Science & Technology REVIEW

December 2000

U.S. Department of Energy's
Lawrence Livermore
National Laboratory

Revolution in Materials Science

Also in this issue:

- Tools for Decision Making
- Storing Carbon Dioxide in Geologic Formations
- Seismic Analyses Get Site Specific

About the Cover

The simulations of material behavior being performed by Livermore scientists are closely tied to laboratory experiments. Pictured here is a vacuum cryostat resistivity irradiation chamber in which one of the experiments is being conducted. The chamber is used to measure radiation damage in plutonium (shielded inside the gold tube); the resulting data are used to refine the codes that predict the aging of plutonium. The article beginning on p. 4 discusses this and other research activities in advanced computational materials science, whose rapid progress is being assisted by the Laboratory's latest, most powerful supercomputers.

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str/.

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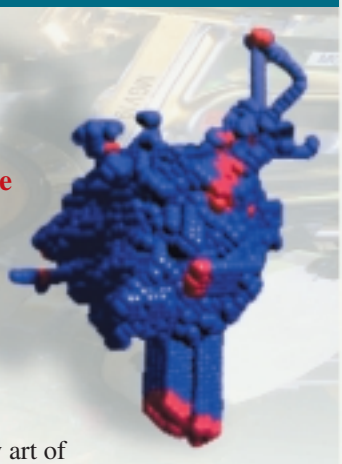
Lawrence Livermore National Laboratory

Contents

Features



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FDA approves Lab's cancer treatment technology

The U.S. Food and Drug Administration has approved a Lawrence Livermore–developed cancer treatment tool. Peregrine, named after the patron saint of cancer patients, is a computer-based system for calculating where radiation goes in the body. It allows doctors to more accurately target tumors with radiation, permitting them to increase the dose needed to eradicate tumors without increasing damage to healthy surrounding tissues.

Peregrine has been under development since 1994 by the Laboratory, in collaboration with researchers at the University of California at San Francisco and other academic institutions. Along the way, it has won the prestigious R&D 100 Award and a Federal Laboratory Consortium technology transfer award. Its principal investigator, Christine Hartmann Siantar, was named a Teller Fellow for her work on the project.

Peregrine combines the Laboratory's 50 years of expertise in radiation physics with advanced computer architectures to produce a system that determines radiation dose information in minutes. Using the Monte Carlo mathematical technique, it simulates the trillions of radiation particles that enter the body during treatment and accurately predicts the energy—that is, the radiation dose—deposited by the particles. The system uses a patient's computed tomography scans to tailor precise radiation doses based on that individual's anatomy and disease.

The Laboratory is partnering with NOMOS Corporation of Pennsylvania, a leading supplier of radiation treatment technologies, to bring Peregrine systems to the medical community. NOMOS will deploy Peregrine on its CORVUS radiation treatment system to accurately calculate the actual dosage for each patient.

Peregrine resulted from a multidisciplinary research effort at the Laboratory. Its development required the expertise of physicists, computer scientists, and electrical engineers, among others. Rosemary Walling, the current program manager of Peregrine, says of the FDA approval, "This was not just about physics. Everyone worked hard to see this project get the validation and verification it needed to get it through to a commercial channel." Now, says Hartmann Siantar, "Peregrine will touch lives. It is a breakthrough technology that could be used in treatment clinics everywhere."

Contact: Christine Hartmann Siantar (925) 422-4619 (hartmannsiantar1@llnl.gov).

Growing protein crystals to fight tuberculosis

The Macromolecular Crystallography and Structural Genomics group at the Laboratory will receive a $4-million grant to perform research to aid the design of tuberculosis drugs. The work will be a key component of a National Institutes of Health–funded program to fight tuberculosis, the number-one infectious disease in the world. The NIH program involves 6 nations and 13 institutions. It will be led by Los Alamos National Laboratory, which is receiving a 5-year, $28-million grant to coordinate the work and distribute the funds.

The Livermore team, led by Bernhard Rupp, will provide crystals of more than 400 proteins of the tuberculosis bacterium. Specific proteins are the means by which the tuberculosis bacterium invades cells and unleashes its virulence; therefore, the proteins are the prime targets for drug intervention. The molecular structure of those proteins must be known in detail so scientists can design effective, specific drugs to interact with them, and crystals are the means of determining the structures.

The Macromolecular Crystallography team will design computer-controlled, robotic devices that enable fast production of protein crystals. Rupp says that it will take "many, many experiments to find the proper conditions in which this crystal forms." After the crystals are made, the researchers will expose them to x radiation. The patterns of x-ray diffraction can then be used to reconstruct three-dimensional protein molecular structures.

"Obtaining crystals of proteins is a key challenge in determining the molecular structure," says Rupp. "Without crystals, there is no crystallography. Proteins are complex biological material, and protein crystals thus are fragile and difficult to grow." Rupp says the team has had great success in crystallizing a variety of bacterial pathogens and determining the structures of tetanus and botulinum toxins. "We are excited about the possibilities of making significant contributions to the understanding and the final defeat of TB. Drug design is at the forefront of biomedical research and a great challenge for the whole TB structural genomics team."

The tuberculosis research program is one of seven NIH pilot studies that build on the discoveries of the government's Human Genome Project and other DNA sequencing research.

Contact: Bernhard Rupp (925) 423-3273 (rupp1@llnl.gov).

Commentary by Hal Graboske

Computational Know-How Advances Materials Science

PREDICTING how materials will behave and perform is central to the success of major industries, the manufacturing of a vast range of consumer goods, and scientific research programs like those at Lawrence Livermore. For years, scientists have longed for computer simulations that could track changes in material properties on scales ranging from the atomic to the engineering. Such simulations would accurately predict material performance. But until recently, such simulations have been relatively crude or even impossible.

Now, because of the extraordinary computational capabilities of Department of Energy parallel-processing supercomputers, that has all changed. For the first time, we are successfully simulating the evolution of mechanical and chemical changes in materials and the performance of these materials in a variety of environments and conditions. These simulations, described in the article beginning on p. 4, are showing us in unprecedented detail how materials form and how they react under different environments. In so doing, the simulations suggest how we can change formulations or manufacturing methods to improve materials.

The advanced simulations are based on software that exploits the capabilities of thousands of small processors working together. Multiprocessing helps scientists solve some of the most perplexing problems in materials science, including understanding how and why materials crack, age, and ultimately fail; how semiconductors can be manufactured to greater tolerances for better performance; and how the three-dimensional structures of biological materials determine their function.

Because of the very nature of materials science, the simulation research is multidisciplinary. Livermore physicists, engineers, computational scientists, materials scientists, and bioscientists team up to develop the new simulations. The research is also based in part on laboratory experiments that serve to both motivate and validate them. We are thus confident that the simulations faithfully recreate the physical processes at work in materials.

One of the most significant attributes of our pioneering work is the vast range of the length and time scales of the simulations, from nanometers to meters and nanoseconds to tens of years. In this way we can trace, for example, the consequences of atomic-scale defects as they accumulate in time and space and eventually affect the performance of a vital part. Computer codes that successfully bridge different scales are essential because changes in material properties, such as radiation damage, can depend on phenomena occurring over many length and time scales.

The most immediate payoff for the simulations is stockpile stewardship—the Department of Energy's program to assure the safety and reliability of the nation's nuclear stockpile. The new simulations are also applicable to a large number of other Livermore research efforts, such as modeling optics damage for the National Ignition Facility, a 192-beam laser.

The potential of computational materials science has become obvious to American industry. The new generation of simulations will allow companies in almost every field to reduce the development time of new materials and more quickly ascertain the causes of material failures.

Clearly, we are entering an exciting era for materials science. Advanced computer simulations amount to a revolution in the field, one that will forever change this centuries-old discipline. Increasingly, computational modeling will complement both laboratory experiments and development of materials science theory. We even foresee the simulations minimizing the role and reducing the number of some traditional experiments that are largely based on trial and error. I am proud that Livermore scientists are among the leaders in the national computational materials science effort.

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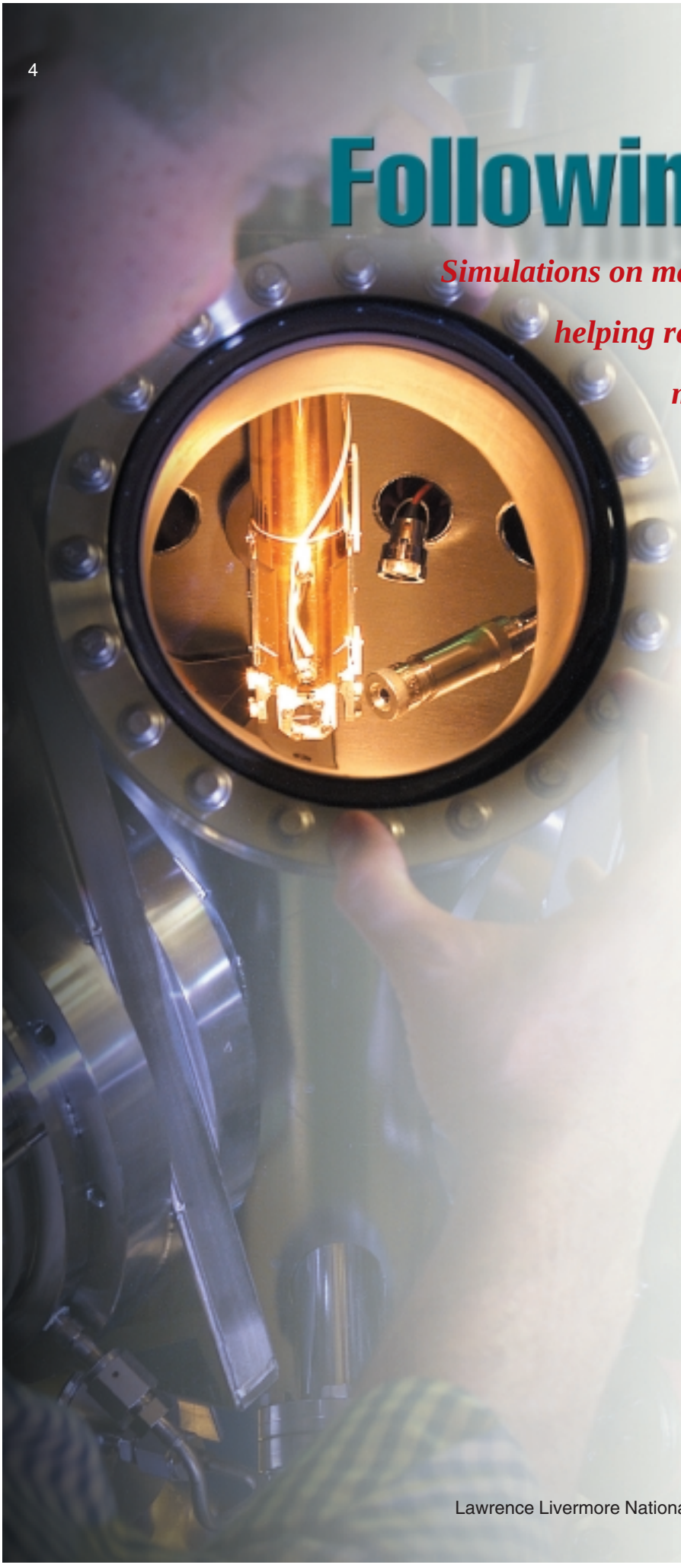
n Hal Graboske is Associate Director, Chemistry and Materials Science.

Following Materials

Simulations on massively parallel supercomputers are helping researchers understand how and why materials change and ultimately fail.



FROM breakthrough computer chips to new alloys for automobile engines, advances in materials shape our day-to-day lives and drive economic growth. For Lawrence Livermore scientists, predicting the performance of advanced materials is essential to success in countless research programs in national security, lasers, energy, and biotechnology.

In the past, advances in materials were accomplished by extensive laboratory testing combined with a healthy dose of guesswork, a time-consuming and often costly approach. Recently, a team of Lawrence Livermore scientists has begun to tap the vast computational power of Department of Energy supercomputers to simulate and accurately predict the performance of advanced materials. These simulations cover a wide range of operating environments and length and time scales.

The new field, called computational materials science, is one of the fastest growing areas within the field of chemistry and materials science. Leading the Livermore effort is materials physicist Tomas Diaz de la Rubia. He heads a team of 20 materials scientists, metallurgists, chemists, computer scientists, and physicists as well as graduate students from the United States and Europe.

The simulation research team works closely with Livermore computer scientists and collaborators from U.S. universities such as Princeton, Washington State, the University of Pennsylvania, MIT, and UCLA, and American companies such as IBM, Intel, and Applied Materials. The work is funded by Lawrence Livermore research programs, the Laboratory Directed Research and Development Program, the Department of Energy's Office of Science, and U.S. industry.

Diaz de la Rubia notes that Livermore research programs need many different classes of materials—including ceramics, glasses, plastics, and metals—and biological products. As a result, his group has assembled a broad research portfolio, one that includes simulating the mechanical properties of materials under extreme conditions, the accumulation of radiation damage in metals, the interaction of laser light with glass, the integrity of canisters for nuclear waste

over Time and Space

storage, the design and properties of advanced alloys, the actions of biomaterials such as enzymes, the dynamics of metal corrosion and cracking, and the diffusion of dopants in semiconductor manufacturing.

A Major International Presence

While helping Lawrence Livermore programs, the group is also establishing a major presence in the scientific community. The team publishes frequently in scientific journals and is prominent at international conferences. For example, Diaz de la Rubia is co-chair of the spring 2001 meeting of the Materials Research Society, which is expected to attract more than 3,000 scientists from around the world to San Francisco.

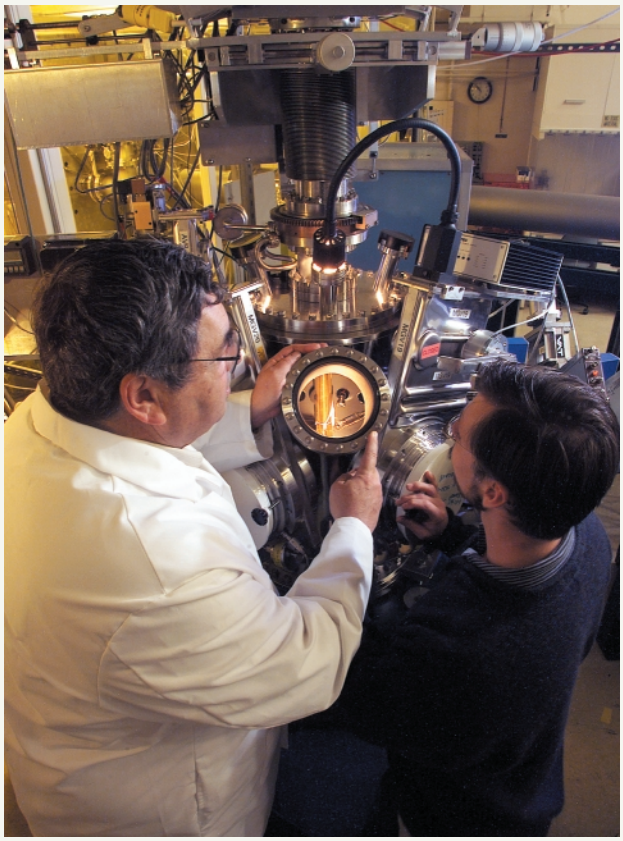
The Livermore work is part of DOE's Office of Science Computational Materials Science Network, composed of multidisciplinary scientific teams at several national laboratories. The network fosters basic materials science research within DOE and also serves to attract the best new talent to the discipline.

Diaz de la Rubia notes that scientists have long used computers to model materials and their performance. However, the newest generation of supercomputers, which employ thousands of microprocessors to tackle simulations once considered intractable, represents a significant advance. The computational materials science team works closely with members of the Laboratory's Center for Applied Scientific Computing to develop simulation tools that take advantage of multiprocessor supercomputers. The most advanced of those computers were acquired through DOE's Accelerated Strategic Computing Initiative (ASCI), a key component of the Stockpile Stewardship Program to assure the safety and performance of the nation's aging nuclear stockpile.

Writing or adapting codes for large parallel machines, in which complex problems are divided up to be jointly solved by multiprocessors, is a large effort. "The task requires people to think about software in new ways," says Diaz de la Rubia. The payoff, however, is a significant improvement in performance, as measured in the time required to run a model and the number of atoms being simulated. On Livermore's ASCI Blue supercomputer, about 350 million atoms could be simulated, but the newest computing platform, ASCI White, will track 10 billion atoms simultaneously.

The Livermore simulations are closely linked to laboratory experiments on the same materials. Experimental data ensure that the simulations accurately reflect the materials' chemical, mechanical, and thermodynamic properties as well as their manufacturing methods and the ways by which they age and ultimately fail. Only with solid experimental underpinnings, says Diaz de la Rubia, can the models help advance the understanding of how materials form, how they react under changing conditions (especially extreme environments), and how they can be improved.

The codes are so sophisticated that Livermore researchers are beginning to predict what scientists will see when imaging materials through electron microscopes. Their simulations constitute an important bridge between



Livermore materials simulations are closely coupled to a program of laboratory experiments. Researchers Mike Fluss (left) and Brian Wirth measure the atomic transport properties of radiation damage defects in metals, including plutonium; the data are used to refine codes that simulate and predict the performance of stockpiled nuclear weapons.

computer models and experiments. When a computer-generated image of calculated defects in a crystal is superimposed on an image of the same material taken with a transmission electron microscope, the results are remarkably similar. "When we see a certain image in the microscope, we now have a good idea about the mechanisms that produced it," says Diaz de la Rubia.

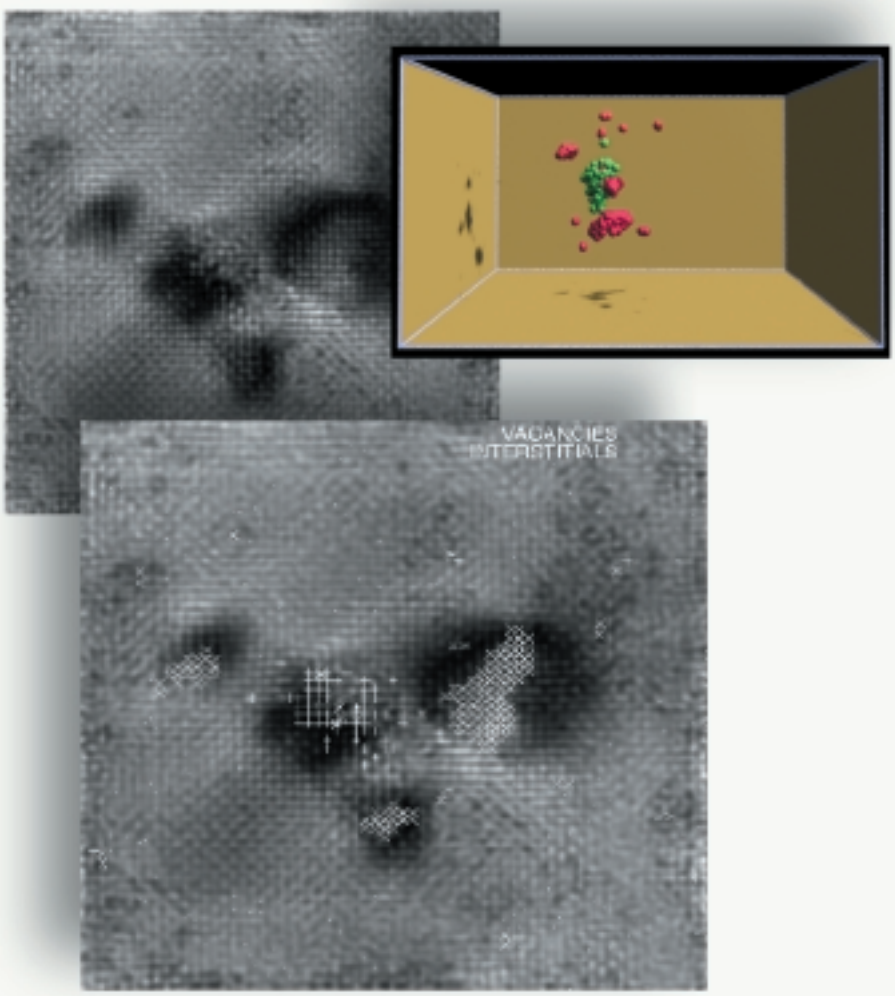
Multiscale Modeling of Materials

The Livermore codes incorporate multiscale modeling, an approach that is needed because material properties often depend on phenomena that take place at all length scales, from nanometers to meters. Multiscale modeling also incorporates a range of time scales from billionths of a second to tens of years. By combining models that cover the full range of length and time scales, scientists can simulate the evolution of mechanical and chemical changes in materials. Such changes may start with a defect occurring in a metal's crystalline lattice over a few nanometers in length and in a billionth of a second. And yet, multiplied millions of times over several years, such defects may combine to cause catastrophic failure of a computer chip, a glass optic, or a pressure vessel.

The most general approach to multiscale modeling is called information passing. In this method, which was introduced to the Laboratory by materials scientists Wayne King and David Lassila, simulations of matter at one scale are based on the results of simulations at a lower (more finely detailed) scale. The challenge is to form a coherent simulation of a material by building what Diaz de la Rubia calls "hooks between different scales."

The other approach, applicable in a limited number of cases, is called embedded multiscale modeling; its development at Livermore is being spearheaded by physicists Bernie Alder, Robert Rudd, Andrew Quong, and Vasily Bulatov. It uses the same code to solve the motion of molecules at all scales, with different physical models having different levels of approximation at each scale. For example, the way a nanometer-size crack behaves at the smallest lengths is similar to the way larger-scale cracks behave. Thus, it is a candidate for embedded multiscale modeling.

There are four major length scales: atomistic (measured in nanometers), microscale (micrometers), mesoscale (hundreds of micrometers) and



The Livermore simulations are beginning to predict the images that scientists will see when viewing materials through electron microscopes. On the upper left is a high-resolution transmission electron micrograph of a crystal of gold showing clusters of defects, namely interstitial atoms (atoms out of place, in red) and vacancies (points in the crystalline lattice where no atoms reside, in green). At the upper right is a computer simulation of how the defects should appear through the electron microscope. Superimposing the simulated image onto the electron micrograph (lower center) shows an impressive correlation between the two.

continuum (larger than 100 micrometers). In most cases, all four scales must be used to completely model a material's performance over a selected period of time. Each scale also requires a special code. For example, the microscale uses new codes such as micro3D, developed at Lawrence Livermore in collaboration with Washington State University researchers, while the continuum scale uses ALE3D, also developed at Livermore.

Simulations Begin with the Atom

The atomistic scale, which involves the properties and interactions of electrons and atomic nuclei, has been studied in great detail since the discovery of quantum mechanics. Atomistic simulations based on so-called first principles help scientists understand how atoms are arranged in crystals, how they bond to other atoms, and how impurities affect them. It is impossible, however, to use only atomistic models to simulate all material properties because of the sheer number of atoms that would be required for such a simulation.

Microscale simulations determine many materials properties, such as strength. But until the advent of ASCI machines, computers did not have the computational horsepower to perform microscale simulations with great fidelity. "People had been studying the collective behavior of dislocations in crystals for 40 years, but they couldn't simulate it until now," says Diaz de la Rubia. The microscale, he says, is the critical link between the atomistic and mesoscopic scales.

Likewise, the mesoscale links the microscale to the continuum scale. The mesoscale determines the structure of grains (a portion of a crystal in which all the atoms are oriented the same). Computer codes essential to understanding the performance of many nuclear weapons are based on this scale.

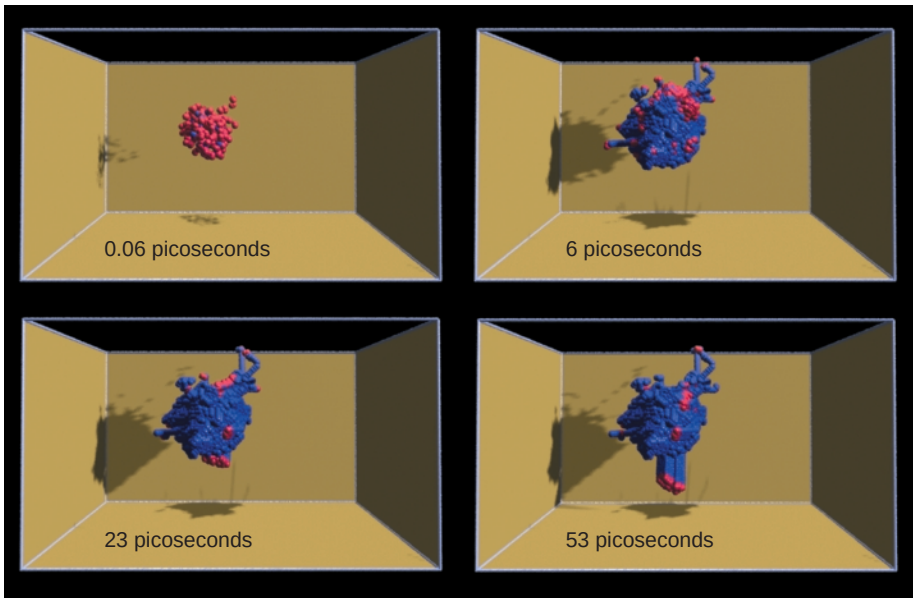
Finally, simulations on the continuum scale provide engineers with the likely behavior of materials in such areas as the damage that occurs in crash testing. At this level—visible to the naked eye—simulations using finite-element methods and experimentally derived equations model physical structures with element sizes that approach those studied individually with mesoscale models.

One essential aspect of multiscale modeling is its interdisciplinary nature. At Livermore, the effort is led by physicist Elaine Chandler and brings together scientists in the Defense and Nuclear Technologies, Physics and Advanced Technologies, Engineering, and Chemistry and Materials Science directorates to accomplish the goals of the modeling programs.

A major focus of the collaborative multiscale modeling effort is predicting the strength of metals in a variety of environments. Diaz de la Rubia notes that a general relationship between a metal's composition and its strength has been well established for decades. However, a detailed understanding of the mechanisms that confer strength based on the metal's crystalline microstructure has been lacking. Such knowledge is particularly vital to making predictions of performance under extreme conditions of pressure and temperature. "We want to predict how metals will deform under all conditions, and multiscale modeling is showing us the way," Diaz de la Rubia says.

Dislocations Are Key

He explains that in a metal, atoms are stacked in an ordered, crystalline lattice. However, there are also regions of less ordered stacking that can affect mechanical properties. These disordered areas can be caused by impurities, point defects in the crystal's lattice, or especially dislocations, which are misaligned planes of atoms that are sometimes referred to as line defects. When dislocations move through a crystalline lattice, they create plastic deformation, the ability of a material to bend without breaking. Without some plasticity, a metal becomes brittle and vulnerable to fracture and failure.



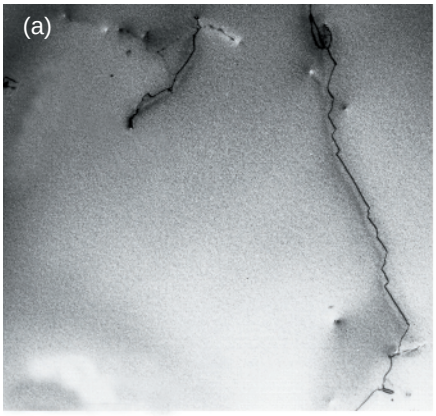
Atomistic simulations of radiation damage in copper atoms show the accumulations of defects over time, particularly those caused by clusters of interstitials (atoms that are not in their correct place in the copper crystal) or by replacements of the original atoms in the lattice. Data from atomistic simulations are used as the basis for microscale simulations.

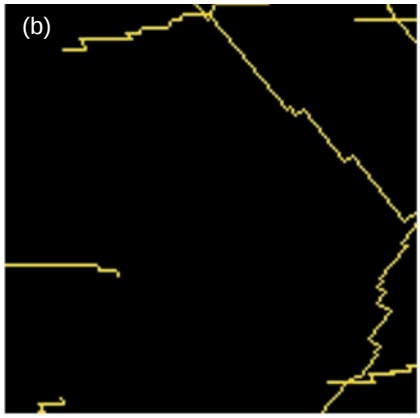
Livermore microscale simulations model the motion, multiplication, and interaction of dislocations, a phenomenon called dislocation dynamics. The simulations show the collective and complex behavior of millions of dislocations per cubic centimeter and how they determine a material's plastic deformation. The simulations are helping researchers better understand how certain manufacturing methods, such as the addition of selected impurities (alloys), harden a metal by interfering with dislocation movement.

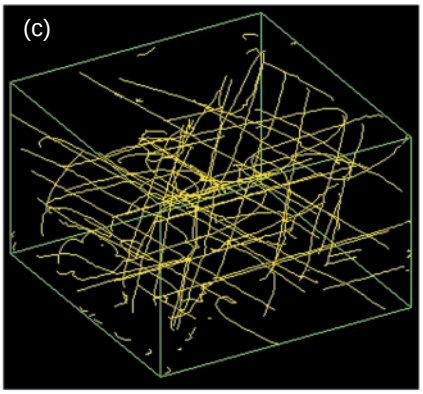
The strength simulation work is closely tied to experiments. The overall effort is headed by David Lassila and is based on the behavior of dislocations in molybdenum and tantalum crystals because these crystals are similar to materials found in many Laboratory programs and the nuclear stockpile. The experiments provide well-characterized dislocation structures to validate the results of the simulations. The experimental results are aided by directly observing dislocation mobility with transmission electron microscopes.

The current parallel version of the simulation code has been run on Livermore's ASCI Blue supercomputer using 80 processors and 260 hours of processing time. Led by Lassila and Bulatov, the researchers are revising the code to run on ASCI White. Lassila and Bulatov, together with physicist John Moriarty, are looking to extend the simulation work to areas of extreme pressure and temperature to improve the accuracy of current material models.

Predicting the strength of materials is important in almost all aspects of stockpile stewardship. Indeed, stockpile stewardship–related projects comprise the majority of the group's work. Diaz de la Rubia notes that materials are at the heart of most of the issues associated with the nation's enduring nuclear stockpile and that a central goal of ASCI is to acquire full-scale materials simulation tools to more accurately predict the lifetimes of weapon components. In particular, scientists want to improve their ability to predict the effects of aging or the performance of a remanufactured weapon part (see *S&TR*, June 1999, pp. 22–25).







(a) An electron micrograph of molybdenum under pressure determines (b) the initial conditions used in the model for simulating dislocation dynamics. (c) The simulation shows a compressed sample of molybdenum with many dislocations running through the crystalline lattice.

Radiation Damage Is Multiscale

One of the most challenging stockpile stewardship–related simulation problems is radiation damage to warhead components and materials. The problem is inherently a multiscale phenomenon. The individual events occur over a scale of 100 nanometers and a small fraction of a second, but the effects build up over decades throughout a material (see box on p. 10).

The materials scientists are applying multiscale modeling to predicting the performance of nonweapons materials in nuclear radiation environments. One team led by physicist Maria Jose Caturla and materials scientist Brian Wirth is modeling materials that could be used in future fusion reactors. Another team headed by physicist Patrice Turchi is modeling the long-term performance of waste canisters manufactured from exotic metal alloys. The canisters are being considered for storage of high-level nuclear waste at Yucca Mountain, Nevada (see *S&TR*, March 2000, pp. 13–20). Livermore scientists are performing simulations to determine how the canister will react over a 100,000-year period in response to extreme conditions of high humidity, temperature, and radiation. The assignment is a huge challenge because

it involves length scales ranging from the atomistic to the entire 45,000-kilogram, 3-meter-long waste canister.

One related area of interest is stress corrosion cracking, the most common mode of failure for a wide range of materials, including not only nuclear waste containers, but also bridges, fiber-optic cables, and nuclear reactor pressure vessels. Because microscopic cracks grow slowly, it is difficult to predict when a part will fail. For the first time, Livermore scientists led by Andrew Quong and materials scientist Wayne King are making the connection between the breaking of single atomic bonds at the tip of a growing crack and the ultimate failure of a part. They are planning to further their research through collaborations with materials scientists from IBM's Almaden Research Center in San Jose, California.

Advancing Semiconductors

An area of great potential is applying multiscale modeling to gain a better understanding of processes in the semiconductor industry. Diaz de la Rubia explains that the semiconductor industry has traditionally used simple models to explain the actions of dopants (impurities deliberately added to semiconductors to achieve a desired property) and defects. However, semiconductor manufacturing involves more than 200 steps in a process that is far too complex to be treated with these models. What's more, the industry is building increasingly smaller features on their chips, and the lack of accurate modeling, particularly on the atomistic scale, is proving to be a serious impediment to the development of next-generation devices. As a result, new atomistic-level models are required.

"Semiconductor companies want to be able to predict the outcome of a process from a given set of manufacturing conditions," says Diaz de la Rubia. To aid the manufacturers, Livermore researchers investigated the kinetics of defect and dopant migration in silicon chips, using funding from DOE's Office of Science and U.S. corporations such as Intel and Applied Materials. The approach provides a fundamental database for use in developing predictive simulations. It combines both experiments and theoretical advances and uses the same methods applied to other multiscale modeling projects.

The simulation results, when compared to results from laboratory experiments, showed the models to be very accurate. The project's success and the promise of the Livermore approach led to a Cooperative Research and Development Agreement with Intel and Applied Materials to create predictive modeling tools for semiconductor manufacturing.

In like manner, says Diaz de la Rubia, researchers are creating a family of tools for simulating biochemical processes. These tools will permit more accurate and rapid protein structure predictions. They will contribute to the study of DNA and aid predictions of protein function, drug activity, and the effects of chemical hazards such as carcinogens.

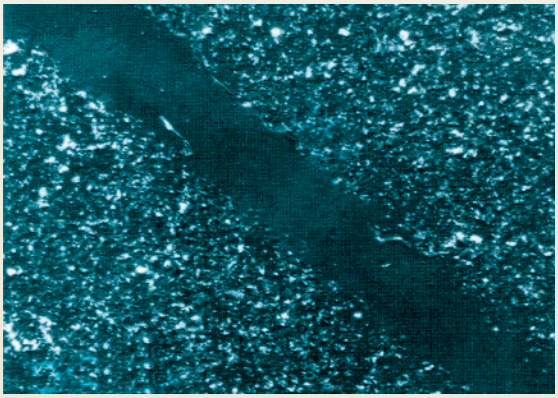
Materials scientist David Lassila, left, discusses the results of dislocation dynamics simulations with his team while they are directly observing dislocations with a transmission electron microscope. Mark Wall is seated at the transmission electron microscope, while Mary Le Blanc and R. Ann Bliss look on at right.

Simulations Reveal Damage from Radiation

Radiation damage is a ubiquitous phenomenon that affects many Lawrence Livermore research programs, the nation's nuclear weapons stockpile, and the nuclear power industry. Radiation damage can significantly degrade mechanical properties, seen most notably in increased brittleness and outright failure of a component.

The damage shortens the lifetime of pressure vessels in nuclear power plants and limits the choice of materials for fusion energy research. The problem is of particular concern for weapons materials such as plutonium. When plutonium-239 decays, it emits an alpha particle (a helium nucleus) and an atom of uranium-235. The resulting buildup of gaseous helium atoms and displaced plutonium atoms from the recoiling uranium could produce unacceptable changes in the plutonium metal. (See *S&TR*, June 2000, pp. 15–22.)

Although radiation damage has been studied for many years, the underlying mechanisms that relate damage to degradation of mechanical properties had not been clearly demonstrated until recently by a Livermore team. Headed by Diaz de la Rubia, the team reported its findings in the August 24, 2000, issue of *Nature* magazine. Because the damage evolves over a wide range of length and time scales, Diaz de la Rubia believed it could only be understood through multiscale modeling whose results are then validated by laboratory experiments.

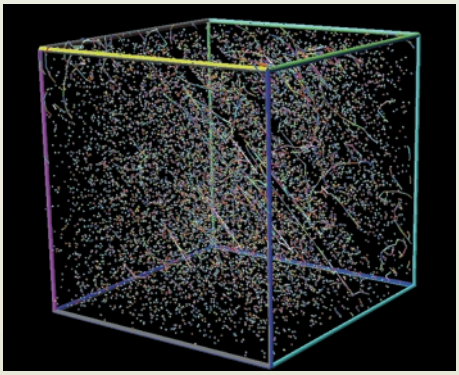


Simulations show that some of the dislocations in irradiated copper form defect-free channels.

The team used atomistic and then three-dimensional microscale simulations of irradiated metals. The simulations showed defects (both vacancies and out-of-place atoms) accumulating at the shortest scales (nanometers and picoseconds) and quickly growing into clusters. These clusters served to pin or prevent the movement of dislocations, which are misaligned planes of atoms. The free movement of dislocations confers plasticity or strength properties on metals.

The simulations showed that as some of the dislocations moved through the metal, they annihilated any defects along their path, thereby forming 200- to 300-nanometer-wide channels along particular directions (see figure below, left). The defect-free channels resulted in plastic instability, that is, areas of reduced strength. The team then compared the simulations to images taken with electron micrographs of irradiated copper and saw a very close correlation between the two (see figure below, right). While electron micrographs had previously revealed the presence of clear channels, scientists could not explain their formation.

Diaz de la Rubia notes that in the case of modeling radiation damage in metals, length scales are not as important as the time scales and energy scales of particles (for example, neutrons) involved in causing damage. The critical information, he says, is "figuring out how fast the changes happen so we can make predictions." To accomplish that requires first simulating the evolution of the smallest changes at the atomistic scale, using kinetic Monte Carlo software, and then applying the results as input to dislocation dynamics models to determine how mechanical changes occur.



Electron micrographs of irradiated copper reveal the same clear channels predicted by the simulations. The clear channels are areas of reduced strength.

Another major area of materials simulation work is for the National Ignition Facility (NIF), which will be the world's largest laser and is now under construction at Lawrence Livermore. Because the facility will have the largest concentration of optics anywhere, scientists need a more accurate method for predicting how the extremely pure optical glass will respond to the laser's high fluence levels.

Diaz de la Rubia is embarking on an effort to predict the lifetime of NIF optics with experiments and multiscale modeling. The project focuses on the final optics system, where the frequency of each laser beam is tripled into the ultraviolet with crystals of potassium dihydrogen phosphate and then focused onto a target through a fused silica lens. "We want to be able to model the response of fused silica in the presence of high intensity laser light," he says.

The modeling effort, led by physicist Michael Feit, involves performing atomistic calculations based on the fundamental properties of silica when exposed to laser light and the methods by which cracks propagate in glass. All of the information will be passed up to continuum-level simulations using the ALE3D code to model large-scale fractures. As with other multiscale modeling work, the NIF project involves a multidisciplinary team that includes experts in optics, lasers, materials science, and mechanical engineering.

With the advent of multiprocessor supercomputers, scientists can finally execute simulations with unprecedented accuracy and with seamless integration over all length and time scales. The Livermore simulation studies will help stockpile stewardship scientists to confidently predict the performance of stockpiled weapons.

The multiscale modeling work affects much more than DOE research programs. Use of the supercomputers amounts to a revolution in the materials science community. In this new era, simulation will guide advanced materials development and will show how materials form, how they react under changing conditions, and how they can be optimized for better performance. Simulations will also provide basic information about material behavior of interest to the nation's industrial products manufacturers.

—Arnie Heller

Key Words: Accelerated Strategic Computing Initiative (ASCI), ASCI Blue, ASCI White, Center for Applied Scientific Computing (CASC), dislocation dynamics, Laboratory Directed Research and Development, multiscale modeling, National Ignition Facility (NIF), plutonium, radiation damage, stockpile stewardship, Yucca Mountain.

For further information contact Tomas Diaz de la Rubia (925) 422-6714 (diazdelarubia1@llnl.gov).

About the Scientist

TOMAS DIAZ DE LA RUBIA is the deputy division leader for Science and Technology in the Chemistry and Materials Science Directorate. After completing his Ph.D. in physics at the State University of New York at Albany, he joined Lawrence Livermore in 1989 as a postdoctoral fellow working on supercomputing applications for fusion materials research. On becoming full-time staff, he first developed physics-based predictive process models for semiconductor manufacturing, in collaboration with several large semiconductor corporations. Then he began developing multiscale models of materials strength and aging in irradiation environments. He has published over 100 peer-reviewed scientific articles, chaired numerous international conferences and workshops, edited conference proceedings and special journals, served on national and international panels, and is currently on the editorial board of five scientific journals and a member of the American Physical Society's selection panel for the Rahman prize in computational physics. His research interests are in applying large-scale computing to materials problems, developing predictive tools for materials performance, and designing new methodologies for multiscale modeling.

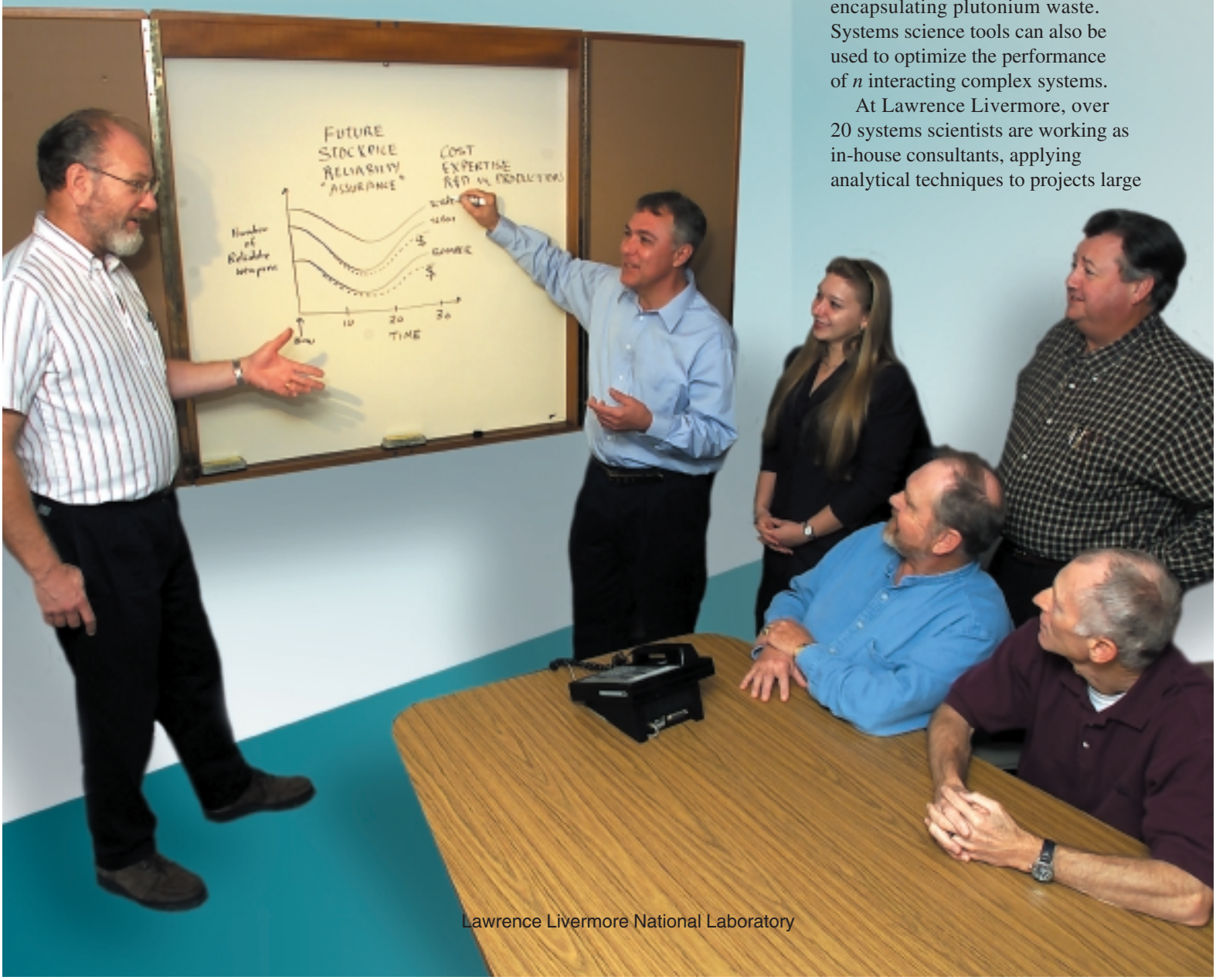
The Art of Systems Science

Which fork in the road should you take? Systems scientists help provide the rational bases for answering that as well as questions involving incredible complexity.

A classic problem in systems science is embodied in the quandary faced by a traveling salesman: what is the best route to *n* cities that passes through each city just once? After a few dozen cities, finding that most efficient route gets extremely complicated. In fact, the computational effort increases exponentially as the number of cities increases. Finding a practical approach to solve that problem is one facet of systems science.

Similarly, *n* interacting systems—facilities, components, machines, processes, and people—are involved in operating the National Ignition Facility (NIF), managing a battlefield, or encapsulating plutonium waste. Systems science tools can also be used to optimize the performance of *n* interacting complex systems.

At Lawrence Livermore, over 20 systems scientists are working as in-house consultants, applying analytical techniques to projects large



Lawrence Livermore National Laboratory

and small. Often, their task is to organize and analyze data to facilitate informed decision making. The information they supply helps managers choose solutions that are the safest, most timely, most productive, or most cost-effective.

The systems scientists work in the Decision Sciences Group led by Tom Edmunds and the Systems Research Group led by Cyndee Annese. The groups, which overlap considerably in expertise and project involvement, are managed as a team by the two group leaders and Annette MacIntyre, a deputy division leader in the Engineering Directorate.

Group members have graduate degrees in statistics, operations research, physics, engineering, economics, and mathematics. They have expertise in decision analysis, computer science, industrial engineering, simulation modeling, and systems engineering. The problems they tackle may involve designing systems to operate in the most effective way; deciding how to allocate scarce human resources, money, equipment, or facilities; or assessing the risks of system options and operations. Systems scientists are typically involved in a variety of projects.

Plethora of Uses

For example, they perform reliability, availability, and maintainability (RAM) analyses look at the big picture of an overall operation and thus assure that the production goals of a facility can be met. The scientists review available design documents, solicit information from experts, talk to vendors and examine their catalogs, and study industrial failure rate data. They examine the interactions among various component systems. In the process, they identify how long it will take to make repairs, how many spare parts will be needed, and so on. Engineers can then incorporate these data in the final design specifications of the facility.

RAM data can be fed into an operating model for the facility, such as a discrete-event simulation that can be used to optimize plant operation (see the box below for more information). It doesn't matter to the model whether the end product is laser shots, shoes, cars, or laundry detergent. The important thing for analyzing performance is that the data going into the model are the best available and that reasonable mathematical representations of the various processes are used. Says Edmunds, "There is an art to structuring and implementing models that can only be developed through experience." The same tools can be applied for a diversity of purposes and problems.

One goal of systems science is to quantify tradeoffs, according to mathematician Mike Axelrod in the Decision Sciences Group, because "you can't always get everything you want at the same time." Quantifiable risks and uncertainties surround each goal. In the Yucca Mountain project, for example, the performance of proposed methods for isolating radioactive nuclear waste must be estimated for tens of thousands of years into the future. Inevitably, uncertainties abound for such long time frames. Systems scientists estimate these uncertainties in a formally traceable manner.

Systems scientists also respond to Department of Energy regulations that require periodic completion of hazard and safety analysis reports for each DOE facility. Experts in probabilistic risk assessment recently completed a number of these reports for buildings at Livermore. They analyzed likely risks and worked with building staff to define preventive and mitigating measures, using system safety tools. One tool was fault-tree analysis, which is deductive

Another Kind of Simulation

Systems science modeling often uses discrete-event simulation, which looks at processes (such as manufacturing) that are made up of a series of individual events. In contrast, simulations of physical and chemical processes examine the state of a process at every instant in time. Examples of the latter include continuous simulations of fluid dynamics and high-explosive detonations. Such simulations comprise the majority of modeling work at Livermore.

The time between events in a discrete-event simulation may be a few seconds or many hours. What matters to the simulation—and what triggers a new event—is a change in some part of the system. Simulations may be run for laser system operations, manufacturing systems, economic markets, or the entire nuclear weapons complex. Analyses seek to predict the feasibility of a design or the performance of existing or proposed systems before their implementation. Design analyses and tradeoff studies can be performed inexpensively via simulation, and the practical implications of proposed systems can be identified and examined. Experiments with simulation models enable engineers to test ideas and proposed operating policies and to suggest alternatives. Key issues typically include throughput, resource utilization, reliability, availability, maintainability, and scheduling.

A large number of simulations have been run to plan the operation of the National Ignition Facility. What happens in terms of downtime when one or more of NIF's 192 lasers is off line? How frequently will parts need to be changed out? What happens when spare parts are not available as planned? Which spare parts matter the most to avoid downtime? What are staffing requirements for the system? These are the kinds of parameters that can be understood and optimized using a discrete-event simulation model.

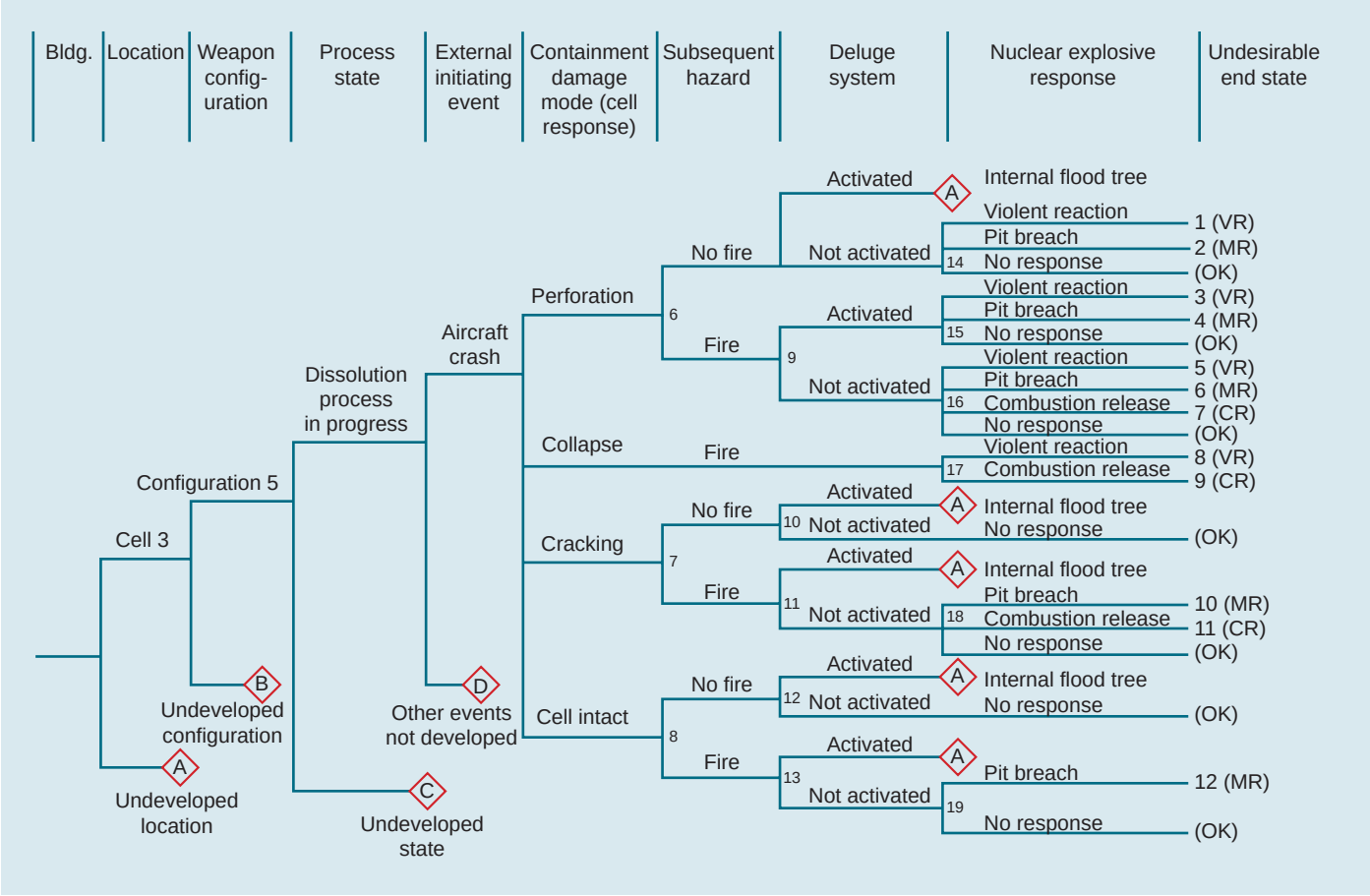
and helps analyze problems from the top down to evaluate many modes of failure both qualitatively and probabilistically.

Systems science statisticians also developed a model for forecasting electric energy demand at the Laboratory. This forecast must be accurate because Livermore contracts for bulk electric power. Usage over or under the forecast results in extra costs.

Livermore statisticians have developed a statistical sampling method for property management at Livermore. DOE requires a periodic audit of the records of more than 50,000 items in capital and attractive property inventory. The statisticians used statistical sampling theory to satisfy the DOE requirements without having to check every record. They reduced sampling costs by 90 percent, well worth the investment. The sampling method can be used for years to come, and DOE is considering applying this technique to property management throughout the DOE complex.

Systems scientists have assessed the risk associated with transporting spent nuclear fuel. They looked at a wide range of accidents and developed a probability distribution of the radiation that might be released from each one. For another project, they analyzed the hazards of assembling and disassembling nuclear weapons, developing a systematic and traceable method to assess the hazards from each part of the operation. This project required a marriage of traditional hazard–risk analysis and time-and-motion studies. To define appropriate controls, the team used database techniques, talked to experts in the field, developed simulations of the processes, and used specialized statistical methods that handle sparse data, rare events, and uncertainty.

Because of the diverse ways that systems science can be applied to Laboratory projects, systems scientists are involved in numerous projects at



An event tree developed as part of a probabilistic risk assessment for the processing of a nuclear weapon. This part of the tree shows what might happen if an aircraft were to crash into the building while processing was under way.

any given time. A few of the larger ones are discussed here.

	Availability		Reliability	
		Estimated lost opportunities		Estimated ruined shots
Conventional facilities	0.9915	(8.1%)	0.9985	(0.6%)
Laser system	0.9894	(10.1%)	0.8878	(53.3%)
Beam transport	0.9956	(4.2%)	0.9852	(6.7%)
Computer control	0.9448	(54.0%)	0.9941	(2.7%)
Optical components	0.9911	(8.5%)	0.9852	(6.7%)
Laser control	0.9920	(7.6%)	0.9493	(23.3%)
Target area	0.9921	(7.5%)	0.9852	(6.7%)
Goals	0.90		0.80	

The first-cut allocation of availability and reliability among the eight major systems at Livermore's National Ignition Facility. The goal was 90-percent availability and 80-percent reliability.

Analysis for NIF

The National Ignition Facility (NIF) is a cornerstone of the Department of Energy's Stockpile Stewardship Program to assure the safety and reliability of our nuclear arsenal without nuclear testing. It is also the largest single project under way at Livermore. NIF's 192 laser beams will be used to heat and compress a tiny deuterium–tritium fuel pellet with the goal of achieving thermonuclear ignition for the first time in a laboratory.

The NIF Conceptual Design Report specifies a goal of 90-percent facility availability for operating three shifts round-the-clock, that is, having no more than 10-percent downtime (lost opportunities) due to unscheduled maintenance and unexpected equipment failure. The goal for laser system reliability is 80 percent. To meet those goals, design engineers must know what the unavailability and unreliability allowances are for each NIF system. They need answers to such questions as: If the quality of a component is lower to save money, what effects will the reduced quality have on reliability and availability? Where would redundancies improve performance and be most cost effective? What preventive measures can be incorporated into the design to reduce maintenance and downtime?

Because of NIF's enormous size and importance, systems scientists approached this RAM study in two steps. They first allocated unavailability and unreliability from the top down, looking at the interaction of major functions to determine where the most downtime might occur. Then from the bottom up, they assessed individual component performance to determine overall system performance. The bottom-up estimates were used to monitor how evolving designs were addressing RAM performance goals and to check on the plausibility of the top-down allocations. As design of NIF progressed, designs were modified and allocations were iterated to meet system performance goals. If goals could not be achieved, availability could be increased by on-site backups, on-hand spares, and on-call maintenance. The table above shows the breakout of how availability and reliability were allocated throughout the major NIF systems in the first-cut allocation.

Because no laser facility truly compares to NIF, Bayesian statistical techniques were used to help handle the problem of sparse data and uncertainty. Systems scientist Alan Sicherman, who headed the top-down study, was pleased to note, "The top-down and bottom-up assessments were close to each other, which was pretty remarkable."

To integrate the RAM studies over all systems and to assess whether the total facility goals could be met, Laboratory scientists developed a discrete-event simulation model known as NIFSim. The NIFSim model used subsystem availability estimates from the RAM assessment as input to produce estimates of the availability of NIF as a function of the failure rates of its components and subsystems under various scenarios. In addition to failure-rate data, the NIFSim model reflected planned maintenance, personnel allocations, and operating modes such as all 192 or fewer beams, shots every 4 or every 8 hours, and periodic high-power (2- to 20-megajoule) shots.

NIFSim was used to check plans for facility operations to maintain a desired shot schedule. It showed what happens under different assumptions, such as performing maintenance only on planned maintenance days or having spare parts readily available. NIFSim predicted that at the completion of final design, NIF can be available for approximately 766 shots per year for an 8-hour shot cycle. For a 4-hour shot cycle, 1,360 shots are possible. The importance of spares availability and planned maintenance was illustrated by the simulation showing that if no spare parts are available, only 15 shots per year are possible.

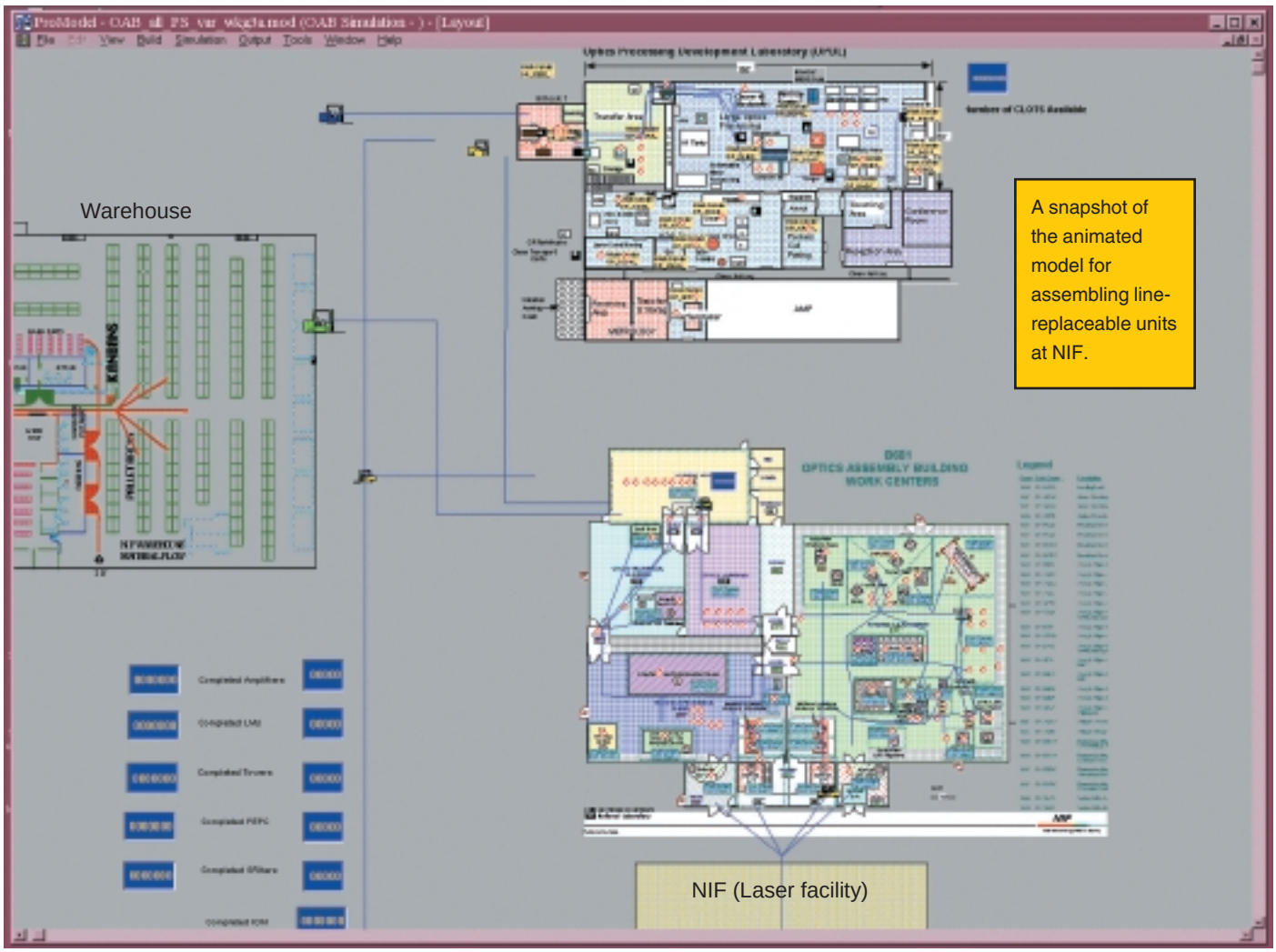
NIFSim can be customized to evaluate various scenarios of shot schedules, spare part availability, maintenance deferral, staffing levels, and operating practices related to unexpected equipment failures.

Systems scientists are helping to plan for the production of certain spare parts known as line replaceable units, or LRUs, for NIF. These are limited-life components and include some laser mirrors, spatial filter lenses,

transport spatial filter diagnostic and alignment towers, cavity spatial filter towers, amplifier slab cassettes, plasma electrode Pockels cells, and flashlamp cassettes. Assembly of many LRUs from smaller components will take place at Livermore. Many of the LRUs are as large as a refrigerator and cannot be stored easily. Instead, they will be manufactured "just in time."

For just-in-time manufacturing to work effectively, planners must work backward from the time new parts are to be installed during the first five years as well as from the start time of later refurbishments. What's more, they must consider random failures so they can minimize operational downtime. The model for assembly, installation, and refurbishment of NIF LRUs analyzes and verifies production capabilities under varying constraints. It is a decision-analysis tool for identifying risk, allocating resources, scheduling staff, and assuring that the activation schedule can be met within given time, resource, and budget constraints. As a cost- and time-saving device, perhaps its most important use is for estimating where resources may be most strategically allocated.

Systems scientists on another NIF project developed a statistical method for measuring "how clean is clean" on metallic surfaces in proximity to optics. The intense energy of the laser beam can drive microscopic particles from laser vessel surfaces onto nearby optics. As the laser beam passes through the optics, energy is deposited in any dust and dirt particles that are present, thus damaging the optics by punching microscopic holes in their surfaces. A cleanliness level for optics has been



A snapshot of the animated model for assembling line-replaceable units at NIF.

established, but to check every optical surface is not practical. The challenge, then, is to establish a process for performing random checks that ensure, to an acceptable level of confidence, the cleanliness of all vessel surfaces interfacing with optics.

Finally, systems scientists have simulated the process for manufacturing KDP (potassium dihydrogen phosphate) optics for NIF. In modeling the manufacturing process, the scientists presented questions and facts that optics producers had to consider to improve efficiency. The developed model is now used for estimating production (how many finished crystals can be produced per month) and for determining process bottlenecks. This information is then used in making decisions about process parameters such as the number of machines of each type needed, the number of shifts for each machine, or whether more than one vendor at a time should be producing optics for NIF to meet its installation and maintenance goals.

Forecasts for the Stockpile

Recently, systems scientists completed development of decision aids to forecast the reliability of the nuclear stockpile and select an optimal set of science-based activities (stockpile surveillance, physics experiments, weapon simulations, and plant production) to enhance confidence in the future performance of the stockpile. Using reliability and process modeling as well as discrete-event simulation and multiattribute utility theory, Livermore systems scientists developed a forecast framework that projects the status of various weapon systems into the future. As shown in the figure below, future reliability depends on the activities that the DOE invests in today.

Systems scientists also developed a database and simulation model framework of facilities and associated capabilities throughout the DOE weapons complex. The framework focused on readiness and technical base facilities that will be used to develop the new generation of weapons codes and physical experiments to validate the codes.

Although the model still requires more detailed data to realize its full potential, the framework is designed to address issues such as: How well can experimental throughput capacity address the goals and timelines of the overall research campaign? Is available expertise adequate for experimental design, execution, and data interpretation? Is there sufficient funding for ongoing experimentation as well as for the construction and maintenance of facilities? Is the Laboratory hiring and training the right disciplines to maintain design, experimentation, code development, theory, and refurbishment capabilities to continue stockpile certification?

Modeling Waste Processing

Discrete-event simulation modeling is helping to find the best method for processing 13 metric tons of plutonium that are no longer needed for national defense. Livermore and several partners are developing a ceramic material in which the plutonium will be immobilized, a production process for fabricating the material, and a process for placing the finished ceramic– plutonium "pucks" in waste canisters. The plutonium comes from several sources with varying levels of impurities. It must be blended to evenly dilute the impurities before the pucks are fabricated. The challenge is to accomplish the blending operation with as few reblends as possible to minimize handling costs and personnel exposures.

Systems scientists developed an impurity blending model, whose logic

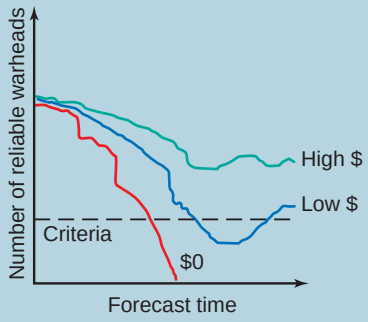
Problem: Forecasting stockpile reliability

The nuclear weapons stockpile must continually be certified as safe and reliable, a challenging task in the absence of nuclear testing. The problem is to select an optimal set of science-based investments (in stockpile surveillance, physics experiments, weapon simulations, and plant production) that maximize confidence in the near- and far-future performance of the stockpile.

Approach: Reliability, process, and cost modeling and discrete-event simulation

This effort requires modeling nuclear weapons complex enterprises in three fundamental areas: (1) determining how weapons expertise, physics experimentation, and computer simulation capability will affect the future ability to detect and assess problems and to design and certify remedial actions and certify the results; (2) modeling weapons production facilities, capacities, and costs; and (3) assessing past and predicting future failure types and rates in the stockpile.

Result: Forecasts weapon system and investment decision scenarios



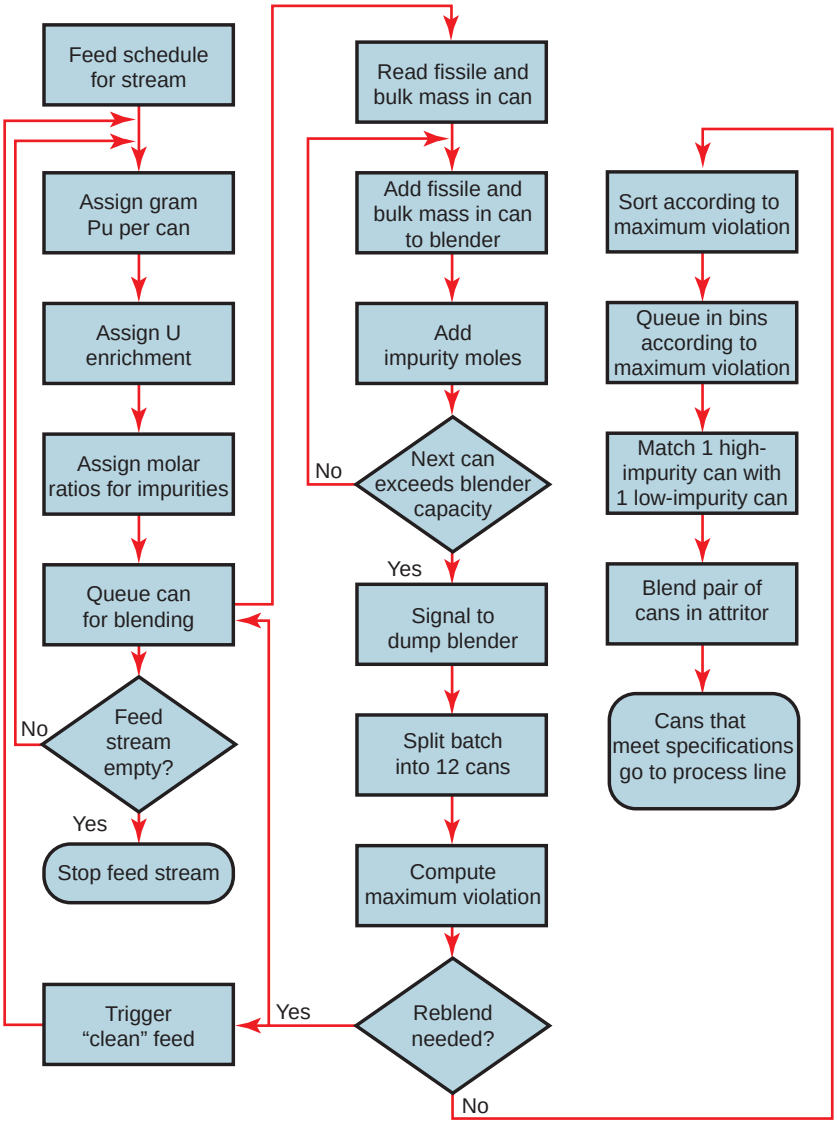
Systems scientists forecast the future reliability of various weapon systems as a function of investments in science-based activities.

flow is shown in the figure below. The model used Monte Carlo simulation techniques to account for uncertainty in the impurity content of incoming cans of plutonium. With this model, the team developed feed-stream schedules and material staging methods that minimize reblend requirements for 13 feed and plant design cases. The model provides the capability for rapid evaluation of new feed scenarios and operating constraints as they arise, including variations in isotopic mixtures.

Buying Uranium from Russia

Systems science data analysis methods have found their way into a major DOE nonproliferation project that is monitoring the purchase of highly enriched uranium from the Russians. In several formerly closed cities in Russia, highly enriched uranium is being removed from nuclear weapons, processed to reduce its enrichment level, and shipped to the United States where it is used for fuel in nuclear reactors. Personnel from several DOE laboratories spend from a few weeks to several months at a time in Russia monitoring these processes. Monitors check inventory, measure the reduced level of enrichment, and seal canisters that are sent to the U.S. Monitoring began in 1995 and is expected to continue until 2013.

Currently, four Russian sites require monitoring and typically, six monitoring visits are made to each site per year. From five to ten monitors participate in each of those 24 visits every year, producing reports of what they saw. The Russians also supply records for in-plant processing, interplant transfers, and shipping. They send about 8,000 pages of data per year—all requiring sifting and analyzing for holes or inconsistencies. In 1998, Livermore was assigned to be the repository for these data. A relational database keeps the information organized. From Livermore, the monitoring information travels via a secure network to analysts around the U.S. who examine it and prepare reports for DOE. Together, the Livermore team makes recommendations to DOE about



A logic flow of the simulation model for processing surplus plutonium. Plutonium from several sources has varying levels of impurities that must be diluted evenly. The goal is to perform as few reblends as possible to minimize handling costs and personnel exposures.

Sealed canisters of uranium shipped from Russia.

the effectiveness of the visit and prepares a new set of instructions for the next group of monitors.

Consistency tests for the data include developing tags and seals for chain-of-custody observations, standardizing monitoring forms and trip reports, performing mathematical and statistical analyses, reconciling apparent inconsistencies by seeking Russian clarifications of anomalous observations, and performing a final assessment.

On the Move

Systems science is applicable to a wide range of problems, so systems scientists at Livermore move from one project to another very different one on a regular basis. Whether working on seismic discrimination for treaty verification, allocating resources for contaminant cleanup at Livermore's experimental test site, or developing a model of energy use in China, they take their kit of decision analysis tools to help solve problems.

—Katie Walter

Key Words: decision analysis; discrete-event simulation; National Ignition Facility (NIF); nonproliferation; operations research; reliability, availability, maintainability (RAM); plutonium disposition; risk analysis; statistics; Stockpile Stewardship Program; systems engineering.

For further information contact Cynthia Annese (925) 422-0264 (annese1@llnl.gov) or Annette MacIntyre (925) 423-7254 (macintyre1@llnl.gov) .

About the Scientists

CYNTHIA ANNESE is group leader of the System Research Group, a systems science team at Livermore that focuses on innovative analysis of information, technical and safety risk assessments, and integrated simulation modeling. She received a B.S. in physics from the University of Idaho at Moscow, and an M.S. and Ph.D. in nuclear engineering from the University of California at Berkeley. Following work as a test engineer for the Fast Flux Test Facility and the Fusion Materials Irradiation Test Facility at the Hanford Reservation in Richland, Washington, she joined the Laboratory in 1985 as a physicist working in laser diagnostics for the Nova laser. Her current assignment is in the Nonproliferation, Arms Control, and International Security Directorate where, in addition to leading the systems science group, she conducts research to characterize design, manufacturing, and testing programs for nuclear weapons in countries of concern to the U.S. government. She also analyzes data to resolve questions about activities involving the international nuclear fuel cycle.

ANNETTE MACINTYRE is a deputy division leader for the Electronics Engineering Technology Division in the Engineering Directorate. She also helps manage the systems science groups, teaming with their group leaders to lead a sizable number of technically diverse scientists and engineers who perform risk, safety, and reliability analyses. She has over 20 years of experience in risk, safety, reliability, and discrete-event simulation modeling in the areas of waste management, economics, public and worker safety, and operation tradeoff studies. Most recently, she has worked on the issues of control reliability and effectiveness in real environments. MacIntyre received a bachelor's degree in German and European Affairs and a master's degree in operations analysis, both from the American University in Washington, D.C. She joined Lawrence Livermore in 1987 as the deputy program manager for reliability, availability, and maintainability in the Laser Isotope Separation program. Prior to that, she was a risk analyst and safety engineer at Rockwell Hanford Operations in Richland, Washington.

A Solution for Carbon Dioxide Overload

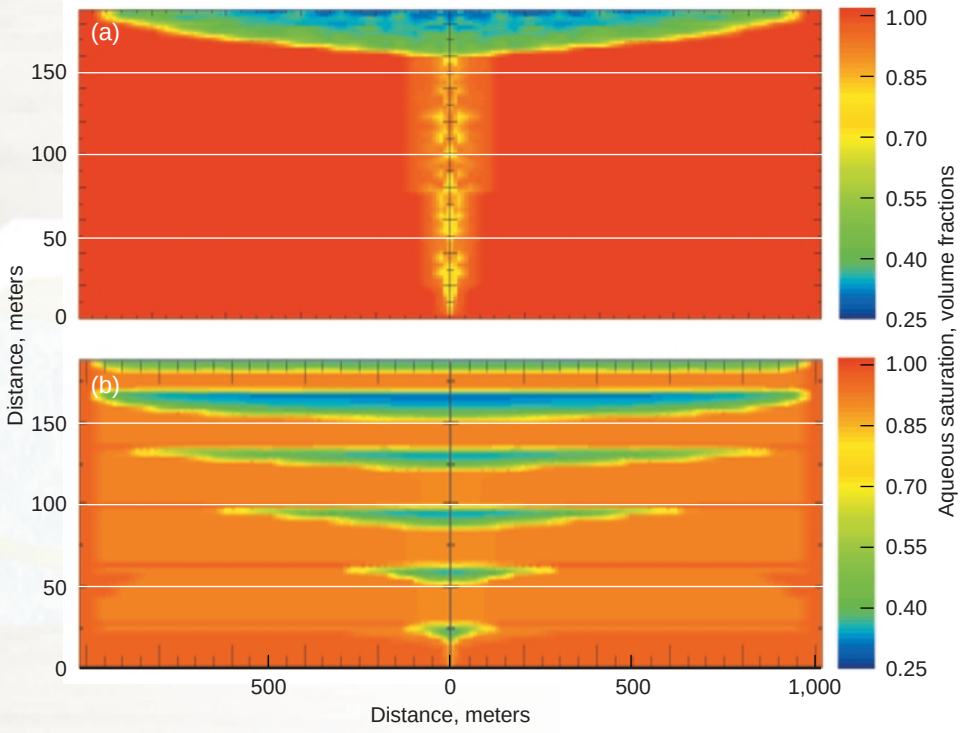
MORE carbon dioxide is making its way into our atmosphere as we burn fossil fuels and deforest tropical lands. Most experts agree that increased emissions of greenhouse gases—especially carbon dioxide—are responsible for an overall warming of our planet over the last 150 years.

In 1991, Norway became the first country to impose a federal tax on atmospheric CO_2 emissions from combustion-based point sources such as coal-fired power plants. Shortly thereafter, this tax—$55 per ton of CO_2—was extended to include emissions associated with offshore oil and gas production. The day is not far off when other countries, possibly including the U.S., will follow Norway's lead, thus creating a strong financial incentive to develop strategies for safe disposal of CO_2 waste streams.

One such strategy is to capture excess CO_2 and inject it underground, where it will remain sequestered from the atmosphere for thousands of years. Geochemist James W. Johnson is heading a Livermore team that is developing criteria for identifying subsurface geologic formations that could be used for CO_2 sequestration. "Our work is part of a long-term Department of Energy effort to identify optimal sites for sequestering CO_2," says Johnson.

Although CO_2 injection is a technique commonly used for enhancing the recovery of oil, large-scale injection for the sole purpose of isolating CO_2 from the atmosphere is occurring at just one place today: the offshore Sleipner facility, owned and operated by Statoil, Norway's state oil company. Located beneath the Norwegian sector of the North Sea, the extensive Sleipner West natural gas field is characterized by a high (9 percent) concentration of CO_2, well above the 2.5-percent limit imposed by European export specifications. Statoil strips excess CO_2 from the recovered gas in a tower on its offshore production platform before exporting the gas to the European community. Injecting the captured CO_2 into a confined aquifer—800 meters below the seabed and 2,500 meters above the Sleipner West hydrocarbon reservoir—results in no tax on Statoil for its atmospheric emissions.

Since 1996, Statoil has injected about a million tons of CO_2 per year and saved $55 million per year in taxes. The injection facility cost just $80 million to construct, and its operation accounts for less than 1 percent of overall production costs. At Sleipner, geologic sequestration has proved to be an



Sequestration performance depends on the geology of the proposed sequestration site. (a) In an aquifer with no shale layers, the CO_2 plume rises quickly to the aquifer caprock, where it migrates laterally beneath this impermeable seal. (b) When shale units are present, they effectively retard the plume's vertical migration while promoting its lateral extension, thus enhancing the effects of solubility and mineral trapping.

environmentally sound and financially prudent disposal option for excess CO_2.

Starting with simulations of CO_2 injection at the Sleipner site, Johnson and his collaborators, Carl Steefel and John Nitao, are developing a general modeling capability for analyzing CO_2 sequestration in geologic formations. This Livermore team is uniquely qualified to forge this capability, given their experience in developing an internationally recognized suite of reactive transport simulators (GIMRT, NUFT), supporting geochemical software (SUPCRT92), and thermodynamic-kinetic databases (GEMBOCHS). Using this integrated toolbox, they have begun to identify the geochemical, hydrologic, and structural constraints on successful geologic CO_2 sequestration. Eventually, they will correlate these constraints with the characteristics of potential geologic formations, rank their overall sequestration performance based on this correlation, and thus identify optimal injection sites.

Modeling a Dynamic System

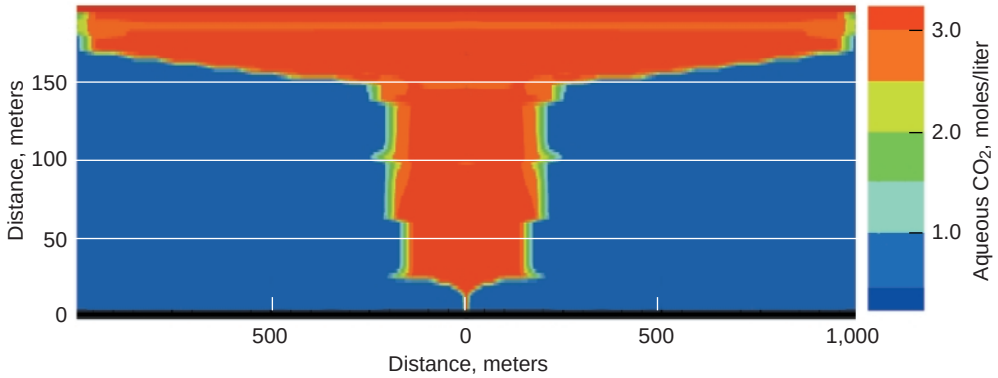
Reactive transport modeling integrates the geochemical, hydrological, and mechanical processes that characterize dynamic geologic systems. These processes, which include chemical reactions, fluid flow, heat transfer, and mechanical stress and strain, are interdependent and must be modeled simultaneously to simulate the true behavior of geologic systems. Simultaneous modeling was not possible for complex geologic systems until the advent of massively parallel supercomputers. Now, Johnson's team is producing the first-ever reactive transport simulations of CO_2 injection and sequestration within geologic formations.

Their initial Sleipner simulations examine what happens to CO_2 after it is pumped into its watery grave. At Sleipner, the storage formation is a highly porous, fluid-saturated sandstone aquifer, sealed at both the top and bottom by thick, relatively impermeable shale. The CO_2 moves through the formation via several migration processes and at the same time is trapped by various sequestration processes. The CO_2 migrates by displacing ambient water, with which it is largely immiscible, and by rising relative to this water, owing to its lower density. It also moves faster than the ambient fluid because of its lower viscosity. As the CO_2 plume migrates, some of it may react with formation minerals to precipitate carbonates (mineral trapping), some dissolves into the formation waters (solubility trapping), and some may eventually be isolated within anticlinal structures bound by the shale cap (hydrodynamic trapping).

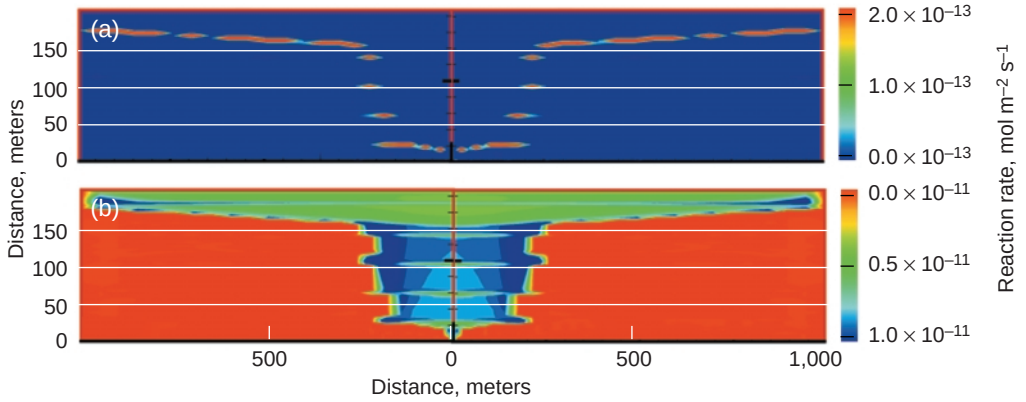
Understanding the relative effectiveness of these competing migration and sequestration processes is the key to identifying sites that will provide optimal sequestration performance. Reactive transport modeling represents a unique capability for quantifying this balance of processes.

First Results

The results of preliminary, two-dimensional NUFT and GIMRT simulations of CO_2 injection at Sleipner are shown in the three figures here, which illustrate the relative effectiveness of various sequestration processes after one year of injection. The figure on p. 20 illustrates the profound dependence of the CO_2 plume's location on the absence or presence of thin shale barriers within the aquifer. Without these layers, the CO_2 plume rises quickly to the aquifer caprock, where it then migrates laterally beneath this impermeable seal. When low-permeability shale units are present, as they are at Sleipner, they effectively retard the plume's vertical migration while promoting its lateral extension. The shale layers not only delay the arrival of the CO_2 plume at the caprock but also increase tremendously the volumetric extent of plume interaction with the aquifer and thus the potential for solubility and mineral trapping.



When shale layers are present, aqueous CO_2 concentrations are as high as 3 moles per liter within a large part of the aquifer. The overall distribution indicates that solubility trapping has sequestered about 3 percent of the injected CO_2 after 1 year, a small but measurable amount.



When shale layers are present, mineral trapping is limited to (a) minor calcite precipitation, which occurs at the expense of (b) plagioclase dissolution. Both are dependent on the effects of CO_2 solubility. Mineral trapping has sequestered less than 1 percent of the injected CO_2 after 1 year, a small but measurable amount.

The figure on p. 21 shows the spatial distribution of aqueous CO_2 concentrations when shale layers are present. It indicates that about 3 percent of the total injected CO_2 has dissolved into the ambient formation waters. Thus, solubility trapping represents a small but measurable contribution to aggregate sequestration.

The contribution of mineral trapping is also small but measurable. Precipitation of carbonates requires the presence of appropriate elements within formation minerals. In this Sleipner simulation, only a small concentration of one such element (calcium) is present in a single formation mineral (plagioclase), also of small concentration. Hence, mineral trapping is limited to minor calcite precipitation at the expense of plagioclase dissolution—a very slow process relative to solubility trapping. After 1 year, calcite precipitation has sequestered less than 1 percent of the injected CO_2.

In this preliminary 1-year simulation, solubility and mineral sequestration account for less than 4 percent of the injected CO_2. However, the relative effectiveness of solubility and especially of mineral trapping may be significantly increased over longer time frames within formations whose ambient fluid composition and mineralogy are different from Sleipner's. Johnson is quick to note, "Our research is first-cut reactive transport modeling of the complex CO_2 injection–sequestration problem." Other potentially significant effects will be evaluated in future work.

A Collaboration Begins

The preliminary reactive-transport simulations of CO_2 injection that Johnson's team carried out at Sleipner used site-specific technical data available in the public domain, but these data are insufficient for further detailed modeling efforts. Livermore recently initiated a collaboration with the International Energy Association (IEA), which coordinates research and development and monitoring of the Saline Aquifer CO_2 Storage (SACS) project at Sleipner. As part of the collaboration, IEA–SACS will supply Livermore with additional Sleipner data, which will permit more highly resolved simulations. These improved models will yield new insights into the current injection process and perhaps ways to improve sequestration performance at Sleipner.

For Livermore and the Department of Energy, obtaining more data for the unique Sleipner CO_2 sequestration project—and developing a general modeling capability based on Sleipner simulations—is invaluable. The problem of excess CO_2 must be solved, geologic sequestration represents a potentially promising solution, and reactive-transport modeling provides a unique way to identify optimal geologic formations for sequestration in the U.S.

—Katie Walter

Key Words: carbon dioxide sequestration, reactive transport modeling.

For further information contact James W. Johnson (925) 423-7352 (jwjohnson@llnl.gov).

Preparing for Strong Earthquakes

NOTHING like a mighty earthquake demonstrates the power of nature. People who live through one remember it forever.

California's Loma Prieta and Northridge earthquakes were disastrous, but experts warn that more and possibly bigger earthquakes threaten the state. We're powerless to prevent them, but we can prepare. That is just what the University of California (UC) is doing, with the help of the Campus Earthquake Program (CEP), a partnership of Lawrence Livermore National Laboratory and seven UC campuses. The CEP is helping UC prepare for large earthquakes by determining what can be expected at specific sites on various campuses.

Livermore's François Heuze, a geotechnical engineer in the Energy and Environment Directorate, initiated and leads the CEP. Heuze explains, "Campus structures were damaged from the moderate Loma Prieta and Northridge earthquakes. In larger tremors, University campuses could suffer loss of life and serious damage."

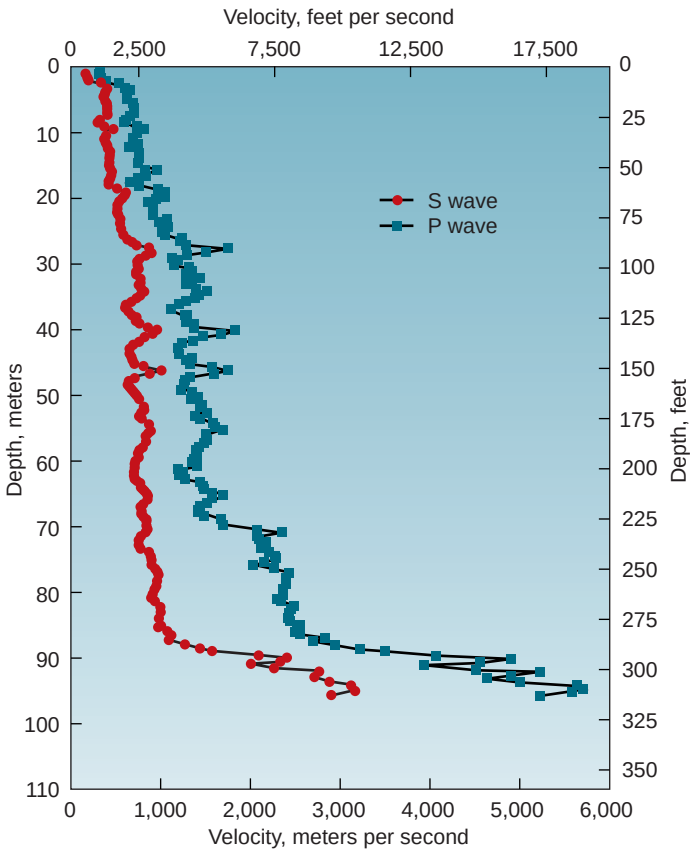
The work has been funded under the Campus–Laboratory Collaboration Program of the UC Office of the President. It has also received funding from the campuses that had sites evaluated as well as from Lawrence Livermore's University Relations Program.

From Research to Reality

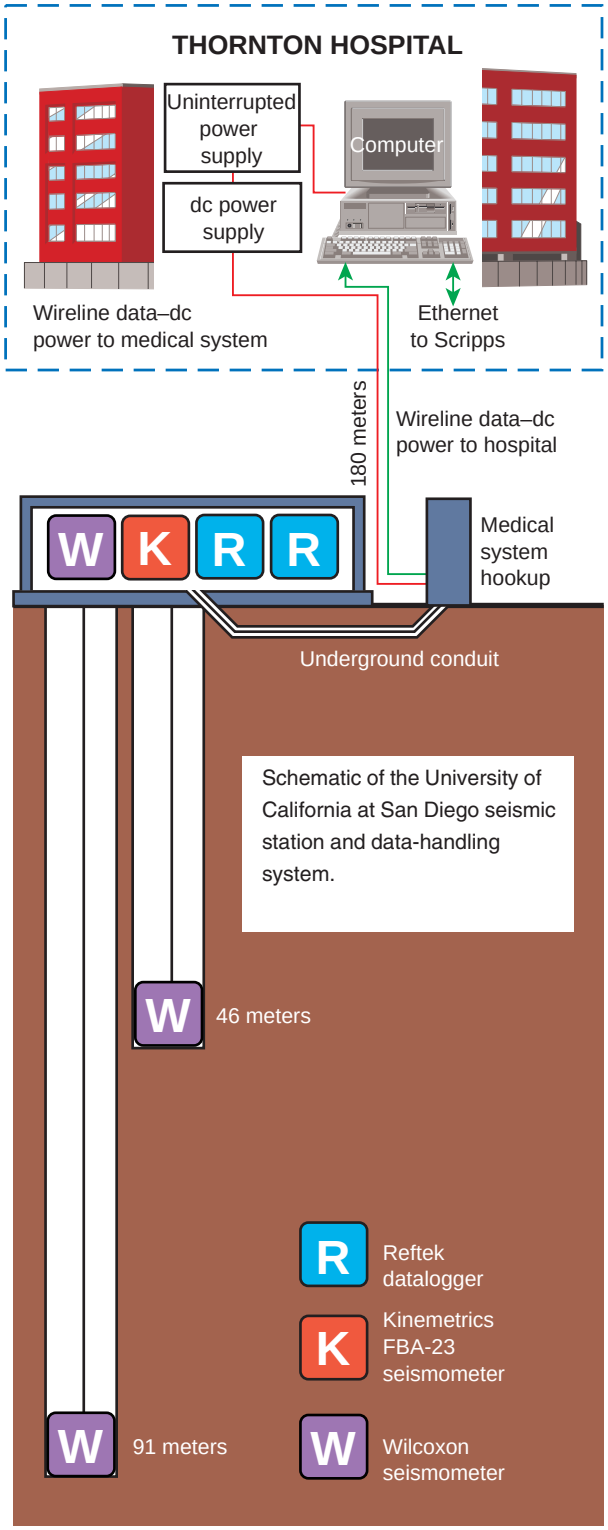
The Campus Earthquake Program had its genesis as a research project in Livermore's Laboratory Directed Research and Development (LDRD) Program in 1991. In this project, started by the Engineering Directorate's Gerry Goudreau, Laboratory seismologists and geotechnical engineers used site-specific records from small earthquakes to predict strong ground motions at those same sites during large earthquakes. Then structural engineers on the team used these strong-motion estimates to calculate the response of specific structures, such as the Dumbarton Bridge crossing San Francisco Bay (see *Energy & Technology Review*, September–October 1993, pp. 7–17).

With LDRD results in hand, Heuze met with UC officials to determine their interest in conducting similar studies at the campuses. At the time, UC's seismic policy was quite brief. "It basically said that if you had any earthquake concerns, you should call a structural engineer," recalls Heuze. UC campuses at Riverside, San Diego, and Santa Barbara expressed interest in acquiring additional information about specific sites on their campuses.

About the same time, the UC Office of the President initiated the Campus–Laboratory Collaboration program to encourage cooperative research between the national laboratories and the campuses. Of 120 proposals submitted to the program in 1995, the CEP was one of five that were funded. Bringing together experts in geology, seismology, geophysics, and geotechnical engineering, the CEP in 1996



Graph of compressional- (P) and shear- (S) wave velocities at the University of California at Riverside. The water table is indicated by the velocity increase in the P wave without an increase in S wave at the 71-meter depth, and the hard granite can be "seen" starting at 88-meter depth.



began a four-year examination of three specific sites: the Engineering 1 Building at Santa Barbara, the Thornton Hospital at San Diego, and the Rivera Library at Riverside.

Listening to the Underground

Given a site's ground motion—that is, how the site's geology responds to earthquakes—a structural engineer can design a building to withstand that motion. However, estimating the range of possible ground motions at a particular site requires a detailed knowledge of the site geology, the regional earthquake faults, and the site's response to seismic waves.

A geotechnical engineer draws on a variety of methods to determine what level of ground shaking should be considered in designing a structure to withstand earthquakes. One method, deterministic hazard estimation, focuses on designing a structure that could survive the largest earthquake expected at that site. Before this method is applied, the source (fault) and size (magnitude) of the threat must be determined. Another method, Probabilistic Seismic Hazard Estimation (PSHA), combines a variety of uncertainties—such as the likelihood of an earthquake of a certain magnitude occurring on a given fault—to estimate the probability of the structure experiencing a certain level of ground motion (or greater) during a specified time period.

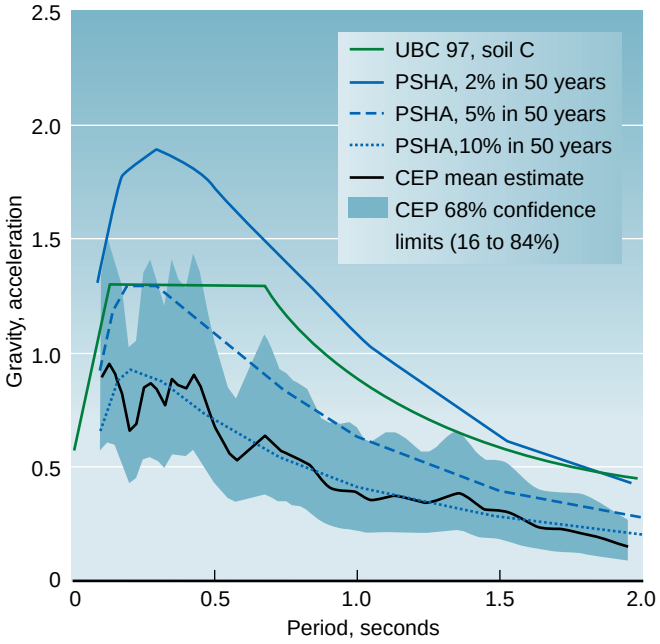
The CEP provides site-specific seismic analyses by characterizing the geology of a given site, monitoring small local earthquakes at depth and on the surface, and using this information to model the strong motions of large earthquakes. The first step is to identify faults that could produce moderate to strong ground motion (defined as earthquakes of magnitude 6 and above on the Richter scale). The next step—characterizing the site—involves working out the details of the geology and the stratigraphy (the succession of geologic layers or strata). This work consists of drilling and sampling boreholes, collecting geophysical soil logs, making geotechnical measurements on soil samples, and pulling it all together to paint a detailed picture of subsurface geology. "This kind of exhaustive site characterization is seldom performed," says Heuze. "It is expensive and goes well beyond common site investigations. However, that is the price we must pay to obtain the credible site-specific knowledge required for predicting strong earthquake effects."

On each campus, the researchers placed seismic stations in vertical arrays as deep as 90 meters, far beyond the 30 meters typical of most geophysical examinations. The stations recorded small earthquakes from the local faults as well as regional events. Large earthquake motions for a

given site were simulated using these data in combination with rupture scenarios of the faults identified as the main threats. Heuze explains, "For our calculations, we divide the fault surface into many subzones, sum up the contributions from small events in each subpart, and thus obtain the strong motion in rock under the site. We then calculate how that earthquake propagates up to the surface through the different soil layers." Rock's response to earthquakes is linear and fairly straightforward. But soils respond nonlinearly.

What can't be predicted is how an earthquake will break on a fault. It could fracture at one end and travel the length in one direction, or start at the opposite end. It could begin anywhere along the fault surface and travel in both directions, splitting the energy. Typically, the CEP analyzes over 100 rupture scenarios for each fault for a given earthquake magnitude. At the UC Santa Barbara site, for example, the team used 240 scenarios. The results of these estimates are then presented in terms of a stochastic distribution of possible motions for the campus.

"It is important to understand the difference between our approach, which is stochastic but deterministic, and the PSHA, which is strictly probabilistic," says Heuze. "We are not putting probabilities on our motions. We say that, whether the likelihood is low or high, they can happen, because nobody knows how the fault will rupture."



Graph of surface strong-motion estimates for the University of California at Santa Barbara's Engineering 1 Building. The estimates are for the Uniform Building Code (UBC) 97 (green line), the Probabilistic Seismic Hazard Analysis (PSHA) with different earthquake likelihoods in a 50-year period (blue lines), and the Campus Earthquake Program (CEP) approach (the teal area defines the range for the mean ±1 standard deviation of the estimated earthquake motions).

Rock-Bottom Line

Study results will be presented in a series of Lawrence Livermore reports, prepared with the campuses and available to the general public. In the reports, the site-specific ground motions calculated by CEP are compared to results obtained by other methods.

Heuze says, "Eventually, the University's decision on which motions to use as the design basis will depend on the combination of all the information it acquires. We are working closely with UC's consultants to combine the deterministic and probabilistic assessments, while also accommodating the regulatory constraints of building codes."

The CEP also has a proposal to perform a similar assessment for the site of the future UC Merced. Merced is the ideal study site, Heuze notes, because its ground-motion information would be available to the architects and structural engineers before they design any campus buildings.

Heuze adds, "This program is unusual in drawing, for the first time, upon the brain power within the UC system—professors, postdocs, and students at the campuses, scientists and engineers at Lawrence Livermore—to address the ground-motion problem facing the University. I see earthquake exposure to be the single greatest threat to the welfare of the University. Now, through this multidisciplinary effort, we can understand much more clearly the earthquake exposure that each campus faces."

—Ann Parker

Key Words: Campus Earthquake Program (CEP), Campus–Laboratory Collaboration Program, ground-motion analysis, Probabilistic Seismic Hazard Analysis (PSHA).

For further information contact
François Heuze (925) 423-0363 (heuze@llnl.gov).

Patents and Awards

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Abraham P. Lee Joseph P. Fitch	**Micro Devices Using Shape-Memory-Polymer Patches for Mated Connections** U.S. Patent 6,086,599 July 11, 2000	A method and microdevice for repositioning or retrieving miniature devices located in inaccessible areas—for example, medical devices (stents, embolic coils) located in a blood vessel. The microrepositioning or retrieving device and method use shape-memory-polymer (SMP) patches formed into mating geometries (for example, a hoop and a hook) for reattachment of the deposited medical device to a catheter or guidewire. For example, SMP or other material hoops are formed on the medical device to be deposited in a blood vessel, and SMP hooks are formed on the microdevice attached to the hoops on the medical device, or vice versa, enabling deposition, movement, redeposit, or retrieval of the medical device. By changing the temperature of the SMP hooks, microdevices can be attached to or released from the hoops located on the medical device. One method for forming the hooks and hoops involves depositing a sacrificial thin film on a substrate, patterning and processing the thin film to form openings through it, depositing or bonding SMP materials in the openings so that they are attached to the substrate, and removing the sacrificial thin film.
Paul R. Coronado John F. Poco	**Flexible Aerogel Composite for Mechanical Stability and Process of Fabrication** U.S. Patent 6,087,407 July 11, 2000	A flexible aerogel and process of fabrication. An aerogel solution is mixed with fibers in a mold and allowed to gel. The gel is then processed by supercritical extraction or by air drying to produce a flexible aerogel formed to the shape of the mold. The flexible aerogel has excellent thermal and acoustic properties and can be used in numerous applications, such as for energy absorption and insulation (temperature and acoustic), to meet the contours of aircraft shapes, and in limited spaces—because an inch of aerogel is four to five times better as an insulator than an inch of fiberglass. The flexible aerogel may be inorganic (silica) or organic (carbon) and can contain glass or carbon fibers.
William D. Daily Clifford Schenkel Abelardo L. Ramirez	**Electrical Resistance Tomography from Measurements inside a Steel-Cased Borehole** U.S. Patent 6,088,655 July 11, 2000	Electrical resistance tomography (ERT) produced from measurements taken inside a steel-cased borehole. A tomographic inversion of those measurements was then made to image, remotely from the borehole, the electrical resistivity distribution in the formation. The ERT method involves combining electrical resistance measurements made inside a steel-cased borehole, to determine the electrical resistivity in the formation adjacent to the borehole, with the inversion of electrical resistance measurements made from a borehole not cased with electrically conducting material, to determine the electrical resistivity distribution remotely from a borehole. It has been demonstrated that by using these combined techniques, highly accurate current-injection and voltage measurements made at appropriate points within the casing can be tomographically inverted to yield useful information outside the borehole casing.
M. Leslie Carman Robert T. Taylor	**Laboratory Method Used for Bioremediation** U.S. Patent 6,090,287 July 18, 2000	An improved method for in situ microbial filter bioremediation that increases the operational life of an in situ microbial filter emplaced into an aquifer. A method for generating a microbial filter of sufficient catalytic density and thickness so that it needs to be replenished less frequently has improved bacteria attachment and detachment characteristics. It is endogenously more stable under in situ conditions. A system for in situ field water remediation.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Jeffrey S. Haas Fredrick R. Kelly John F. Bushman Michael H. Wiefel Wayne A. Jensen	**Hand-Portable Thin-Layer Chromatography System** U.S. Patent 6,096,205 August 1, 2000	A hand-portable, field-deployable thin-layer chromatography (TLC) system and a hand-portable, battery-operated unit for illuminating, developing, and acquiring data from the TLC plates. The TLC system contains many miniaturized features that permit a large number of samples to be processed efficiently. It includes a solvent tank, a holder for TLC plates, and a variety of tool chambers for storing TLC plates, solvent, and pipettes. After processing in the TLC system, a TLC plate is positioned in a collapsible illumination box. The box and a charged-coupled device (CCD) camera are optically aligned for optimal pixel resolution of CCD images from the TLC plate. The TLC system also includes an improved development chamber for chemical development of the TLC plates, which prevents solvent overflow.
John F. Cooper G. Bryan Balazs Peter Hsu Patricia R. Lewis Martyn G. Adamson	**Integrated System for the Destruction of Organics by Hydrolysis and Oxidation with Peroxydisulfate** U.S. Patent 6,096,283 August 1, 2000	An integrated system for destruction of organic waste comprises a hydrolysis step at moderate temperature and pressure, followed by direct chemical oxidation using peroxydisulfate. This system can be used to quantitatively destroy volatile or water-insoluble halogenated organic solvents, contaminated soils and sludges, and the organic component of mixed waste. The hydrolysis step results in a substantially single phase of less volatile, more water-soluble hydrolysis products, thus enabling the oxidation step to proceed rapidly and with minimal loss of organic substrate in the offgas.
Tri D. Tran Kimio Kinoshita	**Surface Modifications for Carbon Lithium Intercalation Anodes** U.S. Patent 6,096,454 August 1, 2000	A prefabricated carbon anode containing predetermined amounts of passivating film components is assembled into a lithium-ion rechargeable battery. The modified carbon anode enhances the reduction of the irreversible capacity loss during the first discharge of a cathode-loaded cell. The passivating film components, such as Li_2O and Li_2CO_3, of a predetermined amount effective for optimal passivation of carbon, are incorporated into carbon anode materials to produce dry anodes that are essentially free of battery electrolyte prior to battery assembly.
Robin R. Miles Phillip Belgrader Shanavaz L. Nasarabadi	**Microsonicator for Spore Lysis** U.S. Patent 6,100,084 August 8, 2000	A microsonicator for spore lysis. The microsonicator uses ultrasonic excitation of spores to perform spore and cell lysis. The microsonicator comprises a container with a cavity in it for retaining the sample in an ultrasonic transmission medium. The cavity is closed by a silicon membrane to which an electrode and piezoelectric material are attached, with the electrode and piezoelectric material being electrically connected to an ac signal generator. The membrane flexes and vibrates at the frequency of the ac voltage applied to the piezoelectric material.
Duncan J. Maitland Abraham P. Lee Daniel L. Schumann Luiz Da Silva	**Shape-Memory-Polymer (SMP) Gripper with a Release Sensing System** U.S. Patent 6.102,917 August 15, 2000	A system for releasing a target material, such as an embolic coil, from an SMP located at the end of a catheter that uses an optical arrangement for releasing the material. The system includes a laser, laser driver, display panel, photodetector, fiber-optic coupler, fiber optics and connectors, a catheter, an SMP-based gripper, and a release sensing and feedback arrangement. The SMP-based gripper is heated by laser light through an optic fiber. The heat causes the gripper to release a target material (for example, embolic coil for therapeutic treatment of aneurysms). Various embodiments are provided for coupling the laser light into the SMP, including positioning the coils specifically, removing the fiber cladding adjacent to the coil, metal-coating the SMP, doping the SMP with a gradient-absorbing dye, tapering the fiber-optic end, coating the SMP with low-refractive-index material, and locating an insert between the optic fiber and the coil.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Abraham P. Lee M. Allen Northrup Dino R. Ciarlo Peter A. Krulevitch William J. Benett	**Release Mechanism Utilizing Shape Memory Polymer Material** U.S. Patent 6,012,933 August 15, 2000	Microfabricated therapeutic actuators are fabricated using a shape-memory polymer (SMP), a polyurethane-based material that undergoes a phase transformation at a specified temperature (Tg). At a temperature Tg, material is soft and can be easily reshaped into another configuration. As the temperature is lowered below temperature Tg, the new shape is fixed and locked in as long as the material stays below temperature Tg. When reheated to a temperature above Tg, the material returns to its original shape. Use of SMP for microtubing makes the microtubing a release actuator for the delivery of embolic coils through catheters into aneurysms, for example. The microtubing can be manufactured in various sizes, and the phase-change temperature Tg is determined for an intended temperature target and use.
Ai Quoc Pham Robert S. Glass	**Hydrocarbon Sensors and Materials Therefore** U.S. Patent 6,013,080 August 15, 2000	An electrochemical hydrocarbon sensor and materials for use in sensors. A suitable proton-conducting electrolyte and catalytic materials are applied to the detection and measurement of nonmethane hydrocarbons. The sensor comprises a proton-conducting electrolyte sandwiched between two electrodes. At least one of the electrodes is covered with a hydrocarbon decomposition catalyst. Two different modes of operation for the hydrocarbon sensors can be used: equilibrium versus non-equilibrium measurements and differential catalytic. The sensor has particular application for on-board monitoring of automobile exhaust gases to evaluate the performance of catalytic converters. In addition, the sensor can be used in monitoring any process where hydrocarbons are exhausted, for instance, in industrial power plants. The sensor is low- cost, rugged, sensitive, simple to fabricate, and miniature and does not suffer cross sensitivities.
William C. Moss	**Impedance-Matched, Joined Drill Pipe for Improved Acoustic Transmission** U.S. Patent 6,018,268 August 22, 2000	An impedance-matched jointed drill pipe for improved acoustic transmission. A passive means and method that maximize the amplitude and minimize the temporal dispersion of acoustic signals that are sent through a drill string. It is used for measurements made while drilling telemetry systems. The improvement in signal transmission is accomplished by replacing the standard joints in a drill string with joints constructed of a material that is impedance-matched acoustically to the end of the drill pipe to which it is connected. Provides improvement in the technique of measuring while drilling, a technique that can be used in well logging, directional drilling, and drilling dynamics. It is also useful in gamma-ray spectroscopy while drilling post-shot boreholes.
Albert E. Brown	**High Energy, Low Frequency Ultrasonic Transducer** U.S. Patent 6,109,109 August 20, 2000	A wide-bandwidth, ultrasonic transducer to generate nondispersive, extensional, pulsed acoustic pressure waves into concrete-reinforced rods and tendons. The wave propagation distance is limited to double the length of the rod. The transducer acoustic impedance is matched to the rod impedance for maximum transfer of acoustic energy. The efficiency of the transducer is approximately 60 percent, depending upon the type of active elements used in the transducer. The transducer input energy is, for example, approximately 1 megajoule. Ultrasonic reflections will occur at points along the rod where there are changes of 1 percent of a wavelength in the rod diameter. A reduction in the rod diameter will reflect a phase-reversed echo, as compared with the reflection from an incremental increase in diameter. Echo signal processing of the stored waveform permits a reconstruction of those echoes in an image of the rod. The ultrasonic transducer has use in the acoustic inspection of long (over 12 meters) architectural reinforcements and structural supporting members such as in bridges and dams.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Stefan Swierkowski	**T-Load Microchannel Array and Fabrication Method** U.S. Patent 6,110,332 August 29, 2000	A three-dimensional T-load for planar microchannel arrays for electrophoresis, for example, which enables sample injection directly onto a plane perpendicular to the ends of the microchannels' axis. This injection is accomplished by forming input wells that extend beyond the ends of the microchannel, thereby eliminating the right angle connection from the input well into the end of the microchannel. In addition, the T-load input well eases the placement of an electrode in or adjacent to the well and thus enables very efficient reproducible electrokinetic (ek) injection. The T-load input well eliminates the prior concerns about input well–microchannel alignment, since the input well can be drilled after the top and bottom microchannel plates are bonded together. The T-load input well may extend partially or entirely through the bottom microchannel plate, which enables more efficient gel and solution flushing and placement of multiple electrodes to assist in the ek sample injection.
Claude Montcalm Paul B. Mirkarimi	**High-Reflectance, Low-Stress, Mo–Si Multilayer Reflective Coatings** U.S. Patent 6,110,607 August 29, 2000	A high-reflectance, low-stress molybdenum–silicon (Mo–Si) multilayer reflective coating particularly useful for the extreme ultraviolet (EUV) wavelength region. While the multilayer reflective coating has particular application for EUV lithography, it has numerous other applications where high-reflectance and low-stress multilayer coatings are used. Multilayer coatings having high near-normal incidence reflectance (R greater than or equal to 65 percent) and low residual stress (less than or equal to 100 megapascals) have been produced using thermal and nonthermal approaches. The thermal approach involves heating the multilayer coating to a given temperature for a given time after deposition in order to induce structural changes in the multilayer coating that will have an overall "relaxation" effect without reducing the reflectance significantly.
Richard F. Post	**Combined Passive Bearing Element–Generator Motor** U.S. Patent 6,111,332 August 29, 2000	An electric machine includes a cylindrical rotor made up of an array of permanent magnets that provide an N-pole magnetic field of even order (where $N = 4, 6, 8$, etc.). This array of permanent magnets has bars of identical permanent magnets made of dipole elements where the bars are assembled in a circle. A stator inserted down the axis of the dipole field is made of two sets of windings that are electrically orthogonal to each other, where one set of windings provides stabilization of the stator and the other set of windings couples to the array of permanent magnets and acts as the windings of a generator motor. The rotor and the stator are horizontally disposed, and the rotor is on the outside of said stator. The electric machine may also include two rings of ferromagnetic material. One of these rings would be located at each end of the rotor. Two levitator pole assemblies are attached to a support member that is external to the electric machine. These levitator pole assemblies interact attractively with the rings of ferromagnetic material to produce a levitating force upon the rotor.

Awards

A framed **letter of commendation** from Army Lieutenant General John Costello was a surprise honor presented to Laboratory lead engineer **Douglas Faux** during a quarterly Integrated Project Team meeting of the U.S. Army Space and Missile Defense Command. The letter cited Faux's many years of distinguished service working on projects for the Command, particularly in "performing independent analyses that assessed TMD (Theater Missile Defense) and NMD (National Missile Defense) interceptor lethality against a suite of nuclear targets." It continued, "Most recently, your execution of the hydrocode effort supporting the NMD Lethality Program has been exceptional. Your management of the vast workload and competing priorities has been vital to the success of this program." Costello, the three-star general in charge of the U.S. Army Space and Missile Defense Command, said that Faux has made "important and lasting contributions to the nation's defense."

Faux joined the Laboratory 12 years ago. He is currently assigned to the Nonproliferation, Arms Control, and International Security Directorate, matrixed from the Engineering Directorate's New Technologies Engineering Division.

Project leader **Karl van Bibber** represented the Laboratory during the presentation of the **DOE Program and Project Management Award** to the B Factory project at the Stanford Linear Accelerator Center (SLAC). The project comprises two major construction efforts: a two-ring accelerator complex built by a collaboration of SLAC and Lawrence Berkeley and Lawrence Livermore national laboratories; and a 1,200-ton particle detector built by a consortium of nine nations. Van Bibber, along with **Marshall Mugge**, **Lou Bertolini**, and **Curt Belser**, led Livermore's work on the construction of the two-ring accelerator complex while **Doug Wright** and **Richard Bionta** helped develop the BaBar detector. More than 300 Laboratory scientists and engineers worked on the B Factory over the five years of its construction.

With the top category award, the Department of Energy was acknowledging the $239-million project's on-time, on-budget completion. The B Factory accelerator complex is used to collide a beam of electrons with a counterrotating beam of antielectrons to produce subatomic particles called B mesons. Scientists study the disintegration patterns of the B mesons to try to understand why the universe is dominated by matter when it was created with equal amounts of matter and antimatter.

"Building the B Factory and now doing science with it has been an exhilarating experience," said van Bibber. Added SLAC Director Jonathan Dorfan, "I'm delighted that the B Factory was chosen out of a field of such strong contenders. I cannot emphasize strongly enough the wonderful cooperation that existed among the three Bay Area labs during construction. Our colleagues at Livermore and Berkeley were outstanding."

Science & Technology Review 2000 Index — Page

July/August 2000

September 2000

October 2000

November 2000

December 2000

Abstracts

Following Materials over Time and Space

A group of Lawrence Livermore scientists is using the computational power of Department of Energy supercomputers to accurately predict the performance of advanced materials. Their field of research is called computational materials science, one of the fastest growing areas within the chemistry and materials science disciplines. The computer codes they use incorporate a concept called multiscale modeling, in which a material's properties are followed through length scales from nanometers to meters and time scales from nanoseconds to tens of years. In this way, the codes simulate the evolution of mechanical and chemical changes in materials. The Livermore simulation work is closely tied to laboratory experiments to ensure that simulations accurately reflect the physical properties of materials being modeled. The simulation work is clearly showing, for the first time, the physical mechanisms underlying radiation damage.

Contact:
Tomas Diaz de la Rubia (925) 422-6714 (diazdelarubia1@llnl.gov).

The Art of Systems Science

Systems scientists practice the multidisciplinary art of gathering information and constructing the systems models needed to help project managers make informed decisions. Their expertise in decision analysis, computer science, industrial engineering, simulation modeling, and systems engineering is put to use on projects ranging from planning for National Ignition Facility operations to forecasting Lawrence Livermore's electric energy demand. They perform reliability, availability, and maintainability (RAM) analyses and discrete-event simulations to optimize just-in-time manufacturing. They perform probabilistic risk assessments for safety analyses of buildings at Livermore and assess the risk associated with transporting spent nuclear fuel. And they use Monte Carlo simulations to find the best method for processing plutonium no longer needed for national defense. Their mathematical and statistical analyses are used to help discriminate seismic sources for treaty verification, allocate resources for contaminant cleanup at Livermore's experimental test site, and develop a model for energy use in China.

Contact:
Cynthia Annese (925) 422-0264 (annese1@llnl.gov), or Annette MacIntyre (925) 423-7254 (macintyre1@llnl.gov).

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Roger Batzel's Legacy of Leadership

Roger Batzel
1922–2000

When Roger Batzel died on July 29, 2000, he left a legacy of leadership at Lawrence Livermore National Laboratory. This issue of *S&TR* commemorates his long tenure as director (1971 to 1988) and the quiet, self-assured man who led the Laboratory during a period of tremendous growth, research diversification, and technical achievement. In addition to a lead article surveying Batzel's accomplishments as director, separate articles report on the following aspects of the Batzel years:

- *The growth and change in Livermore's defense and national security mission.*
- *The development of the Laboratory's biomedical and biotechnology capabilities.*
- *The diversification of the Laboratory's energy mission to include the peaceful use of nuclear energy, the development of nonnuclear energy resources, and the safe disposal of the waste from nuclear power plants.*

Coming Next Month

University of California
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P.O. Box 808, L-664
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