and aeration chamber. A blower evacuates VOCs volatilized during aeration through an activated-charcoal filter.*

concentration than allowed by drinking water standards).

To meet discharge limits for VOCs, we designed and built a water aeration system to polish the effluent from the UV/H_2O_2 unit. A baffled 530-liter tank receives effluent directly from the UV/H_2O_2 unit. A centrifugal blower injects air at a rate of ~50 m^3/min to subject the water to intense aeration. Another centrifugal blower extracts the VOCs volatilized during the aeration process. The exhaust air stream is then passed through a carbon filter before being discharged to the atmosphere. The total concentration of VOCs in water entering the polishing tanks is about 10 ppb. The aeration process removes these residual untreated VOCs to concentrations much less than 5 ppb. Thus, we can safely discharge treated water to the recharge basin south of the Laboratory. The carbon filter adsorbs all volatilized VOCs so that no VOCs are discharged to the atmosphere.

Table 1. **VOC destructive efficiency of the UV/H_2O_2 system (ND = nondetectable).**

Compound	Concentration, ppb		Polishing-system discharge, ppb
	Influent	UV/H_2O_2 effluent	
1,1-dichloroethene	12	ND	ND
1,1-dichloroethane	3	2	ND
Chloroform	2	1	ND
1,1,1-trichloroethane	7	6	ND
Freon 113	6	6	ND
Trichloroethene	5	ND	ND
Tetrachloroethene	170	3	ND

The extraction well servicing Treatment Facility A has direct influence on about half the VOC contaminants in the groundwater plume. Installation of other extraction wells is being evaluated to accelerate the removal of all contaminants in the plume.

Data from the operation of Treatment Facility A are being used to evaluate the merits of this treatment technology and provide guidance for the selection of future treatment technologies at LLNL. These data are also being used to verify the predictive computer models designed for hydrogeologic analyses. These models provide information concerning water table drawdown as a function of well location, contaminant migration, and estimates of total remediation time. Thus, Treatment Facility A is remediating the VOC-contaminated groundwater and is also helping advance the techniques of hydrogeologic predictive modeling.

Contact: W. Isherwood (415) 423-5058.

Testing Self-Contained Breathing Apparatus

Our test of the performance of self-contained breathing apparatus should set the standard for designing and building these devices to make sure that they function properly in a flashover.

Self-contained breathing apparatus (SCBA) are critical devices for firefighters and other emergency-response personnel—many times, their lives depend on the proper performance of their SCBA. The Special Projects Division (SPD) of the Laboratory's Hazards Control Department has, over the past two decades, evaluated and sought ways to improve the performance of SCBA. Our leadership in this area is widely recognized. An SPD staff member sits on the National Fire Protection Association (NFPA) Subcommittee on Self-Contained Breathing Apparatus; this group sets the standards for test methods that simulate the use of SCBA in realistic, worst-case fire conditions. The 1987 revision of the standard added test methods to evaluate high-volume air flow, accelerated corrosion, vibration and shock, lense abrasion, thermal cycling, particulate exposure, and communication. We designed and built the prototype of the high-performance breathing machine now specified in this standard for measuring SCBA air flows before and after each test. At least ten replicate breathing machines are in use by major U.S. and European SCBA manufacturers.

Evaluation of SCBA performance also requires a flame and heat test to assure that the apparatus will function in a flashover (the rapid ignition of superheated gases that collect under the ceilings of rooms involved in fires). Often in a flashover, a large overpressure propels the firefighter some distance before he is knocked down. The NFPA committee defines the laboratory simulation to be a 15-min exposure at 95°C while the unit operates at a 40-liter/min breathing rate, followed by a breathing rate of 100-liter/min during a 10-s exposure to an 815°C flame and heat source. Within 30 s after this test, the mannequin and SCBA must be raised some 15 cm and allowed to free fall. To pass, the apparatus must sustain no flame on any component for more than 2 s and must maintain positive pressure in the SCBA facepiece. To meet these test parameters, we have designed, constructed, and evaluated the test apparatus shown in Figure 1. The insert shows the SCBA engulfed in flames during the short, high-temperature part of the test.

After final review by the full NFPA technical committee, in mid-1990, this test can be incorporated into the next revision of the standard. Our preliminary test results suggest that SCBA manufacturers will have to make many changes in component-part materials. The resulting respiratory equipment will provide the improved protection that firefighters and emergency-response workers need to work safely and will increase their survivability in a flashover.

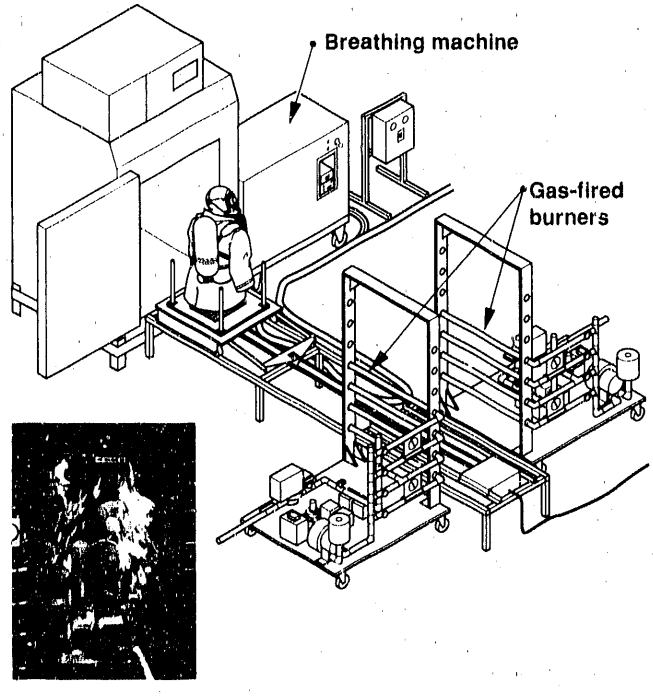


Figure 1. *Arrangement of equipment for performing flame and heat test of SCBA. The breathing machine is a high-performance design developed at LLNL for measuring the airflow rates achieved by the SCBA. Inset: commercially available SCBA engulfed in flames to simulate typical flashover thermal conditions.*

Contact: J. Johnson (415) 422-5165.

Index of 1990 Laboratory Achievements

For further information on the activities reported in this issue, contact the individuals listed below.

The State of the Laboratory, **1**	J. H. Nuckolls	(415) 422-5435
Defense Systems (overview), **4**	W. F. Scanlin	(415) 423-6810
High-Explosives Applications Facility, **6**	R. M. Alire	(415) 422-2419
W89 Engineering Development Program, **8**	J. V. Tyler	(415) 423-1307
Cost-Effectiveness of Modernized U.S. Strategic Forces, **10**	P. L. Chrzanowski	(415) 422-6522
Numerical Simulation of Electromagnetic Effects in Realistic Geometries, **12**	J. Ambrosiano	(415) 423-6634
Three-Dimensional Calculations of Material Strength, **14**	D. W. Baum	(415) 423-2236
Opacity Experiments with the Nova Laser, **16**	T. S. Perry	(415) 423-2065
	P. T. Springer	(415) 423-9221
New Streak Cameras, **18**	J. J. Ronchetto	(415) 422-3795
Applying Nuclear Testing Technology to ES&H Issues, **20**	D. A. Leich	(415) 422-6609
Arms Control and Treaty Verification Activities at LLNL, **22**	D. W. Dorn	(415) 423-5196
Laser Research (overview), **24**	J. I. Davis	(415) 423-9818
	A. J. Levy	(415) 423-8729
The Nova Laser, **26**	D. R. Speck	(415) 422-0681
Pulse-Shaped Implosions on Nova, **28**	R. E. Turner	(415) 422-8112
Multiframe Gated X-Ray Image Camera: The Fastest Movie Camera in the World, **29**	J. Kilkenny	(415) 423-4213
Damage-Resistant Optical Materials, **30**	J. Campbell	(415) 422-6497
Laboratory X-Ray Lasers, **31**	M. D. Rosen	(415) 422-5427
	D. L. Matthews	(415) 422-5360
Subpicosecond 7-TW Tabletop Laser, **32**	M. Perry	(415) 423-4915
AVLIS Laser Technology for the Next Generation of Microlithography, **33**	H. W. Friedman	(415) 422-2257
	E. R. Ault	(415) 422-6209
Advanced Laser Applications, **34**	E. V. George	(415) 423-3939
	K. R. Manes	(415) 423-6207
Industrial-Scale AVLIS is Approaching its Deployment Goals, **36**	E. R. Ault	(415) 422-6209
Uranium AVLIS Program, **38**	R. W. O'Neil	(415) 422-6222
Plutonium Laser Isotope Separation, **40**	J. G. Harri	(415) 422-6157
Magnetic Fusion Energy and Beam Research (overview), **42**	A. J. Glass	(415) 422-9804
Microwave Tokamak Experiment, **44**	B. Hooper	(415) 423-1409
	S. Allen	(415) 423-2676
The International Thermonuclear Experimental Reactor, **46**	C. D. Henning	(415) 422-0235
Free-Electron Lasers, **48**	T. J. Orzechowski	(415) 422-6709
	M. K Sheaffer	(415) 422-6292
Energy and Earth Sciences (overview), **50**	R. N. Schock	(415) 422-6477
	L. W. Younker	(415) 422-0720
Prototype Heater Test of the Environment around a Simulated Nuclear-Waste Package, **52**	A. L. Ramirez	(415) 422-6909
Modeling Radionuclide Release from Nuclear Wastes, **53**	C. J. Bruton	(415) 423-1936
	W. L. Bourcier	(415) 423-3745
Hot-Recycled-Solid Retort for Oil Shale Processing, **54**	R. J. Cena	(415) 422-7336
Environmental Restoration and Waste Management, **55**	J. Yow	(415) 422-3521
Discriminating between Nuclear Explosions and Earthquakes, **56**	S. R. Taylor	(415) 423-0616
A Test of Newton's Inverse-Square Law of Gravity, **58**	P. W. Kasameyer	(415) 422-6487
Numerical Simulation of Solute Transport in Porous Media, **59**	A. F. B. Tompson	(415) 422-6348
	R. B. Knapp	(415) 423-3328
Biomedical and Environmental Science (overview), **60**	M. L. Mendelsohn	(415) 422-5765
A Human DNA Repair Gene with High Evolutionary Conservation, **62**	C. A. Weber	(415) 423-8155
	L. H. Thompson	(415) 422-5658

Analysis of Trace Chemicals in Complex Mixtures by Liquid Chromatography/Immunoassay, **64**
DNA Probes from Human Chromosomes, **65**
AMS Validation of Neutron Doses, **66**
Biodegradation of High-Explosive Wastes, **67**

Engineering (overview), **68**
Algorithms to Improve Atmospheric Imaging, **70**
Development of a 20-GHz Integrated Optical Modulator, **71**

High-Power Microwave Generation, **72**

Predicting Thermal Loads that Cause Crack Growth and Failure, **73**
Fiber Composite Materials for Extreme Environments, **74**
Computer-Simulated Sheet-Metal Hydroforming, **75**
Physics (overview), **76**
Brilliant Pebbles, **78**
Reflection Grating Array for an X-Ray Satellite, **80**
The PEGASYS Project at SLAC, **81**

High-Temperature Superconductors: Novel Quantum Spin Liquids?, **82**

Determining Why Climate Models Disagree, **83**
Advanced Modeling of Thermonuclear Reaction Cross Sections, **84**

Chemistry and Materials Science (overview), **86**

The Chemistry and Physics of Modified Superconductors, **88**

Fingerprinting Petroleum Problems, **90**
Chemical Dynamics of Solid-Combustion Reactions, **91**
Electronic Structures of Surfaces, **92**
From Electronic Structure to Phase Formation in Alloys, **93**
Computations (overview), **94**

Archival Storage System, **96**
Adaptive Methods for Fluid Dynamics in Three Dimensions, **97**
TERPSICHORE: A New Plasma Physics Code, **98**
The SISAL Language Project, **99**
Laboratory Administration (overview), **100**

LLNL and Education, **102**
LLNL and Community Relations, **104**
Technology Transfer: LLNL Partnerships with Industry, **105**

Challenging Times Require Innovative ES&H Solutions, **106**
Center for Technical Studies on Security, Energy, and Arms Control, **108**
Measuring the Size Distribution of Radon Decay Products, **109**
Groundwater Treatment at the Laboratory, **110**
Testing Self-Contained Breathing Apparatus, **112**

M. Vanderlaan (415) 422-5721

P. J. de Jong (415) 423-8145
T. Straume (415) 422-5138
J. P. Knezovich (415) 422-0925
J. I. Daniels (415) 422-0910
E. A. Lafranchi (415) 422-8355
T. W. Lawrence (415) 422-5322
D. Lafaw (415) 423-4604
M. Lowry (415) 423-2924
M. D. Pocha (415) 422-8664
W. W. Hofer (415) 422-1636
R. A. Riddle (415) 423-7541
S. F. Groves (415) 422-1331
B. N. Maker (415) 422-1385
C. B. Tarter (415) 422-4169
W. S. Scott (415) 422-7288
C. Hailey (415) 422-4511
F. S. Dietrich (415) 422-4521
K. A. van Bibber (415) 423-8949
R. B. Laughlin (415) 422-7354
A. K. McMahan (415) 422-7198
J. B. Grant (415) 423-4415
W. L. Gates (415) 422-7642
R. M. White (415) 422-9668
D. A. Resler (415) 423-0451
C. Gatrousis (415) 423-2851
T. T. Sugihara (415) 423-8351
M. J. Fluss (415) 423-6665
H. B. Radousky (415) 422-4478
B. Andresen (415) 422-0903
J. Wong (415) 423-6385
A. Gonis (415) 422-7150
P. Turchi (415) 422-9925
R. R. Borchers (415) 422-9870
J. E. Ranelletti (415) 422-3782
S. Coleman (415) 422-4323
J. Bell (415) 422-7105
D. Anderson (415) 422-9818
J. Feo (415) 422-6389
P. E. Coyle, III (415) 423-7788
D. K. Fisher (415) 422-3343
G. W. Campbell (415) 422-5217
Science Education Program (415) 423-3177
Public Affairs (415) 422-4599
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R. C. Ragaini (415) 423-8875
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