April 2002

Science & Technology REVIEW

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Simulating Quantum Molecular Activity

Also in this issue:

- Forensic Science Extends Crime-Solving Powers
- Compact, Powerful Laser Has Tactical Weapons Use
- 50th Anniversary Highlight: Engineering Makes Big Science Work

Lawrence Livermore National Laboratory

Making History
Making a Difference

1952-2002

About the Cover

Simulations of quantum molecular dynamics are for the first time allowing scientists to get an accurate look at what happens to individual atoms and molecules during high-pressure experiments. On the cover is a simulation done on Livermore's ASCI White supercomputer of the extremely rapid dissociation, or coming apart, of water molecules under intense pressures. The article beginning on p. 4 reports on innovative quantum molecular dynamics simulations, which have also been done of high-pressure hydrogen experiments and to model the quantum molecular behavior of DNA and other biomolecules.

Cover design: Kitty Tinsley

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. 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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Arnie Heller, Ann Parker,
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Art Director and Designer
Kitty Tinsley

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Kitty Tinsley

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Livermore rated “outstanding”

For the first time, the Laboratory has achieved an overall rating of “outstanding” on its annual assessment by the Department of Energy’s National Nuclear Security Administration (NNSA).

This fiscal year 2001 assessment (October 2000 through September 2001) covers Livermore’s performance in institutional management, science and technology, and operations and administration. The comprehensive evaluation system, along with annually negotiated performance standards, is defined in the University of California’s contract with DOE.

Institutional management was rated “outstanding”—the highest rating possible and an increase over last year’s “excellent”—and is the result of improvements by the director and his management team in strategic planning, establishing and communicating performance expectations, internal and external communications, asset and infrastructure management, accountability and commitment, and community relations.

Livermore science and technology also received an overall rating of “outstanding,” an improvement over last year’s “excellent” rating. “We continue to prove ourselves as a world leader in science and technology,” says Jeff Wadsworth, deputy director for Science and Technology. “Every single employee contributed to these outcomes, and we can all be proud of what the Lab has achieved.”

The “outstanding” rating for operations and administration is the highest since the rating system went into effect in 1992. For John Gilpin, director of Contract Management, this rating “demonstrates the professionalism and commitment of all employees and managers to accomplishing missions and achieving long-term performance improvement.”

Contact: Lynda Seaver (925) 423-3103 (seaver1@llnl.gov).

Tiny fuel cell boosts battery power

Livermore’s Center for Microtechnology Engineering has developed and demonstrated a prototype miniature thin-film fuel-cell power source, which may provide portable electric power for consumer electronics and remote, autonomous military, environmental, and security electronics and sensor applications.

The miniature fuel-cell technology incorporates a thin-film fuel cell and microfluidic fuel-processing components in a common package. This power module uses easy-to-store liquid fuels such as methanol and provides more than three times the operating time possible with rechargeable batteries.

“Livermore’s fuel cell can be cheaper, smaller, with more energy capacity than any battery or alternative fuel-cell technology,” says Jeffrey Morse, principal investigator on the fuel cell project.

The patented design and method for making thin-film fuel cells combines microcircuit processes, microfluidic components, and microelectrical-mechanical systems (MEMS) technology. Morse predicts that the lighter-weight, longer-lasting MEMS-based fuel-cell power source will replace rechargeable batteries such as lithium-ion and lithium-ion polymer in a range of consumer electronics, including cell phones, handheld computers, and laptops. Other applications include military electronics and sensors for remote and autonomous uses that require extremely long-lasting power.

Contact: Jeffrey Morse (925) 423-4864 (morse3@llnl.gov).

Full-system nuclear simulation complete

Scientists at Lawrence Livermore and Los Alamos national laboratories have completed the largest computer simulations ever attempted, the first full-system, three-dimensional simulations of a nuclear weapon explosion.

These simulations represent the achievement of an important milestone for the National Nuclear Security Administration’s Stockpile Stewardship Program, which is responsible for maintaining the safety, security, and reliability of the nation’s nuclear deterrent. Both calculations ran on ASCI White—the world’s fastest and most capable supercomputer—at Livermore.

Two years ago, Livermore and Los Alamos scientists completed the first three-dimensional simulations of, respectively, a weapon primary and a weapon secondary, the two stages of modern nuclear weapons. The new simulations of a weapon’s complete operation built on those achievements.

The Livermore and Los Alamos teams used different approaches to meeting the full-system milestone, and both completed their simulations more than two months ahead of schedule. A Laboratory-sponsored external review panel of distinguished physicists and computer scientists conducted a detailed independent review of the computational methods and results of these simulations and affirmed the success of both approaches.

The Los Alamos simulation ran remotely on the ASCI White machine at Livermore, more than 5,500 kilometers away, through the secure network connecting the laboratories. Researchers in New Mexico viewed data on the ASCI Blue Mountain supercomputer and its EnSight graphics package at Los Alamos. The amount of data transmitted between the laboratories was about 35 times the information contained in the Library of Congress.

The Livermore simulation ran on more than 1,024 processors of ASCI White and took 39 days to execute.

Contact: Lynda Seaver (925) 423-3103 (seaver1@llnl.gov).

Physics Changes Focus

THE preeminent goal of physics in the 20th century was to understand the workings of the world at the most fundamental level. This moving target shifted to ever-smaller scales as the technology of observation—driven in turn by advances in physics—became more and more powerful.

As physicists studied atoms and their constituents, they learned that Newton's laws of motion did not apply. For example, the particles that make up water molecules evidently do not follow the same set of rules as bulk samples of water. Convinced, however, that the world becomes more understandable as its basic constituents and interactions are exposed, physicists rarely considered systems of more than two interacting particles, unless they skipped directly to infinity. This reductive approach led to the triumphs of modern physics, including quantum mechanics and the standard model of the strong nuclear, weak nuclear, and electromagnetic interactions. To this day, however, many bulk properties of water remain a mystery.

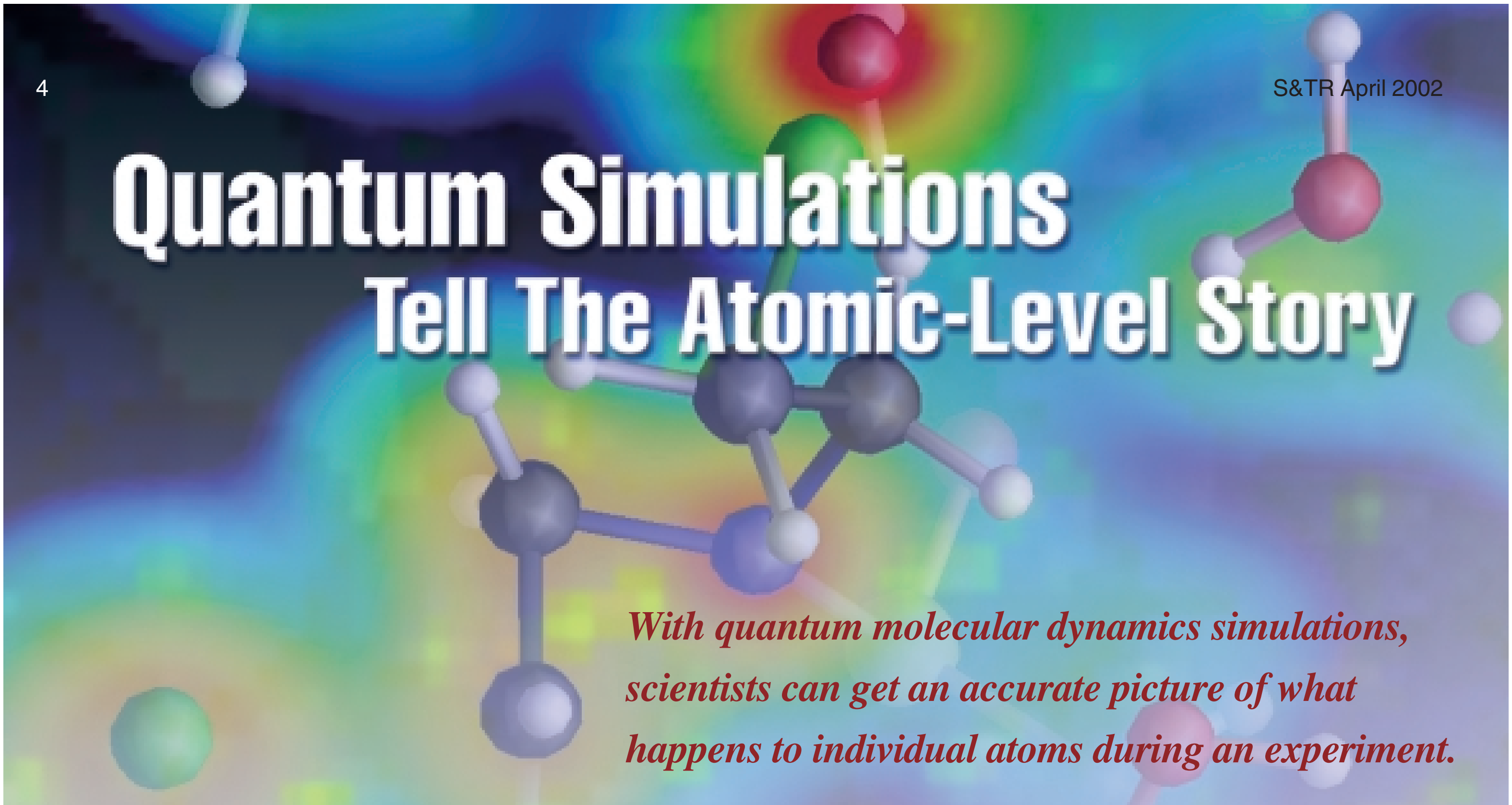
As we enter a new century, geometric growth in computing power—also engendered by modern physics—has positioned physicists to address anew the complexities of many particles interacting to produce the bulk properties of materials. Using Advanced Simulation and Computing (ASCI) supercomputers to simulate the quantum mechanics of matter being shocked, researchers can now see in detail the dynamic activity of the atoms and molecules in the sample.

The article beginning on p. 4 describes the first-ever quantum molecular dynamics simulations of shocked hydrogen. Those simulations, the largest ab initio simulations ever done on the ASCI White computers, sought to find physical reasons for differing results from two sets of high-pressure experiments on deuterium, an isotope of hydrogen. Other simulations have examined the mechanical properties of water molecules under ambient conditions and at extreme pressures. For stewardship of the nation's nuclear stockpile as well as for other programmatic applications, knowledge of how materials shock and fracture at the molecular level is essential.

An especially exciting area for quantum simulations is in the growing field of nanoscience. Nanomaterials—one nanometer is a billionth of a meter, or 100,000 times smaller than the width of a human hair—are the ultimate challenge to the way physicists count: one, two, . . . infinity. Ranging from around 10 to 1,000 atoms in size, nanoparticles behave in a complex way that is different from the behavior of both their atomic constituents and bulk matter. For the silicon nanoparticles known as quantum dots, quantum simulations reveal unique optical properties that vary with size and surface characteristics. Not only will lasers made of silicon be possible for the first time, but silicon dots may also be useful as fluorescent markers in biological research and as biological sensors. Quantum simulations are also exploring the behavior of DNA and how best to exploit a cancer-fighting drug.

As a tool for biological research, quantum simulation may engender progress akin to the advances in structural biology that followed the introduction of another physics tool, x-ray diffraction using synchrotron light sources. In fact, quantum simulations will play a key role in advancing biological imaging using fourth-generation light sources to illuminate proteins with the world's most brilliant x-ray pulses. But that's another story.

■ William Goldstein is associate director of Physics and Advanced Technologies.



Quantum Simulations Tell The Atomic-Level Story

With quantum molecular dynamics simulations, scientists can get an accurate picture of what happens to individual atoms during an experiment.

FOR almost as long as Lawrence Livermore has existed, scientists have been experimenting with materials to learn what happens to them under high pressure. In the brief instant of a high-explosive detonation, for example, shock waves produce pressure up to 500,000 times that of Earth's atmosphere, detonation waves travel as fast as 10 kilometers per second, and temperatures soar to 5,500 kelvins.

Early high-pressure experiments were designed to investigate the properties of weapon materials under these mind-boggling conditions and thus support the development of new weapons. Today, experiments seek out the fundamental properties of such deceptively simple materials as water and hydrogen. This very basic information is being applied to work in high explosives, planetary science, and materials science.

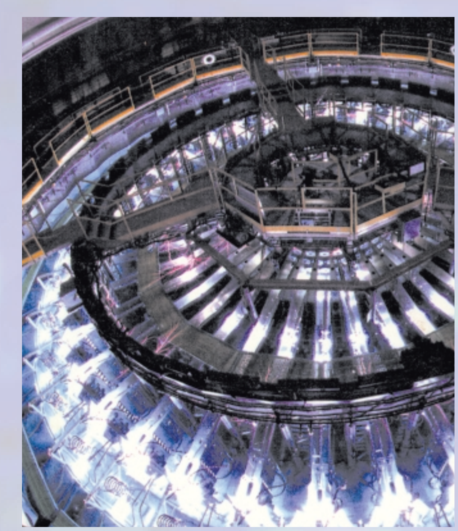
Experiments with a gas gun that shocks a sample or with a diamond anvil cell that applies static pressure demonstrate the changes brought about by pressure—the "after" conditions that scientists can compare to the "before." Now, for the first time, using computer simulations, researchers can get an accurate look at what happens to individual atoms and molecules during those experiments.

Simulations based on quantum molecular dynamics make it possible to view experimental activity as it happens. Quantum molecular dynamics is quite different from classical molecular dynamics, which is primarily concerned with the classical motion of atoms interacting with a given potential. The interesting chemistry and physics of many molecules take place at the atomic and subatomic level. But Newton's laws of classical mechanics no longer apply here. Physicists developed quantum mechanics early in the 20th century to appropriately describe the physics and chemistry of matter at the microscopic level. Quantum molecular dynamics focuses on all the interactions between atoms and electrons and does not involve fitting interactions to experimental data.

First-principles, or ab initio, molecular dynamics models use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. (See the box on p. 8.) These models in combination with Livermore's powerful computers allow scientists to create accurate, reliable simulations of complex physical phenomena.

Physicist Giulia Galli leads the Quantum Simulations Group at Livermore. In the four years since this group was established, it has explored entirely new territory. Early work included simulations of the mixing of water and hydrogen fluoride, DNA, and the elasticity of silicon carbide, a semiconductor material. (See *S&TR*, July/August 1999, pp. 20–22.) Their more recent simulations of shocked liquid hydrogen were the largest ab initio simulations to date on Livermore's terascale computers, which are part of the National Nuclear Security Administration's Advanced Simulation and Computing (ASCI) program. "Our hydrogen simulations were the first to look at an experiment in action," says Galli. "We could actually see how a real experiment had gotten from 'before' to 'after.'"

Quantum simulations are an excellent tool for predicting the properties of materials that cannot be measured directly. They provide accurate information about the properties of materials subjected to extreme conditions (for example, high temperature or high pressure) that are difficult to achieve experimentally. Simulations also help experimental physicists to interpret their results. "Simulation results neatly complement experimental results and may also guide the choice of new experiments," says Galli.



Experiments on (left) Livermore's Nova laser and (right) Sandia National Laboratories' *Z* accelerator shocked liquid deuterium, an isotope of hydrogen. In both experiments, a short, intense shock caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. The experiments found different compressibilities, which could affect the equation of state for hydrogen and its isotopes. Quantum simulations sought to point out physical reasons for the differences.

Codes Make It Work

The computer code used to simulate dynamic processes is JEEP, which physicist Francois Gygi began developing about eight years ago when he was at the Swiss Federal Institute of Technology. Some physical properties of matter, such as optical properties, can be obtained more accurately using static calculations performed with quantum Monte Carlo codes, which are the specialty of physicists Andrew Williamson, Jeff Grossman, and Randy Hood.

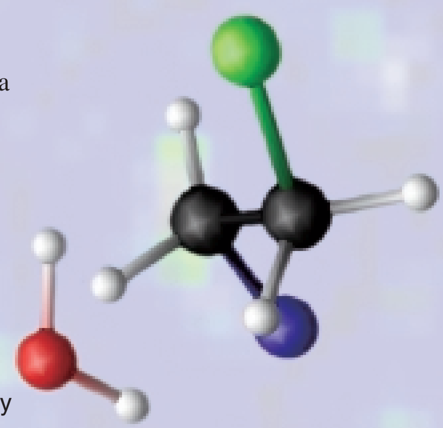
JEEP and quantum Monte Carlo codes operate differently. Both have to make approximations in their equations, but quantum Monte Carlo codes make very few. JEEP operates faster and excels at deriving the location of atoms and molecules. The more accurate quantum Monte Carlo simulations cannot give dynamic properties but are a better tool for determining the optical properties of molecules. Quantum Monte Carlo calculations are also useful for testing the validity of approximations made in the JEEP code's theory and for improving the accuracy of this theory.

Simulations Resolve Differences

Quantum simulations by Galli and Gygi may point out the differences found during two sets of high-pressure experiments on deuterium, an isotope of hydrogen with one proton and one neutron. One set of experiments was performed on Lawrence Livermore's Nova laser. The other set was performed on Sandia National Laboratories' *Z* accelerator, the world's most energetic pulsed-power machine, in Albuquerque, New Mexico.

The Livermore experiments in 1997 and 1998 and the Sandia experiment in 2001 subjected a sample of liquid deuterium to a short, intense shock that caused the hydrogen to form a hot plasma and, very briefly, become a conducting metal. In the Nova experiments, a laser beam produced a steady shock wave aimed at the target cell holding the sample. The wave was smoothed to ensure a spatially planar and uniform shock front, critical for obtaining accurate measurements.

The experiment at Sandia used an entirely different technique for producing a shock wave. Pulsed-power machines have large banks of capacitors used to accumulate electrical charges over many hours. All of that stored energy is discharged in one enormous pulse that lasts for a fraction of a microsecond. The pulse creates a powerful electromagnetic field that slams a flyer plate into the deuterium sample capsule. Sandia's magnetically driven plate is faster



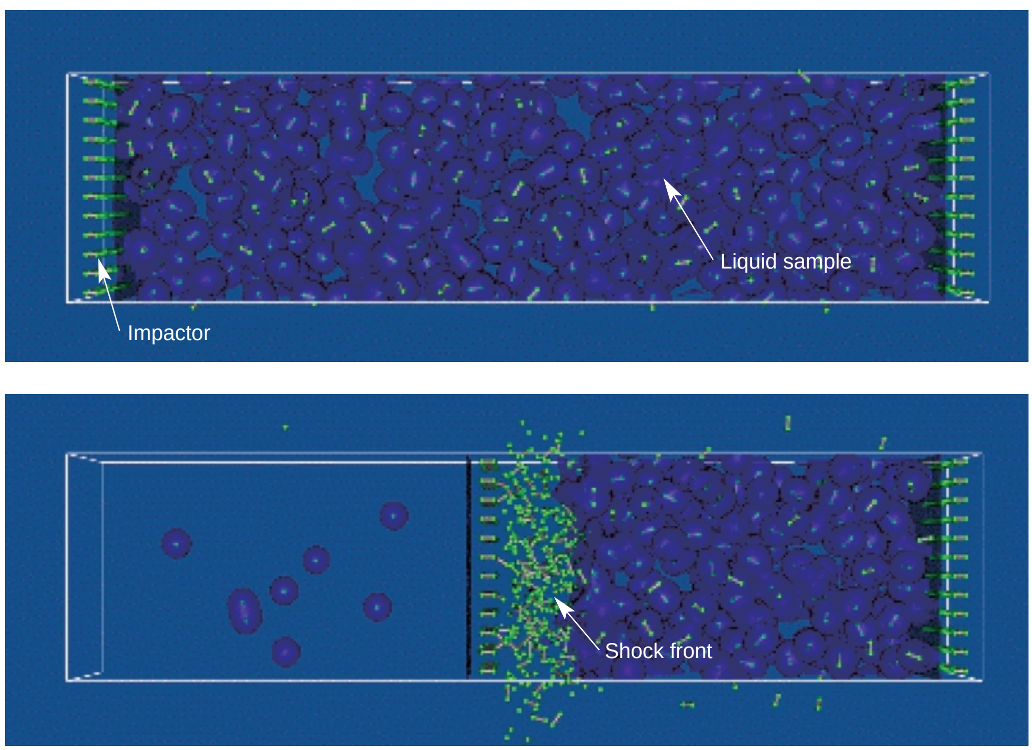
although smaller than the flyers used by Livermore's two-stage gas guns for shock experiments. It thus results in higher shock pressures. The *Z* accelerator also sustains a shock for a longer time than the Nova laser.

The two sets of experiments on the Nova laser showed that the deuterium samples were compressed to a density much higher than anyone had expected. These data differed from those used to predict the then-current model of the equation of state (EOS) for hydrogen and its isotopes. An EOS is a mathematical representation of a material's physical state as defined by its pressure, density, and either temperature or energy. It is a necessary constituent of all calculations involving material properties. Predictions concerning the formation and evolution of large planets, such as Jupiter, strongly depend on the EOS of hydrogen at pressures reached in the Nova experiments.

The *Z* flyer data reached pressures up to 70 gigapascals, which overlapped part of the pressure regime of the Nova laser experiments. The Nova experiments determined the EOS by using an x-ray probe and x-ray microscope to look into the deuterium as it was being shocked. The Sandia experiments simultaneously shocked a deuterium sample and a foil of aluminum. Researchers then found the EOS by comparing deuterium's behavior with that of aluminum. Although the Sandia EOS data required the comparison with aluminum, the *Z* flyer produced a shock in the deuterium that held a constant pressure for much longer than did the experiments with the Nova laser.

At a pressure of 40 gigapascals, the Nova and *Z* data agree, showing that the hydrogen EOS is about 20 percent more compressible than it was earlier thought to be. In other words, at this pressure, hydrogen will squeeze into a smaller volume with a higher density than previous models had predicted. At a pressure of 70 gigapascals, the Nova data show an even larger compressibility compared with equilibrium theory—almost 50 percent higher—while the *Z* flyer data are about 7 percent higher than theory predicted. "This is a considerable and important discrepancy," says Livermore physicist Robert Cauble, who oversaw the experiments on both the Nova laser and the *Z* accelerator.

Galli and Gygi performed two sets of simulations as they sought an explanation for the experimental results. The first simulations were of hydrogen under fixed pressure and temperature. The pressure values ranged from 20 to 120 gigapascals while temperatures ranged from 5,000 to 12,000 kelvins. Galli and Gygi then simulated the behavior of liquid deuterium during a shock experiment. Although the simulations of static conditions gave results that agreed with Sandia's data,



Quantum simulations of shocked hydrogen reveal the atomic-scale structure of the shock front. (top) Thirteen hundred and twenty deuterium atoms are arranged in a periodically repeating molecular dynamic cell that contains an impactor, a wall, and a liquid sample. Four computer experiments used different impactor velocities in an effort to mimic experimental results. (bottom) The shock front and the compression of the deuterium atoms are shown from one computer experiment.

the simulation of a shock in deuterium gave results that agreed with the Livermore Nova shocks.

Gygi notes that the conditions of the Nova and *Z* accelerator experiments differed. For one thing, the time scales of the pulse were different: 2 to 4 nanoseconds in Nova and about 30 nanoseconds in the *Z* machine. "Another variable may be that a laser beam is very different from a magnetic pulse," says Gygi.

Although the simulations did not supply a full explanation for the difference between the two sets of experimental results, Galli and Gygi's calculations did help to point out possible important differences. "In the past," says Gygi, "experimentalists with different results just pointed fingers at each other. Now, we hope that simulations will help to explain the physical reasons causing disagreement between different experiments. Also, big experiments are often expensive to repeat. The Nova laser is gone completely, so reproducing part of the Nova results with simulations can be very useful."

Water, Water Everywhere

Recent experiments also explored one of the most common liquids—water. "You would think that everybody knows everything about water," says Galli, "but that is far from the truth. And water is in practically everything in our world." Water is in many materials studied at Livermore: Biological systems are largely water, high explosives contain water, and water vapor may accumulate inside an aging nuclear weapon.

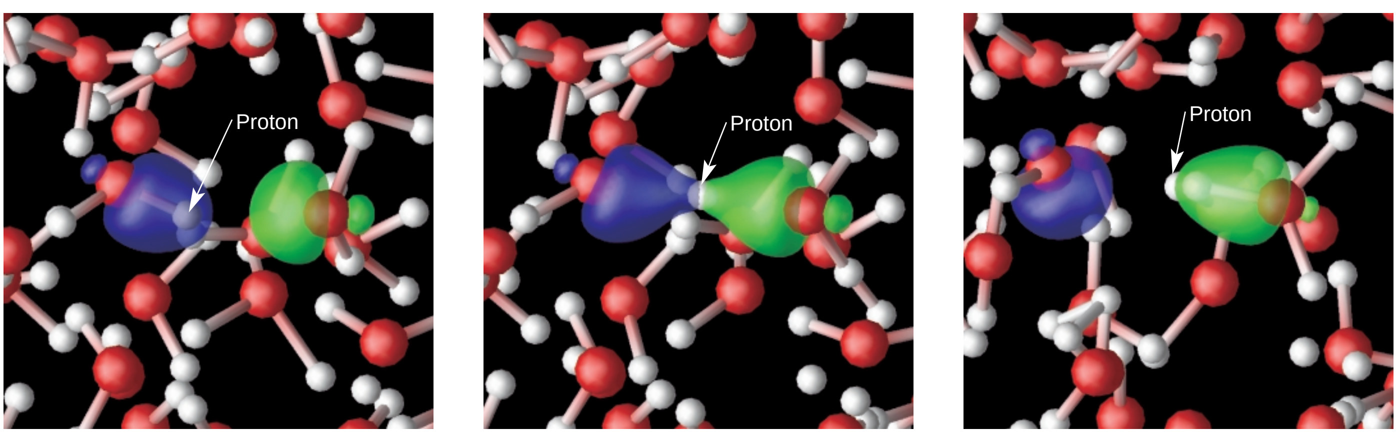
Physicist Eric Schwegler, Galli, and Gygi were interested in what happens to water under pressure, information important to Livermore's U.S. nuclear weapons stockpile stewardship mission. In particular, they were interested in learning how the water molecule comes apart under high-pressure conditions.

First, they developed a model of liquid water at ambient conditions, which compared favorably with recent x-ray data gathered at the University of California at Berkeley and with neutron diffraction data gathered in England. Then they modeled water at moderate pressure and found structural data that agreed with recent diamond anvil cell experiments performed at Commissariat à l'Énergie Atomique (CEA) in France.

Scientists already knew that under ambient conditions, water molecules rarely dissociate (come apart)—just once every 11 hours. When dissociation does occur, two water (H_2O) molecules become hydroxide (OH^-) and hydronium (H_3O^+), with one proton hopping to the other H_2O molecule. How increased pressure affects dissociation has long been debated.

Experiments on water at extreme temperatures and pressures have been few. One pioneering 1985 experiment at Livermore used a two-stage gas gun to shock water with pressures up to 26 gigapascals and temperatures to 1,700 kelvins. This experiment did not find any evidence of H_3O^+ under pressure. These data led to the suggestion that the dissociation mechanism at high pressures might be different from the one at ambient conditions, that perhaps a single H_2O molecule dissociates to H^+ and OH^-.

In quantum simulations of static pressure conditions ranging up to 30 gigapascals, Schwegler's team found that the dissociation process begins in earnest at 14 gigapascals. By 30 gigapascals, dissociation is occurring once every billionth of a second. The team was surprised to discover the same dissociation process that occurs at ambient conditions in which a proton jumps across to another water molecule. The simulations also indicated why the 1985 experiment did not reveal this process. At very high pressures, the lifetime of a H_3O^+ molecule is on average only 9.8 trillionths



Snapshots of the dissociation of a water molecule at high pressure. (left) As the water molecules dissociate, (middle) a proton is transferred to a neighboring water molecule so that (right) a hydroxide (OH^-) and a hydronium ion (H_3O^+) are formed.

of a second, too short to be observed in the 1985 experiment with detection technologies available then.

For Better Health

Schwegler, Galli, and Gygi are also working with researchers in Livermore's Biology and Biotechnology Research Program (BBRP) Directorate to simulate the dynamic behavior of DNA and other biomolecules. The goal is to combine Livermore's expertise in biology, simulation methods, and high-performance computing to nurture a new Laboratory core competency in computational biology. (See *S&TR*, April 2001, pp. 4–11.)

The simulations of water at ambient conditions were a necessary jumping-off point since all biomolecules contain a high percentage of water. Such liquid-phase simulations are far more complicated than those of isolated molecules in the gas phase because of the increased number of atoms that must be modeled.

"Getting water right made our future work much easier," says Schwegler. "And there are lots of experimental data to compare."

Subsequently, the team developed first-principles simulations of the dissolution of sodium and magnesium ions in water. In each case, their simulations agreed with numerous experimental investigations by others, but they also found several interesting features that had not been seen before.

That work was preparation for quantum simulations of the DNA sugar–phosphate backbone connecting the millions of base pairs that make up our genetic code. The flexibility of DNA in solution is central to the formation of DNA–protein complexes, which in turn mediate the replication, transcription, and packaging of DNA. Part of this flexibility comes from rotations around the bonds found in the backbone.

To learn more about how these rotations work, the team modeled the

Simulating Quantum Molecular Dynamics

In the classical molecular dynamics approach, a model of interactions between atoms is supplied as input before a simulation can be carried out. Such models are based on a priori knowledge of the physical system being studied. "Those models work if you know the chemical bonds already," says physicist Francois Gygi.

In contrast, first-principles, or ab initio, molecular dynamics does not require any a priori knowledge of interatomic interactions. These simulations use only the laws of quantum mechanics, the fundamental physics equations that describe electrons. The existence of chemical bonds is the result of electron interactions and the laws of quantum mechanics. Quantum simulations can describe the forming and breaking of chemical bonds, which cannot be done using classical molecular dynamics. Thus, classical molecular dynamics cannot explain complex states of matter such as hot, compressed fluids in which molecules come apart and regroup. Quantum molecular dynamics, however, is an ideal method for showing what happens to fluids under pressure.

The fundamental physics equations that must be solved in quantum simulations are extraordinarily complex. Until powerful computers such as Livermore's ASCI White came along, ab initio quantum molecular dynamics simulations could handle only a few atoms. Even now, a model of a few hundred atoms over less than a millionth of a second takes days of computing time to complete on Livermore's huge computers.

Modeling the behavior of molecules at the quantum level requires not only unprecedented computational power and speed but also specially designed simulation codes. One such code is JEEP, which Gygi began developing when he was at the Swiss Federal Institute of Technology.

JEEP is based on density functional theory, which describes the electronic density of a molecular or condensed system. Walter Kohn of the University of California at Santa Barbara won the Nobel Prize for Chemistry in 1998 for his development of density functional theory. In its original form, this theory was confined to ground-state properties of molecules. Since then, it has been expanded and made applicable to the study of atomic motion and complex dynamic effects of matter. Kohn's work on density functional theory has revolutionized the way scientists approach the electronic structure of atoms, molecules, and solid materials in physics, chemistry, and materials science.

Since coming to Livermore, Gygi has adapted and optimized JEEP for use on the massively parallel computers of ASCI. Now, with ASCI computers, he can examine materials systems with hundreds of atoms and thousands of electrons extremely accurately.

Monte Carlo codes are more accurate but have been extremely demanding of computing time. Every increase in the number of particles (N) being modeled requires N^3 more computing time. Twice as many electrons requires 8 times more computing time, 3 times as many electrons requires 27 times more computing time, 4 times as many electrons requires 128 times more computing time, and so on. Modeling more than a few atoms requires prohibitively long periods of computing time. Recently, however, physicists Andrew Williamson, Jeff Grossman, and Randy Hood developed a technique that allows for linear scaling of computing time for quantum Monte Carlo calculations. In other words, doubling the number of electrons only increases computing time by a factor of two instead of a factor of eight. This important breakthrough is based on techniques also used in some quantum molecular dynamics codes.

smallest part of the DNA backbone, the dimethyl phosphate anion (DMP^-). They observed changes in the shape of DMP^- when it was exposed to a sodium cation, changes that had not been seen in any previous classical molecular dynamics simulation of DMP^- in water. In future simulations, they plan to examine the influence of magnesium and other cations on the shape and flexibility of DNA.

Schwegler's team has also been collaborating on studies of cancer-fighting drugs known as phosphoramides being done by Mike Colvin and his associates in BBRP. These nitrogen-mustard-based drugs have been used to treat cancer for 50 years, so there is plenty of experimental data to compare with simulations. By examining how the phosphoramide molecules are activated, this team hopes to find ways to improve the drug and to make it more effective. (See *S&TR*, April 2001, pp. 9–10.)

Mustard drugs are believed to work by forming cross-links between the two strands of a cancer cell's DNA. Because the cell cannot easily eliminate the cross-links, the cell cannot replicate itself and dies. Before the drug can attach itself to the cancer cell's DNA, it has to lose chlorine ions. With his quantum simulations, Schwegler is learning more about the activation process, examining how the drug loses the chlorine ions and how much energy is required.

Surface Chemistry Is Key

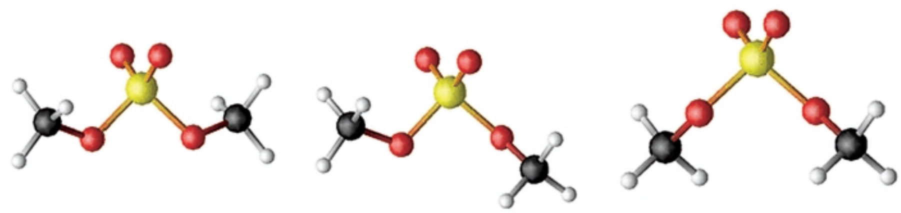
Livermore researchers used both density functional theory (on which the JEEP code is based) and quantum Monte Carlo codes to perform first-principles calculations of silicon nanoclusters, or quantum dots, which are tiny silicon molecules just a few nanometers in size, about 100,000 times smaller than the width of a human hair. These nanoclusters produce different colors of light depending on their diameter and are being considered as replacements for the fluorescent markers that researchers now use to tag proteins during experiments. With the markers, scientists can locate specific proteins and watch them as they go about their business.

Existing fluorescent dyes work well as markers. But they are short-lived. Their fluorescence rapidly fades until they are no longer detectable. They also have to be excited by a specific wavelength of laser light that matches their absorption. If researchers are studying more than one protein at a time and use multiple fluorescent markers, they must also use as many lasers as there are different markers.

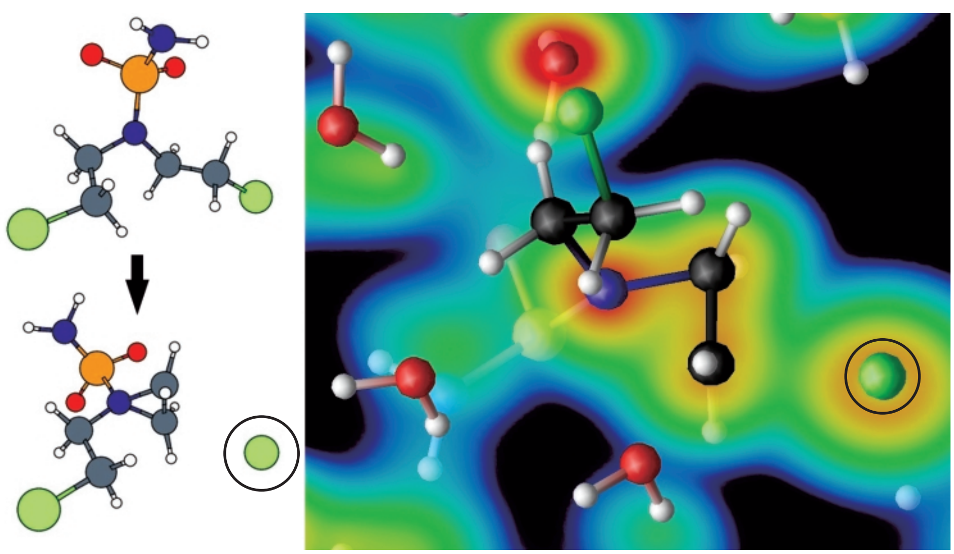
Silicon quantum dots have several advantages as biomarkers. They do not bleach out, and multiple markers can be excited by a single laser. "Given their small size, they would be a gnat on the side of a protein," says Williamson, "and the protein should continue to act and react normally."

The synthesis of silicon dots is still in its infancy. Livermore has several experimental efforts under way to synthesize them. A long-term goal is to use silicon nanoparticles in biosensors to detect biological and chemical warfare agents.

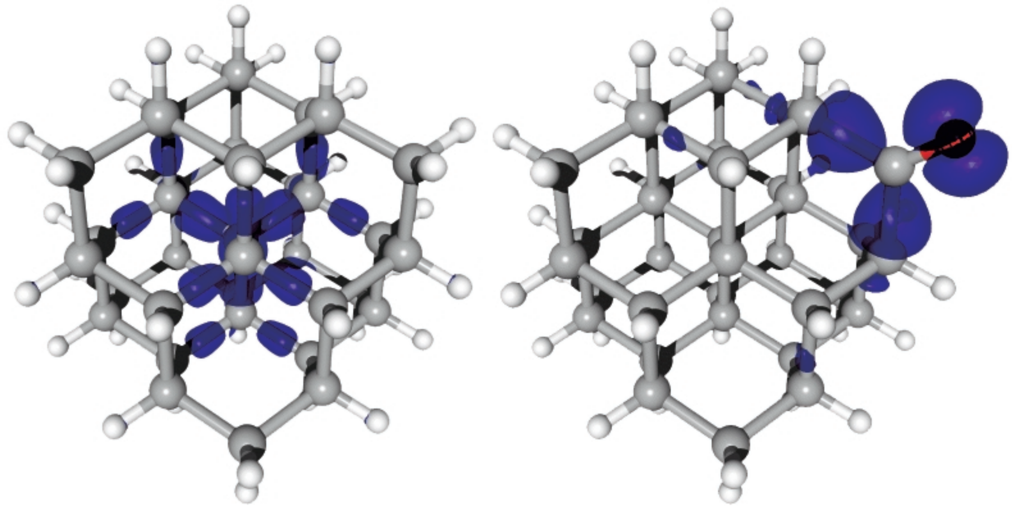
During the manufacture of the quantum dots, contamination is a



Part of the flexibility in DNA comes from rotations around the bonds found in the backbone, which consists of deoxyriboses linked together by phosphodiester bridges. Shown here is a simple model of the phosphodiester linkage found in the backbone of DNA. The molecule can adopt a variety of conformations by rotations around the phosphorus–oxygen bonds.



The cyclization of phosphoramide mustard in solution. (left) As the new carbon–nitrogen bond is formed, a chloride ion (circled) leaves the mustard and (right) is solvated by the surrounding water molecules.



(left) In a 71-atom silicon quantum dot, the white atoms are hydrogen atoms bonded to the surface that are "passivating" the dot and making it less reactive. A silicon dot that is completely passivated by hydrogen will have all its electrons in the center. (right) When two of the hydrogen atoms are replaced by a more reactive oxygen atom, the electron charge cloud is drawn toward the oxygen atom. This dramatically changes the optical properties (wavelength) of the silicon quantum dot.

concern. Oxygen, especially, can be a killer for silicon, notes Williamson. Recent Livermore simulations examined the effect of oxygen on silicon particles. A single oxygen atom, as well as many other contaminants, can make a big difference on a quantum dot because of the dot's large ratio of surface area to volume. Surface chemistry plays a big role in the study of these tiny particles.

The effects of surface chemistry are illustrated in the figure above. The left portion of the figure shows a nanometer-size silicon quantum dot made up of 71 atoms. The white atoms on the surface are hydrogen atoms bonded to the dot in such a way as to "passivate" the surface. This means they attach themselves to the highly reactive surface silicon atoms (gray). The purple cloud shows the region where the electrons that will absorb light are most likely to be located in this silicon quantum dot. For a silicon dot completely passivated by hydrogen, the electrons are located in the center of the dot. The right portion of the figure above shows how the situation changes when two of the hydrogen atoms are replaced by a more reactive oxygen atom. The electron charge cloud is drawn toward the oxygen atom, and this change in the electron density dramatically changes the optical properties of the silicon dot.

The team is currently broadening the scope of its nanostructure investigations to include other semiconductor materials such as germanium and cadmium–selenide.

Bigger and Better

One goal of Galli's group for the next few years is to apply quantum simulations to a wider and broader set of problems and to use quantum simulations on a par with laboratory experiments as a tool for research in science and engineering. Quantum simulations are a fully predictive approach that will provide a new window through which scientists can observe the world at the atomistic level in exquisite detail, avoiding uncontrolled approximations. Galli's group will focus on fluids under extreme conditions—for example, water under shocked conditions—and on building knowledge and expertise in the field of nanoscience, in particular, modeling artificial and biological nanostructures for labeling and sensing applications.

Because of the success of their quantum simulations, Galli and Gygi are working with IBM on the design of the next-generation ASCI computers. When these monster computers arrive, extremely complex simulations may be able to answer questions that cannot now be answered.

—Katie Walter

Key Words: hydrogen, JEEP, nanostructures, quantum dots, quantum molecular dynamics, quantum Monte Carlo calculations, quantum simulations, water.

For further information contact Giulia Galli (925) 423-4223 (galli@llnl.gov).

Forensic Science Center Maximizes the Tiniest Clue

Livermore chemists are coaxing a wealth of information from increasingly small samples.

WHILE Lawrence Livermore's national security accomplishments have received much publicity over the years, one Laboratory organization has gained such a stellar reputation among law enforcement, intelligence, and emergency response agencies that it is cited by Tom Clancy in his novel *Shadow Watch* (Berkley Books, 1999):

"I've requested assistance from the Forensic Science Center in San Francisco. It's at the Lawrence Livermore National Laboratory. I don't know if you're familiar with them."

"They did evidence analysis on the Unabomber case, the Times Square and WTC bombings in New York, probably hundreds of other investigations," Nimec said. "Uplink's had a relationship with them for years, and I've worked with them personally. The LLNL's the best group of crime detection and national security experts in the business."

Founded in 1991, the Laboratory's Forensic Science Center (FSC) offers a comprehensive range of analytical expertise to counter terrorism, aid domestic law enforcement, and verify compliance with international treaties and agreements. The center's combination of human and technological resources has made it among the best of its kind for collecting and analyzing virtually any kind of evidence, some of it no larger than a few billionths of a gram. Its resources, expertise, tools, and techniques are applied to all kinds of cases, from the September 11 World Trade Center attack to the spread of anthrax spores, from multiple homicides to nuclear materials smuggling.

FSC has a staff of 15 personnel, mostly chemists, with expertise in analytical chemistry, organic chemistry, inorganic chemistry, nuclear chemistry, toxicology, pharmacology, special coatings, and forensic instrument design and fabrication. The center also draws upon the resources of experts in Livermore's Chemistry and Materials Science and Nonproliferation, Arms Control, and International Security directorates.

The center's approach to forensic analysis maximizes the information that can be obtained from sometimes extremely small samples of explosives residue, dust particles, hair strands, blood stains, radioactive isotopes, drugs, chemicals, and clothing fibers. As Brian Andresen, until recently FSC director, says, "We're probing the lower limits of detection for many types of compounds isolated during an investigation." Even the tiniest quantities, says Andresen, are usually enough to provide compelling evidence that holds up in court. The minuscule amounts of oils remaining on fingerprints, for example, can tell the general age of suspects, their diet, and whether they smoke. In that respect, says Andresen, "Everything someone does leaves a chemical or biological signature that we can investigate."

Many forensic research projects have required FSC personnel to develop new analytical tools, forensic techniques for analyzing trace amounts of evidence, and unique sampling procedures. Several new, portable instruments have been developed that are capable of detailed analysis in the field. These tools provide important advantages when dealing with substances that may be unstable, perishable, or too toxic to bring back to the Laboratory.

Supporting International Security

Andresen notes that the term "forensic science" used to apply only to the scientific analysis of evidence for civil or criminal law. Increasingly, however, forensic analyses done at FSC are broadening that definition to include support for monitoring or verifying compliance with international treaties and agreements, particularly those involving weapons of mass destruction, and for countering threats of terrorism. For example, the center is contributing to the National Nuclear Security Administration's (NNSA's) Chemical and Biological National Security Program to develop and field advanced technologies to better prepare for, detect, and respond to chemical or biological incidents in the U.S.

Heather King and David Chambers demonstrate Livermore's solid-phase microextraction (SPME) sampling technique for identifying and quantifying the chemical composition of physical evidence.

In light of its demonstrated capabilities to analyze minute specimens, FSC was selected by the U.S. State Department in 2000 to support the Organization for the Prohibition of Chemical Weapons (OPCW) as the second U.S. certification laboratory. (The other facility is the Edgewood Chemical and Biological Analytical Center in Maryland.)

OPCW, based in the Netherlands, is responsible for implementing the Chemical Weapons Convention, which bans the production, stockpiling, or use of such weapons as nerve agents and blister agents. OPCW-designated laboratories test samples collected by OPCW inspectors from sources around the world to determine whether the samples contain chemical weapon agents, their precursor chemicals, or decomposition products. The convention stipulates that all samples must be analyzed at the two OPCW-designated laboratories. Federal legislation requires that all samples taken from a U.S. facility be tested in a U.S. laboratory that is OPCW-certified.

FSC has established a separate chemical weapons analysis laboratory that is certified by the American Association for Laboratory Accreditation. To date, no actual samples have been officially collected from any site or analyzed at any laboratory. FSC, however, has been required to analyze and identify constituents of mock samples supplied by the OPCW as part of a series of proficiency tests.

According to FSC's Armando Alcaraz, "Passing the tests is a very challenging task because the samples might contain literally thousands of chemicals that are linked to chemical weapons manufacturing." He notes that the samples are sometimes spiked with certain materials to deliberately try to throw the analysis teams off track. Like the test samples, the real samples will be extremely dilute (that is, parts-per-million level) so that they can be shipped commercially or sent through the mail.

Helping Law Enforcement

FSC also assists law enforcement agencies with special needs that cannot be handled by standard crime laboratories. "We're not in the business of routine police lab work," Andresen cautions. However, for cases that are particularly difficult, FSC may be a valuable resource capable of providing a conclusive analysis. In this respect, law enforcement agencies benefit from Livermore technologies that were developed initially to support counterterrorism efforts, detect nuclear proliferation activities, and advance stockpile stewardship.

Under the 1998 "Partnership for a Safer America" memorandum of understanding between the Department of Energy and the departments of Justice, Commerce, and Treasury, the center provides law enforcement agencies such as the Federal Bureau of Investigation (FBI), the U.S. Customs Service, and the Bureau of Alcohol, Tobacco, and Firearms with new crime-fighting technologies. This agreement provides a framework for formal working relationships to facilitate the transfer of DOE technology and technical expertise to law enforcement.

FSC deputy director Pat Grant notes that supporting law enforcement increases the center's expertise and shortens the turnaround times for sample analysis. "Anytime we analyze questioned samples important to a real-world investigation, we are honing our skills. It's a much more interesting and stimulating experience than participating in an exercise."

Scientists from the Forensic Science Center have miniaturized thin-layer chromatography to make it suitable for field use. The portable system includes appropriate reagents, glass plates, a digital camera, and a notebook computer.

Shrinking Instruments

Some of the center's most enduring accomplishments are new tools it has developed for intelligence, law enforcement, and health professionals working in the field. These compact, battery-powered tools provide mobile chemistry laboratories. Because they eliminate the need to ship samples back to a standard laboratory for analysis, the portable technologies greatly speed decision making.

For example, FSC scientists have miniaturized and modernized thin-layer chromatography (TLC), a well-established laboratory procedure that identifies compounds belonging to the same general chemical class. FSC chemists made TLC technology suitable for field use with a portable system that fits inside a suitcase and weighs about 23 kilograms. Although the portable system uses minimal equipment and chemical reagents, it is highly specific and sensitive. The kits can be used to analyze two sets of samples simultaneously, with each set containing about 10 samples. Depending on the compounds being analyzed for, the entire process takes 10 to 20 minutes to complete.

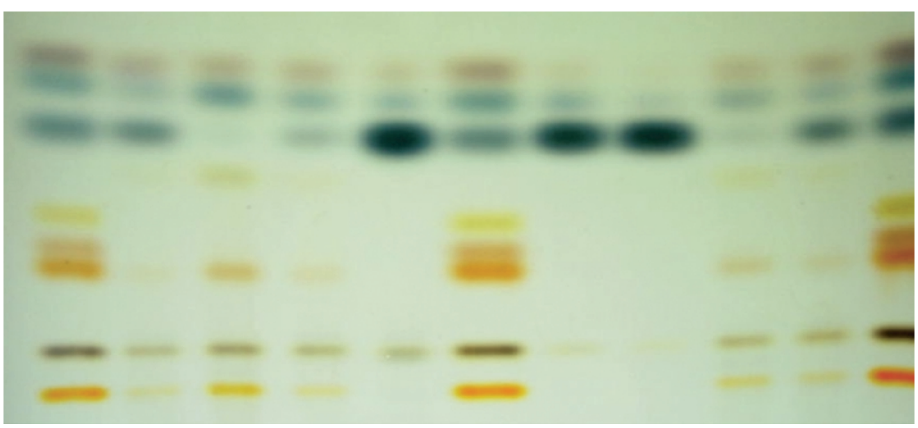
TLC works by separating compounds over the distance they move up a glass plate. Tiny amounts of samples are placed just above the bottom edge of a TLC plate, the plate is placed in a small solvent reservoir, and the solvent moves up the plate by capillary action. A commercial digital camera captures the resulting patterns of dark spots that develop, which are analyzed on a notebook computer using a software program originally developed for the analysis of DNA. Based on the distance the samples have traveled, together with their color and intensity, the computer program identifies the compounds and their relative concentrations.

The center's portable TLC kits are tailored to detect chemicals indicative of chemical weapons, high explosives, propellant stabilizers, or illegal drugs. Each specialized kit includes solvents and developing reagents that are specific to the compounds of interest.

The TLC system was originally developed for the U.S. Army to quickly detect propellant instabilities within the nation's munition storage depots. Propellants (especially high explosives) require stabilizers to prevent them from spontaneously igniting. Because stabilizers are depleted by long exposure to environmental conditions, the Army needed a way to quickly determine the safety of large numbers of munitions. The center's TLC system requires only 50-milligram samples of explosive, instead of the gram quantities typically required by other methods, and 15 minutes for each group of 20 samples, allowing many more samples to be analyzed and at much lower cost than is possible using traditional methods. "Army personnel without a degree or extensive training in chemistry can do this work," says FSC chemist Jeff Haas.

Over a few days in 1998, the portable system successfully characterized the contents of more than 1,200 unearthed mortar rounds discovered in a shallow excavation site at an Army base in Massachusetts. (See *S&TR*, December 1998, pp. 21–23.) The system is now deployed at several other Army facilities as well as by National Guard units.

The system is also used in instances where analysis speed is essential. In light of repeated success by a variety of users, the center is transferring the portable TLC technology to private industry for commercialization and widespread availability to federal and state law enforcement, customs, and environmental agencies.



The portable thin-layer chromatography (TLC) system separates compounds as they move up a glass plate placed in a small solvent reservoir. Based on the distance the compounds travel, together with their color and intensity, a computer identifies the compounds and their relative concentrations. Above is a typical TLC analysis done to detect propellant instabilities by measuring the amount of stabilizer compounds.

Advanced Tools for Field Use

While TLC is effective for identifying classes of chemicals that are specifically targeted, the task of completely characterizing samples in the field requires a more sophisticated instrument such as the gas chromatograph–mass spectrometer (GC–MS). An essential tool in every major analytical laboratory, a GC–MS can detect ultratrace quantities of organic compounds weighing a billionth of a gram or less. The gas chromatograph first slowly heats a sample to about 250°C. As the sample's volatile constituents travel down a long capillary column, they separate according to their vapor pressures and chemical affinities. As they flow into the mass spectrometer, the compounds are bombarded with an electron beam that fragments molecules into ions that constitute a unique fingerprint of that compound for positive identification.

FSC staff scientists have shrunk the standard 114-kilogram laboratory GC–MS to about 28 kilograms; it now fits inside a wheeled suitcase. The self-contained portable device, comparable in sensitivity and selectivity to a standard unit, contains a power generator, vacuum pumps, and laptop computer. The result is an instrument that significantly improves on-scene investigation and evidence collection.

Because of its ability to analyze samples to parts-per-billion sensitivity within 15 minutes, this portable GC–MS can be used to support nonproliferation activities, incident response, and law enforcement investigations. For example, the instrument can precisely identify compounds indicative of the manufacture of chemical warfare agents and illicit drugs. The instrument is currently being manufactured under license to industry.

Identification with Lasers

Although many tools used by FSC personnel depend on analyzing tiny amounts of chemicals that are found in a vapor phase above a liquid or some solid materials, most solid objects, such as human hair or clothing, do not have a significant vapor pressure and thus do not lend themselves easily to GC–MS analysis. However, center personnel can vaporize these solid samples with an extremely fine laser beam to generate wisps of product that contain identifying compounds.

The technology is called imaging laser-ablation mass spectroscopy. The process combines a laser for vaporizing extremely small amounts of material, an ion trap and time-of-flight mass spectrometer for analysis, and a high-powered microscope for viewing. In this way, forensic scientists can collect and rapidly identify suspect chemicals.

The process can be used on almost any solid material—dirt, pieces of glass, paint chips, clothing fibers, strands of hair. The samples are placed inside an ion trap mass spectrometer, irradiated with a laser, and identified within a few minutes by the mass spectrometer. The process allows an investigator to "walk down" a hair shaft by drilling consecutive holes on the same hair with the laser and analyzing each volatile sample. "Because hair grows at a standard rate, the results can reveal a history of drug use or exposure to compounds used in biological or chemical weapons manufacturing," says FSC chemist Greg Klunder. He points out that the method could also be applied to samples of clothing or soil sticking to the shoes of someone suspected of developing chemical weapons.

A similar instrument still under development is capable of detecting chemicals in air and is well suited for high-speed aircraft sampling of exhaust smoke from chemical facilities. Potential applications include identifying hazardous spills, monitoring industrial stacks for certain compounds, and surveying the environment from a remote location to detect chemical releases from a suspect facility.

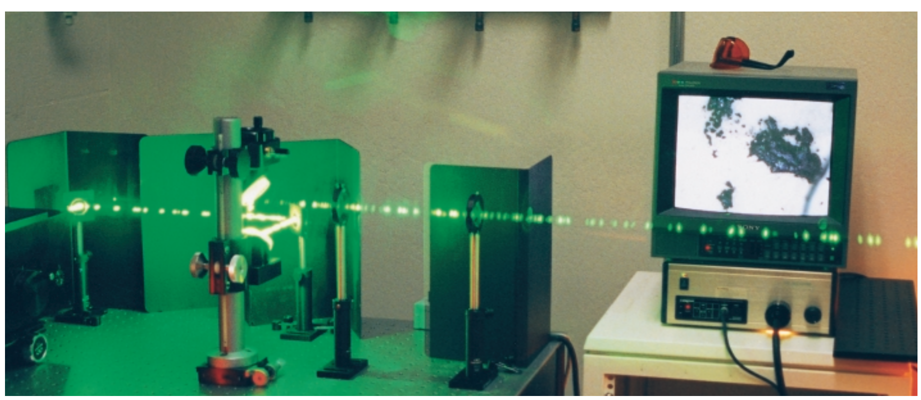
Wands of Collection

One of the center's most important developments has been the solid-phase microextraction (SPME) collection kits that use optical fibers as "chemical dipsticks" for safe and efficient sampling. "The technique has revolutionized the collection of forensic samples in the field," says FSC chemist Pete Nunes.

The technology uses commercial hair-size (100-micrometer-thick) fibers to capture organic vapors. The fiber, residing inside a syringe, is coated with a chemical polymer that, when exposed to the ambient environment for a suitable amount of time, can collect thousands of different compounds by acting as a chemical sponge. The polymer coatings are specific for different types of compounds such as chemical warfare agents, high explosives, or illegal drugs.

The collection technique requires no solvents, sample workup, or additional equipment typically associated with obtaining evidence. The fibers can be inserted directly into a portable or stationary GC–MS for immediate analysis.

Forensic Science Center chemist Del Eckels uses the 28-kilogram portable gas chromatograph–mass spectrometer that fits inside a wheeled suitcase. The portable unit, comparable in sensitivity and selectivity to much larger and heavier units, permits fast on-the-scene chemical analysis.



The imaging laser-ablation mass spectrometer combines a laser for vaporizing extremely small amounts of material, an ion trap time-of-flight mass spectrometer for analysis, and a high-powered microscope for viewing.

Nunes says that because the fibers are fragile, they had never been taken into the field. To overcome their fragility, an FSC team developed rugged aluminum transport tubes, with each tube securing one syringe and fiber. A group of five tubes is contained in each kit. The hermetically sealed tubes prevent any possibility of cross-contamination and support chain-of-custody requirements. A sampling port in the bottom of the tube permits assaying the contents in a glove box before the tube is actually opened.

SPME sampling is being put to good use by FSC weapons scientist David Chambers to monitor nuclear weapon warheads safely. This activity is part of the NNSA's Stockpile Stewardship Program to maintain the safety and reliability of the nation's nuclear stockpile.

Center Plays Role in Famous Law Enforcement Cases

The Forensic Science Center (FSC) has played a pivotal role in several well-publicized criminal investigations. For example, FSC examined the composition and structure of tiny bomb fragments containing trace metal and chemical residues in the Unabomber case.

The center provided analysis and testimony leading to the conviction of Fremont, California, bomber Rodney Blach, a former Chicago Police Department forensic investigator. Blach was convicted of planting bombs during 1998 at the homes of the police chief, a city council member, and others. Former FSC Director Brian Andresen helped investigators from the federal Bureau of Alcohol, Tobacco and Firearms (ATF) to reconstruct what Tom Rogers, assistant district attorney, characterized as "the largest as well as the most electronically sophisticated domestic pipe bombs the ATF had ever encountered." Rogers said, "The electronic aspects of the devices were beyond the expertise of anyone at the ATF."

FSC supported the Democratic National Convention in 2000 by providing a mobile forensic laboratory for the Los Angeles County Sheriff's Terrorist Early Warning Group. The center was also instrumental in interpreting factors surrounding the death of Gloria Ramirez, who made several hospital emergency room personnel violently ill in a well-publicized Southern California case.

FSC helped prosecutors in Glendale, California, rearrest Efren Saldivar, the self-proclaimed Angel of Death and alleged killer of many terminally ill hospital patients. FSC scientists performed toxicology analyses on exhumed tissues from 20 patients. They didn't expect to find anything. However, with the help of completely new techniques, including sample collection procedures developed by the center, they were able to identify the drug Pavulon in the bodies of six of the deceased patients. The rearrest of Saldivar was based primarily on the center's findings

Identifying Bullet Fragments

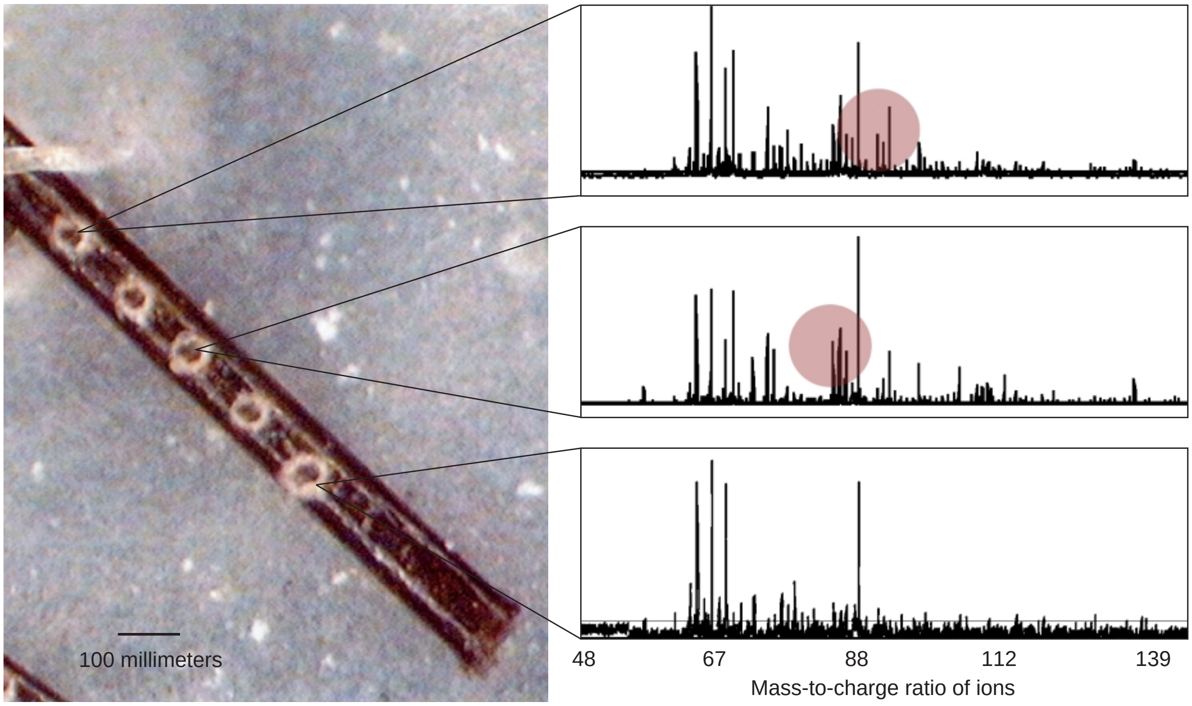
FSC came to the aid of Kings County, California, authorities who were stymied by an execution-style triple homicide. The evidence included a variety of bullet fragments but no weapons. Investigators found corroded, expended casings scattered around the grounds where the suspects lived. FSC personnel led by Rick Randich chemically treated the casings to remove corrosion and then used optical and scanning electron microscopes to match the crime-scene evidence with residence specimens. The staff published its restoration methods as an aid to other agencies.

The center analyzed debris from an explosion that killed a scientist during a 1992 cold fusion experiment at SRI International in Palo Alto, California. In testing the explosion debris, FSC chemists discovered a trace amount of oil in the interior of the SRI electrochemical cell. They determined that a likely source of this oil was lubricating fluid that remained from machining the metal cell components. They concluded that the high-pressure oxygen atmosphere of the electrochemical cell possibly created the potential for an explosive reaction with the oil.

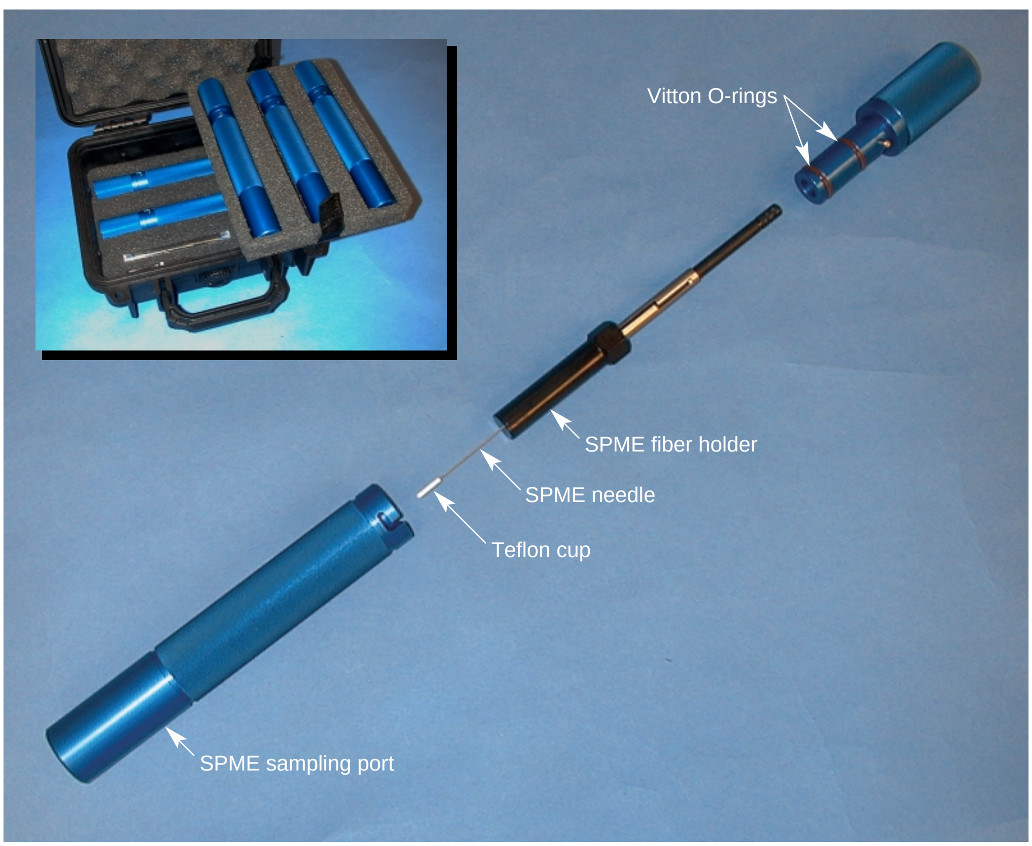
Many FSC investigations involve identifying unknown substances. One specimen brought to the center was a suspicious green liquid uncovered by the Federal Bureau of Investigation (FBI) during a search of a stolen cache of weapons. The container of the liquid was labeled "poison" and gave a dilution formula for use. FSC chemists analyzed the solution for chemical warfare agents but finally identified it as a concentrated cleaning agent.

Another extraordinary analysis centered on a shipment of white crystals in ampoules from China that was thought to be heroin. The powder was interdicted by the U.S. Customs Service and subsequently investigated by the FBI. FSC analyses identified the material as tetrodotoxin, a deadly marine neurotoxin derived from puffer fish. "The definite identification of tetrodotoxin was a real success story for the center," says Andresen.

In the past several months, FSC has been helping authorities to identify samples of substances suspected of being anthrax. Several of the specimens brought to the center by law enforcement officials were from the local community, while others were from locations at the Laboratory. None was found to be real anthrax; instead, the powders were determined to be food materials, dust, dirt, cell culture medium, and powdered paper.



The imaging laser-ablation mass spectrometer allows an investigator to “walk down” a hair shaft by drilling consecutive holes with the laser on the same hair and analyzing each to obtain a volatile sample for a history of activities such as drug use or exposure to chemical weapon compounds.



The Forensic Science Center’s solid-phase microextraction (SPME) collection kits use optical fibers as “chemical dipsticks” and (inset) rugged aluminum transport tubes for safe and efficient sampling. The technique has revolutionized collecting evidence in the field.

Chambers uses SPME's coated fibers to collect volatile and semivolatile molecules that are formed or outgassed from the nuclear and thermal breakdown of organic polymers and high explosives. Signs of outgassing can indicate problems such as corroded metal parts that need to be replaced. By monitoring for the presence of these chemical vapors, scientists are alerted to problems that may be developing inside the weapon.

The center has provided the FBI and other agencies with SPME field kits for the safe and rapid collection of chemical warfare agents. The kits are equally well suited for drug detection and arson investigations. FSC has also developed a new SPME transport tube that is smaller and lighter so that it can fit inside a shirt pocket. Both versions are being licensed to industry for sale to government agencies.

This solid-phase microextraction device is used to collect molecules that are formed or outgassed from the nuclear and thermal breakdown of organic polymers and high explosives contained in nuclear warheads. Signs of outgassing can indicate problems with parts that need to be replaced.

Always On Call

Although the Forensic Science Center was highlighted in a Tom Clancy novel, it is not fiction. It is a rich resource for the national security and intelligence communities and has proved itself a valuable ally to federal and state agencies alike. Just as they have for the past 10 years, FSC personnel will be on call for the next case and the next sample.

—*Arnie Heller*

Key Words: anthrax, Chemical and Biological National Security Program, Forensic Science Center (FSC), gas chromatograph–mass spectrometer (GC–MS), laser-ablation mass spectroscopy, Organization for the Prohibition of Chemical Weapons (OPCW), solid-phase microextraction (SPME), stockpile stewardship, thin-layer chromatography (TLC).

For further information contact Brian Andresen (925) 422-0903 (andresen1@llnl.gov).

Bright Future for Compact Tactical Laser Weapons

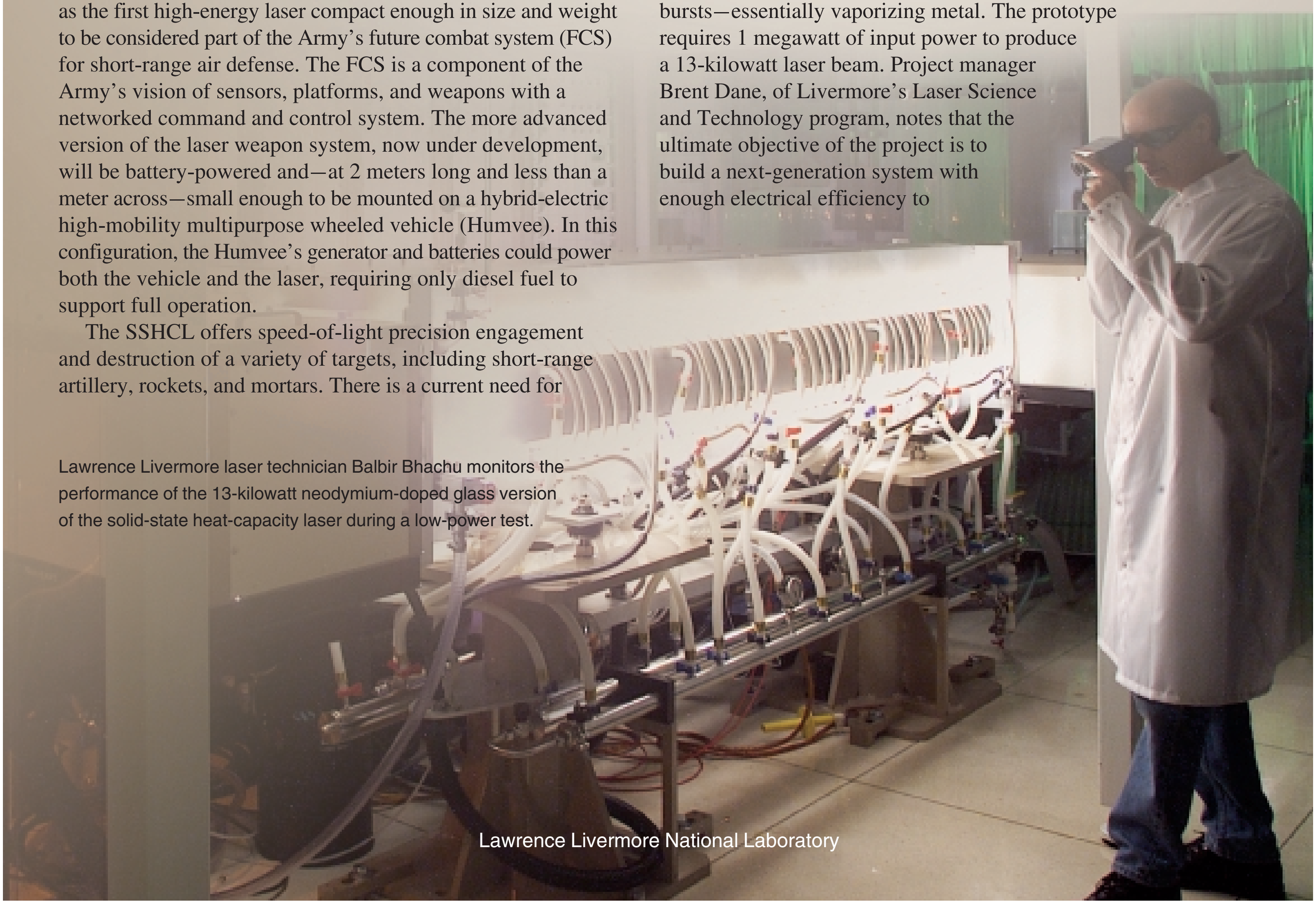
ONCE again, science fiction has predicted science fact. Remember those movies where the hero (or villain) uses a beam from a compact laser to blow a rocket out of the sky? Last December, that generic bit of sci-fi drama took a step closer to reality. In a demonstration at the White Sands Missile Range in New Mexico, the solid-state heat-capacity laser (SSHCL) burned a 1-centimeter-diameter hole straight through a 2-centimeter-thick stack of steel samples in 6 seconds. The electrical current to do so came from a wall outlet and cost no more than 30 cents. While large chemical lasers have successfully shot down tactical rockets, the SSHCL design supports the weight and size requirements for a future mobile deployment.

The SSHCL, designed and developed at Lawrence Livermore, is the prototype of a laser tactical weapon, which shows promise as the first high-energy laser compact enough in size and weight to be considered part of the Army's future combat system (FCS) for short-range air defense. The FCS is a component of the Army's vision of sensors, platforms, and weapons with a networked command and control system. The more advanced version of the laser weapon system, now under development, will be battery-powered and—at 2 meters long and less than a meter across—small enough to be mounted on a hybrid-electric high-mobility multipurpose wheeled vehicle (Humvee). In this configuration, the Humvee's generator and batteries could power both the vehicle and the laser, requiring only diesel fuel to support full operation.

The SSHCL offers speed-of-light precision engagement and destruction of a variety of targets, including short-range artillery, rockets, and mortars. There is a current need for effective protection against these weapons on the battlefield. The project is sponsored by the U.S. Army Space and Missile Defense Command and has a number of commercial partners, including General Atomics, Raytheon Co., PEI Electronics Inc., Northrop Grumman Corp., Goodrich Corp., Armstrong Laser Technology Inc., and Saft America.

Meeting the Challenges

The SSHCL delivered to White Sands for testing last September has an amplifier composed of nine disks of neodymium-doped glass (Nd:glass). In this prototype, an electrical source powers flashlamps, which in turn pump the disks, which then release the energy in pulses of laser light. The average output power of the SSHCL is 10 kilowatts, and it can deliver 500-joule pulses at 20 hertz in 10-second bursts—essentially vaporizing metal. The prototype requires 1 megawatt of input power to produce a 13-kilowatt laser beam. Project manager Brent Dane, of Livermore's Laser Science and Technology program, notes that the ultimate objective of the project is to build a next-generation system with enough electrical efficiency to



Lawrence Livermore laser technician Balbir Bhachu monitors the performance of the 13-kilowatt neodymium-doped glass version of the solid-state heat-capacity laser during a low-power test.

produce a 100-kilowatt laser beam from the same 1 megawatt of input power. The final version will be capable of firing 200 pulses per second.

The Livermore team is focusing on the technological challenges that remain to building the 100-kilowatt system. Dane enumerated the three areas of concentration: growing large crystals of neodymium-doped gadolinium–gallium–garnet (Nd:GGG) for amplifier disks; developing the technology needed to make diode arrays large, powerful, and cost-effective; and defining the laser architecture and technology that will allow high-quality beams to propagate precisely over long distances.

Although the prototype uses Nd:glass for its laser amplifier disks, the final version will use Nd:GGG. "There are many reasons for choosing Nd:GGG," explains Mark Rotter, an electrical engineer who is leading the diode-pumped Nd:GGG effort. "Compared with Nd:glass, Nd:GGG boasts a higher mechanical strength and higher thermal conductivity, which, in combination, will allow us to rapidly cool the disks between runs and reduce the turnaround time between laser firings. The Nd:GGG is also twice as efficient in converting pump energy to output beam energy." The challenge—to grow the crystals large enough to manufacture the nine 13-square-centimeter slabs needed for the 100-kilowatt laser—is well on its way to being met. Northrup/Grumman Poly-Scientific, the commercial partner responsible for growing the crystals, is now producing high-optical-quality Nd:GGG crystals up to 15 centimeters in diameter. The ultimate goal is to grow crystals approximately 20 centimeters in diameter.

To pump these Nd:GGG amplifier disks, the SSHCL will use arrays of laser diodes instead of flashlamps because diode arrays are more compact and efficient than flashlamps and, more importantly, diode radiation generates less heat in the Nd:GGG laser crystals. The challenge is to make the diode arrays large, powerful, and cost-effective and to come up with a cooling scheme that will work in the field.

Lawrence Livermore's Ray Beach, who leads the diode array portion of the project, explains, "Cooling high-average-power laser diode arrays is a unique and challenging problem in the field of thermal engineering. Although laser diodes are extremely efficient devices by ordinary laser standards—they typically convert 50 percent of their electric input power into light output—the remaining 50 percent of the input power shows up as high-intensity heat from a very compact source.

A life-size model, developed by General Atomics and PEI Electronics, of a mobile 100-kilowatt heat-capacity laser built on a prototype of a hybrid-electric, high-mobility multipurpose wheeled vehicle (Humvee) shows the potential compactness of a full-power weapon system.

Because the arrays operate near room temperature, there isn't much opportunity to radiate away heat or use standard electronic cooling techniques such as forced air."

Livermore engineer Barry Freitas came up with a revolutionary packaging technology that solves the problem of creating high-density diode arrays. In this approach, small laser diodes are soldered to low-cost silicon substrates that are etched with thousands of tiny (30-micrometer-wide) microchannels. Cooling water flows through these microchannels, which act as high-performance heat sinks. The team used this packaging design to create the world's highest average-power diode array—41 kilowatts of peak power from a 5- by 18-centimeter package. Arrays that produce 100 kilowatts of power are in production. Work is under way with Armstrong Laser Technology to commercialize the silicon-based diode laser package to support the production needs of the 100-kilowatt laser development.

The team is also working on an optical system that will make a beam of high enough quality—that is, sufficiently narrow, intense, and well-shaped—to propagate 10 kilometers and still hit and disable its target. "In the final system, the laser pulse will travel through nine slabs of crystal, and no matter how good the optics are, the beam will pick up distortions along the way. It's those distortions in the wavefront that we are addressing, because they decrease the power that can be extracted in the laser beam and cause that beam to diverge more on the way to the target," explains Dane.

A team led by Jim Brase in the Physics and Advanced Technology Directorate is developing an adaptive resonator system that will sense distortions in the wavefront and correct them in the system. The resonator—which is based on adaptive optics technology developed at Livermore—includes a deformable mirror, control electronics, and sensors to detect the shape of the laser pulse's wavefront. A deformable mirror will be placed inside the laser resonator, and a wavefront sensor will be used to measure the output beam during operation. The sensor measures the difference between the actual shape and a perfect, flat wavefront. Computer-controlled actuators on the mirror then raise or lower small sections of the mirror's surface to correct distortions in the incoming light so that a high-quality beam is maintained from the laser resonator.

Future Looks Bright

The solutions to these challenges are being incorporated into an SSHCL testbed—a module made up of a three-slab Nd:GGG amplifier pumped by laser diode arrays. This testbed will be configured as a laser system to demonstrate the pulse energy at a high repetition rate in 2003. The final version of the SSHCL, which would have an output power of 100 kilowatts under burst mode for several seconds, is expected to be ready to demonstrate to the Army by 2007.

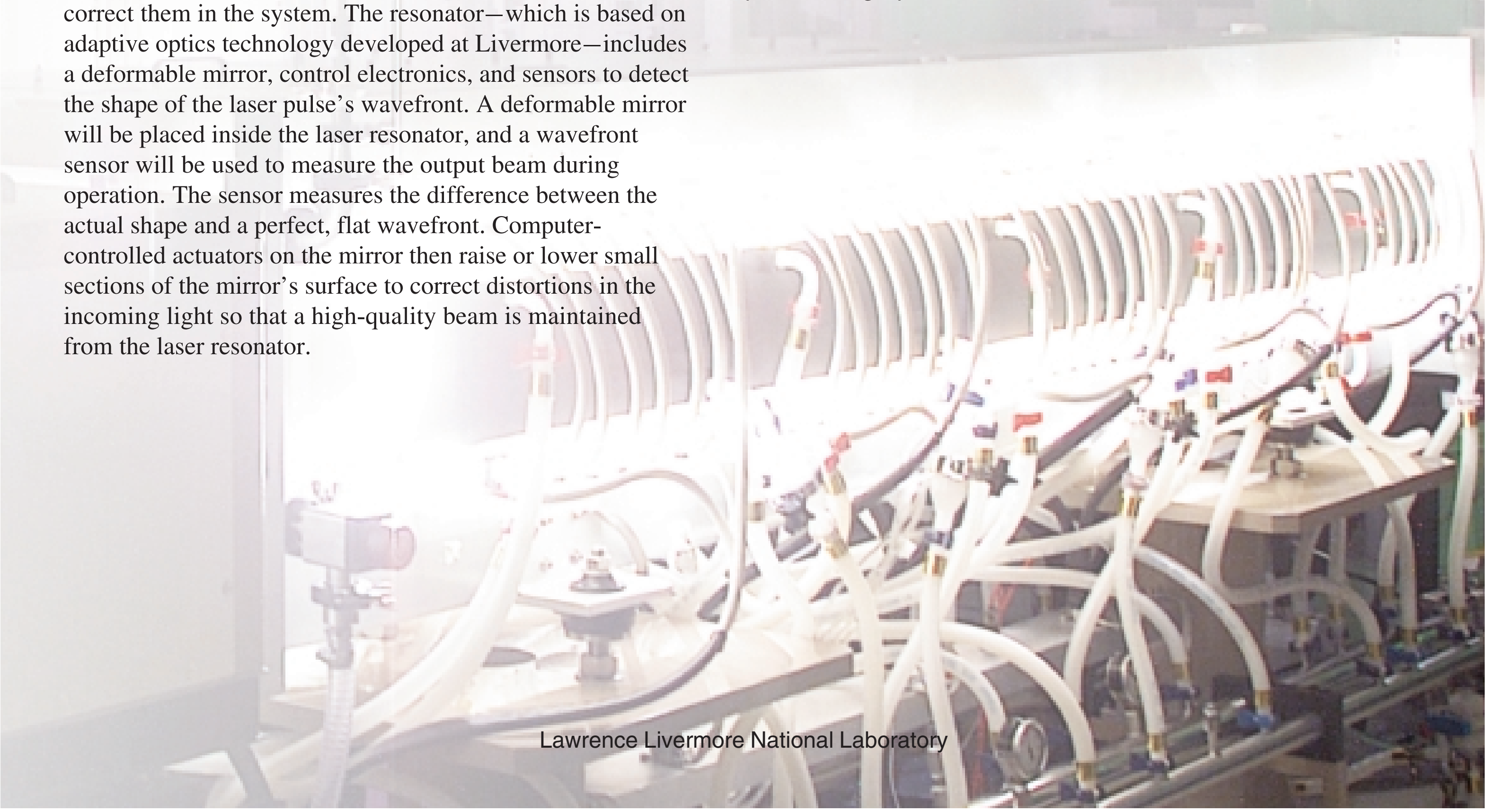
Meanwhile, at the White Sands Missile Test Range, the Army, with Laboratory support, is putting the prototype through its paces, testing it on aluminum and steel to determine what types of power and pulse format will optimize the final weapon system. The Army will also use the prototype to address issues such as lethality, beam degradation due to atmospheric effects, and precision optical pointing and tracking.

The future for the solid-state laser looks promising, notes Dane. "The system we delivered to White Sands is just the starting point. The goal is to have a laser weapon system that is small, cost-effective, and mobile, which protects against tactical threats while meeting the sponsor's other military requirements. We're confident we'll meet these goals."

—Ann Parker

Key Words: laser diode array, neodymium-doped glass (Nd:glass), neodymium-doped gadolinium–gallium–garnet (Nd:GGG), solid-state heat-capacity laser (SSHCL), tactical laser weapon, U.S. Army Space and Missile Defense Command (SMDC).

For further information contact C. Brent Dane (925) 424-5905 (dane1@llnl.gov).



Engineering's Tradition Turns Ideas into Reality

WHEN the Livermore branch of the University of California Radiation Laboratory first opened its gates in September 1952, many of its employees were engineers and machinists recruited from the original "Rad Lab" in Berkeley. Livermore's facilities were primitive—old wooden buildings, no air conditioning, not enough desk lamps or telephones. More important, from an engineer's perspective, the Livermore site—which had previously been the Livermore Naval Air Station—had no shops, no laboratories, no engineering infrastructure. Undaunted, the engineering staff rolled up its collective sleeves and went to work, making and assembling parts for the Laboratory's first nuclear device test in what had been the operating room of the Navy infirmary. Thus, from the beginning, Livermore's engineers and technical staff built a reputation for doing the seemingly impossible.

"Instead of an attic with a few test tubes, bits of wire and odds and ends, the attack on the atomic nucleus has required the development and construction of great instruments on an engineering scale."

—E. O. Lawrence
Nobel Prize Acceptance Speech, 1940

Glenn Mara, associate director for Engineering, notes, "Engineering has a history of collaborating with programs throughout the Laboratory to turn scientific concepts into reality. This approach to 'grand challenge' science is in keeping with the tradition established by E. O. Lawrence of integrating and extending technologies, often simultaneously, and pushing them to their extremes to solve tough technical problems."

For 50 years, Livermore's engineers, designers, technicians, and skilled crafts people have, for example, helped develop and test reliable, safe, secure nuclear weapons; fielded complex high-speed diagnostic systems for nuclear tests; built and operated large magnetic fusion research facilities; designed and built the world's most powerful laser systems and tools for stockpile stewardship; invented compact instruments for detecting biological and chemical agents; and developed microsurgical tools. They made technological breakthroughs to help them do the job—in areas such as precision engineering, nondestructive evaluation, and computational engineering codes—with resulting advances that often had significant applications beyond the Laboratory's gates. (See the boxes on pp. 23, 24, and 26.)

Measuring the Sun's Heat and Density

In Livermore's Nuclear Test program, engineers faced the extreme challenge of creating systems that would measure the performance of an exploding nuclear device. In such an explosion, matter is accelerated to millions of kilometers per hour while experiencing densities and temperatures found only in stars. The Laboratory's early engineers met the challenge, designing instruments and radiation detectors that could capture data on the reaction history, time history, and overall yield of the explosion. The diagnostic systems that evolved over four decades of testing were incredibly complex, often consisting of dozens of specially designed oscilloscopes, hundreds of

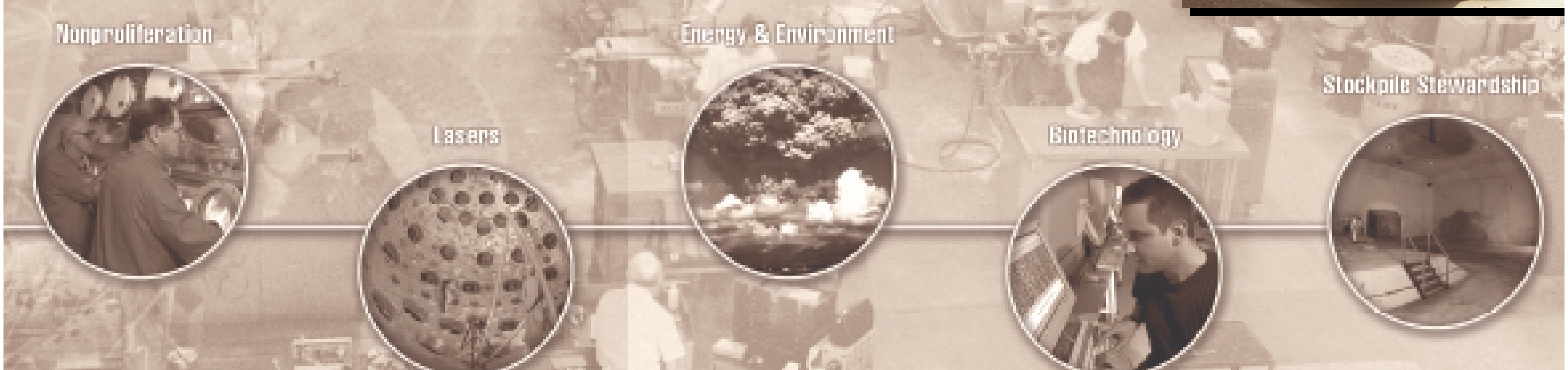
electronic chassis, miles of interconnecting cables, numerous control systems, and thousands of Livermore-developed detectors. Putting the whole together was no less an engineering feat than developing the parts. Timing accuracies, for instance, had to be less than a nanosecond between oscilloscopes connected to detectors over coaxial cables hundreds to thousands of meters long. In addition, because a test offered only one opportunity to gather the data, systems had to be redundant. Thus, detector and oscilloscope systems overlapped the coverage of adjacent systems so that no information would be lost.

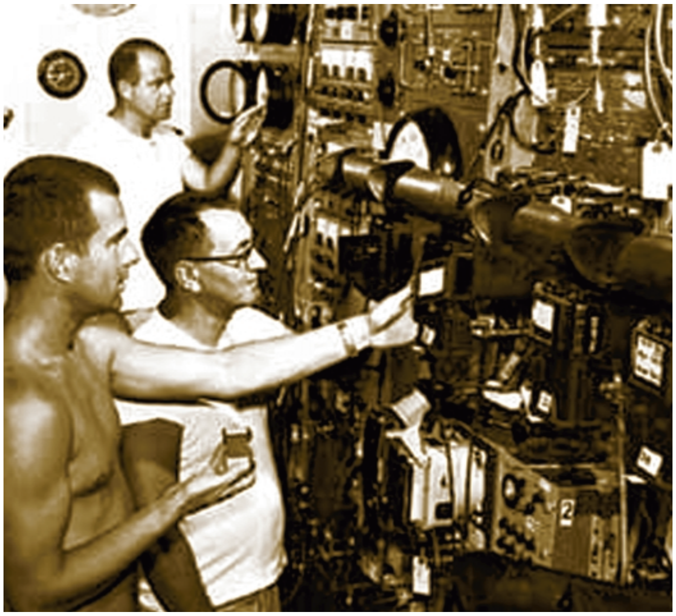
Electronics innovations—from vacuum tubes to solid-state devices to integrated circuits—also revolutionized the systems used in the Nuclear Test program. Livermore engineers designed new oscilloscope systems based on solid-state technology and began exploring digital systems to replace oscilloscopes altogether. One system designed during this time was an extremely fast pulse generator to measure the electrical length of coaxial cables. The generator, which fits into a small box, replaced an entire rack of equipment and reduced dry runs to test simultaneity from days to about an hour. Small digital computers also arrived on the scene. In the Test program, they took over many routine control, timing, and dry-run functions as well as recording or analyzing some of the data. Fiber-optic cables began appearing in underground electronic imaging or spectral analysis systems and were also used to bring digitized data to the surface.

With the cessation of testing in 1992, engineers turned their talents to developing high-speed diagnostic systems for other programs and projects throughout the Laboratory. One such diagnostic device, currently under development in Engineering, will be used in high-explosives tests to measure speeds over 6,000 kilometers per hour in a microsecond timeframe.

Getting the Inside Picture

One area of engineering expertise that grew beyond its initial Nuclear Test program applications is nondestructive evaluation (NDE)—a means of looking at and identifying flaws and defects in materials and finished parts without damaging them (*S&TR*, December 1997, pp. 4–11). Livermore engineers use ultrasonic, acoustic, and other noninvasive techniques to image defects, measure the properties of many kinds of materials, and accurately determine part thicknesses. NDE is used to inspect weapon components, characterize materials, and evaluate solid-state bonds. Engineers have also developed enhanced surveillance techniques, acoustic sensors, array technologies, medical applications, and flight-test sensors—often in concert with industrial partners. Two examples of recently developed NDE systems with applications outside the Laboratory are a system that assays containers of radioactive waste (see *S&TR*, December 2000, pp. 4–11) and the High-Performance Electromagnetic Roadway Mapping and Evaluation System (HERMES), a radar-based sensing system that diagnoses the problems of deteriorating bridge decks (see *S&TR*, October 1998, pp. 8–9). HERMES was successfully tested on a northern California bridge prior to the bridge's demolition.



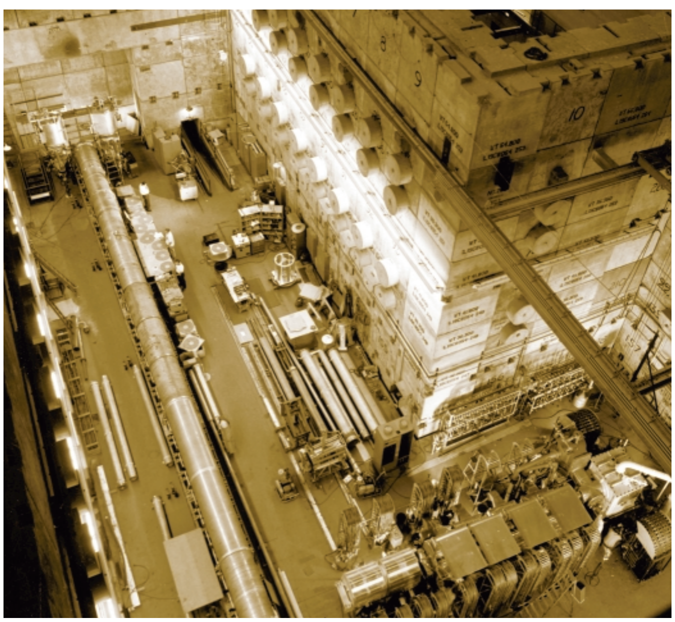


In about 1962, during the days of testing in the Pacific, Livermore engineers and scientists adjust cameras before Operation Dominic, the largest nuclear testing operation ever conducted. These cameras photographed with split-second timing the numerous traces of testing data that streaked across instrument screens in a fraction of an instant during tests. Laser measuring devices and computer techniques eventually replaced these early data-collection and -recording methods.

From Fusion Energy to X Rays

Along with nuclear weapons design and testing, magnetic fusion energy research was an early mission of the Laboratory. The 1970s and 1980s were the heyday of Livermore's research into magnetic mirror machines. Engineers designed and built a series of systems, starting with the Levitrons in the 1950s and moving on to Baseball I and II and the 2XII machine. These early machines led to the development of 2XII-B, which was the first mirror experiment to create a stably confined plasma at temperatures, densities, and durations that approached those needed for a power plant. Success with 2XII-B and the Tandem Mirror Experiment (TMX) in the early 1980s led the Laboratory to design the enormous Mirror Fusion Test Facility, which included the largest superconducting system ever built and equally large vacuum and pulse-power systems.

Livermore's engineers first honed their expertise in linear accelerator design by designing and building the linear induction accelerator Astron for magnetic fusion research in the mid-1960s. After Astron, engineers went on to design a series of linear induction accelerators for the Weapons and Beam Research programs. This series included the Flash X-Ray (FXR), the Engineering Test Accelerator, and the Advanced Test Accelerator. Today's FXR is a major upgrade of the original machine built in the late 1970s. This latest accelerator produces high-energy x rays that can penetrate more than 30 centimeters of steel, providing high-resolution images that show how materials



(left) The linear accelerator Astron, built in the 1960s for magnetic fusion research, was an engineering marvel of its time. No one had ever built such a high-current accelerator before. (right) The Flash X-Ray (FXR) Facility, the nation's most sophisticated linear-induction electron beam accelerator, is a direct descendant of Astron. FXR is an important diagnostic tool in the U.S. weapons research community, enabling scientists to see into the heart of test objects at the very moment they are detonated.

move at ultrahigh speeds. FXR, dedicated in April 1982, remains the nation's most sophisticated linear-induction electron-beam accelerator and one of the most important diagnostic tools in the U.S. weapons research community. (See *S&TR* May 1997, pp. 15–17; March 1999, pp. 4–12.)

Lasers, Large and Powerful

Engineers who supported the Laser program brought with them many of the engineering technologies and systems developed to support the Weapons and Nuclear Test programs and took on a host of new challenges as well. When research into lasers coalesced into a program in the early 1970s, the goal was to produce well-diagnosed thermonuclear microexplosions and to use the laser systems developed at Livermore to study weapons physics and explore the feasibility of producing commercial power.The key engineering words here are "diagnosed" and "developed." Engineers adapted diagnostic systems created for the Nuclear Test program to fit laser researchers' needs. The types of data produced in the tiny explosions—the temperatures, pressures, spectral output—were similar to those of the Test program, as were the time scales.

"In some ways," says Ed Lafranchi, a retired electronics engineer who managed the electronics engineering side of the Engineering Directorate for nearly 15 years beginning in 1973, "the diagnostic requirements and the instrumentation for lasers were very similar to those in the Nuclear Test program, but on a smaller scale." Engineers took high-speed instruments, such as neutron detectors, calorimeters, and streak cameras, and tailored them for laser fusion experiments. As for developing the laser systems themselves, Engineering provided the design and construction expertise that made it possible for the Laboratory to build a series of large neodymium-doped glass lasers of increasing power—lasers that included thousands of high-precision optical components.

New sets of engineering challenges also evolved from the requirements of these enormous optical systems. "We were building some of the largest laser systems existing in the world at that time," explains Lafranchi. "These systems required superclean facilities and new ways to fabricate and polish glass." The National Ignition Facility (NIF), the latest of Livermore's high-energy lasers, will be used for science-based stockpile stewardship and to explore the feasibility of fusion energy for civilian power production and to conduct basic high-energy-density physics research. "NIF is certainly a system of extremes, from an engineering viewpoint," says Monya Lane, operations manager for Engineering. "To begin with, it's enormous in size and power as well as in the number of parts and subsystems involved."

The facility itself is as large as a football stadium and five stories tall. The 1.8-megajoule laser system will have 192 beam lines, 7,500 large optics, more than 30,000 small optics, and 60,000 control points. The 20-nanosecond pulses of laser light from each of the 192 beams must travel 450 meters—through a path of mirrors, lenses, amplifiers, switches, and spatial filters—and converge on a target the size of a BB pellet. Each pulse must be pointed at and hit the target with extreme precision—the equivalent of touching a single human hair from 90 meters away with the point of a needle.

Developing a way to align NIF's 192 laser beams automatically so that they precisely converge on a minuscule target is a formidable task for the engineers working on NIF. The alignment control system is one of NIF's largest systems.

Pioneering Precision

The precision engineering capability that now exists in the Engineering Directorate grew out of the needs of the Laboratory's Weapons program in the 1950s and 1960s. The first few mechanical engineers and machinists who came from Professor Lawrence's Berkeley Rad Lab to support Livermore's weapons design work had to produce high-precision parts from materials that were quite exotic for the times. These engineers and engineering staff became pioneers in the field of precision engineering, inventing new tools and machining techniques such as diamond-coated machine tool bits for improving the finish and accuracy of parts. Among their many accomplishments, Livermore's engineers designed and produced several large diamond-turning machines, each with greater contour accuracy than its predecessor, including the Large Optics Diamond Turning Machine (LODTM). (See *S&TR,* April 2001, pp. 12–14.)

Built in the early 1980s, LODTM was initially developed for strategic defense research to produce large-diameter, nonspherically shaped optics that had to be fabricated with a precision corresponding to a small fraction of the wavelength of light. It has continued to produce extremely precise optical devices for a variety of efforts, including three secondary mirrors for the Keck telescopes in Hawaii and the primary mirrors for a National Aeronautics and Space Administration's Space Shuttle experiment to measure wind speeds using a space-based lidar system. LODTM is still the most accurate large machine tool in the world.

Along with creating systems to machine to extreme precision, Livermore's engineers also developed instruments to measure dimensions, shapes, densities, and surface finishes with greater accuracy than was previously possible. For instance, a recent invention, the absolute interferometer, can measure optical surfaces to within one or two atoms, or less than 1 nanometer. (See *S&TR*, January/February 1998, pp. 12–20, for more information about precision engineering.)

(See *S&TR*, November 1998, pp. 4–11.) It consists of 600 video cameras distributed at 20 points along each beamline, 10,000 stepping motors, 3,000 actuators, 110 racks, 240 kilometers of cable, a high-speed network for transmitting digitized video images, and software to integrate all of these devices.

A Small, Small World

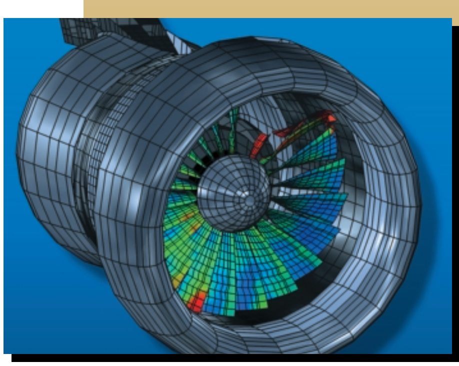
In the world of the very small—where the diameter of a human hair would be considered large—Engineering also made its mark early in the Laboratory's history. (See *S&TR*, July/August 1997, pp. 11–17.) Engineering's focus on microtechnology had its start in the late 1960s when Livermore engineers and scientists began making miniature devices for high-speed diagnostic equipment required for nuclear tests. For many years, before the emergence of Silicon Valley and the ready availability of microchips for a broad array of uses, Laboratory engineers fabricated chips to their own specifications for high-speed switches, high-speed integrated circuits, and radiation detectors. By the early 1980s, Livermore was fabricating thin-film membranes for use as x-ray windows in low-energy x-ray experiments and as x-ray filters. Thin films now serve as debris shields for the Extreme Ultraviolet Lithography program and as targets for high-energy electron experiments that generate x rays.

Microstructures have served as diagnostic devices for Livermore's Nova laser experiments and will do the same for experiments at NIF. In the mid-1980s, Livermore began combining microoptical devices with microelectronics for extremely high-speed, fiber-optic data transmission. Photonic devices have since found their way into many microtechnologies that incorporate optical fibers for transmission of laser light. Livermore's engineers stopped fabricating silicon-based electronic circuits when commercial microchips became available. But they continued to create and apply microfabricated components, including photonic devices, microstructures, and microinstruments, to a variety of Laboratory projects and programs, including stockpile stewardship, nonproliferation, and biomedical research. Recent developments include a silicon microgripper that can be used in microcatheters for medical applications (see *S&TR*, June 1997, pp. 14–21) and a miniature flow cytometer that features ease of alignment and increases the accuracy of flow cytometry, a powerful diagnostic tool used to characterize and categorize biological cells and their content (see *S&TR*, June 1998, pp. 4–9).

Of Computers and Computational Tools

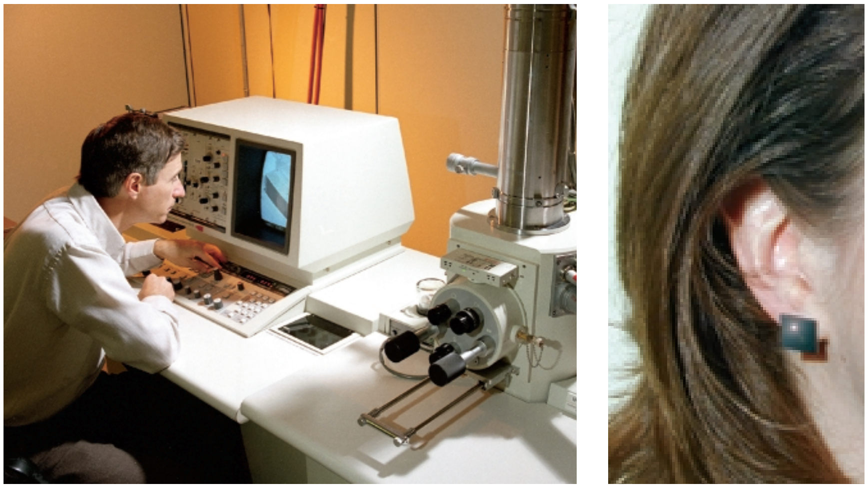
Computers were just becoming a part of the landscape when the Laboratory opened its doors. Some of the Laboratory's first engineers operated, maintained, and modified the Laboratory's first computer, the Univac. Before long, they were also building hardware and designing interfaces, such as the first remote display system—the Television Monitor Display System. When the Laboratory decided to commission computers from commercial suppliers, engineers wrote the specifications. They also wrote "specs" for peripherals that were not commercially available at the time, including a high-speed printer that spat out seven pages a second, an extreme speed even by today's standards. Engineers were among the first to use small computers such as the PDP-11 to automate laboratory experiments throughout Livermore.

In the 1970s, Engineering began developing modeling tools critically needed by Livermore's nuclear weapons projects but unavailable commercially. This work continues to this day. (See *S&TR*, May 1998, pp.12–19.) One of the most well-known of Livermore's early engineering codes is DYNA. An industry observer once wrote: "DYNA is to finite-element codes what Hershey is to chocolate bars and Kleenex is to tissues." Begun in 1979, DYNA3D (the three-dimensional version of DYNA) is an explicit finite-element code that addresses the behavior of structures as they deform and fail. More than 500 companies, universities, and others have applied DYNA3D to problems from crash dynamics to human artery simulations.



In 1992, engineers began developing ParaDyn, the parallel-computing version of DYNA3D. ParaDyn has been used to simulate the structural behavior of weapons and to simulate car crashes, falling nuclear waste containers, ground-shock propagation, aircraft-engine interaction with foreign debris, and biomedical interactions.

In the 1960s, Livermore computational engineers began developing electromagnetic codes that simulate propagation and interaction of electromagnetic fields. Today's electromagnetic field experts study and model wave phenomena covering almost the entire electromagnetic spectrum. One code, EIGER, is a frequency-domain electromagnetic modeling package that has been used recently to model microelectromechanical-system devices, the human neck for speech recognition research, microwave circuits, full-scale Department of Defense systems such as missiles and ships, and phased arrays.



The scale of microtechnology just keeps shrinking. (left) In 1987, Steve Swierkowski inspects a Livermore-designed and -fabricated gallium– arsenide chip, about 3 square millimeters, under a scanning electron microscope. Instruments based on this technology were used at the Nevada Test Site to acquire nuclear test event data and in laser experiments to help shape precise electric pulses for detecting x rays. Today, microtechnology has become nanotechnology, and more features with more capabilities can be squeezed into a smaller area. (right) Livermore's engineers are supporting a Defense Advanced Research Projects Agency project to develop the BioFluidic Chip—essentially a clinical laboratory on a chip, small enough to be worn on an earlobe.

Engineers creating these tiny systems also have an eye to the future. One area showing great promise is that of microfluidic devices. (See *S&TR*, December 2001, pp. 4–11.) These miniature systems move fluids through a maze of microscopic channels and chambers that have been fabricated with the same lithographic techniques used for microelectronics. Microfluidic devices may soon provide a small analytical laboratory on a chip to identify, separate, and purify cells, toxins, and other materials. They might also be used in the future for detecting chemical and biological warfare agents, delivering precise amounts of prescription drugs, keeping tabs on blood parameters for hospital patients, and monitoring air and water quality.

Engineering and Lab Share the Future

Over the past five decades, Livermore engineers have been called upon to use a wide range of materials to build bridges between scientific ideas and useful experiments. The future of Engineering—like its past and present—reflects the evolving national challenges assumed by the Laboratory. In 1992, nuclear testing and engineering development of new nuclear weapon systems halted, and the Stockpile Stewardship Program emerged to help ensure the safety and reliability of the nation's existing nuclear stockpile without nuclear testing. Engineers support this critical national program in many ways. For example, they work on subcritical experiments underground at the Nevada Test Site to help evaluate the dynamic response of plutonium subjected to a high-explosive shock. (See *S&TR*, July/August 2000, pp. 4–11.) They also work on the Lifetime Extension program to extend the stockpile life of Livermore-designed nuclear weapon systems, as well as on NIF, one of the key elements of stockpile stewardship.

Engineering is preparing for future challenges as well. Its five technology centers—in computational engineering, microtechnology, precision engineering, nondestructive characterization, and complex distributed systems—are positioned to solve tomorrow's problems by exploring innovative and cost-effective engineering solutions to emerging technical challenges. "Whatever missions the Laboratory faces in the future," says Mara, "Engineering will be there to supply its special expertise. And if a project involves designing, building, fabricating, or operating a one-of-a-kind experimental facility or system or gathering data at the extreme edges of measurement— the final result will surely show the hand of a Livermore engineer."

—Ann Parker

Key Words: computational engineering, DYNA, DYNA3D, EIGER, Engineering Directorate, Flash X-Ray (FXR) Facility , Large Optics Diamond Turning Machine (LODTM), Laser program, magnetic fusion energy (MFE), microfluidic devices, microtechnology, nanotechnology, National Ignition Facility (NIF), nondestructive evaluation (NDE), nuclear weapons development, ParaDyn, precision engineering, stockpile stewardship, Nuclear Test program.

For more information about Engineering, its projects and its people:
www-eng.llnl.gov/eng_home.html

For information on Engineering's five technology centers:
www-eng.llnl.gov/eng_llnl/01_html/ eng_ctrs.html

For further information about the Laboratory's 50th anniversary celebrations:
www.llnl.gov/50th_anniv/

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

Method for Improving Performance of Highly Stressed Electrical Insulating Structures

Michael J. Wilson, David A. Goerz
U.S. Patent 6,340,497 B2
January 22, 2002
A method for removing the electrical field from the internal volume of high-voltage structures, for example, bushings, connectors, capacitors, and cables. The electrical field is removed from inherently weak regions of the interconnect, such as between the center conductor and the solid dielectric. It is placed in the primary insulation. This is done by providing a conductive surface inside the principal solid dielectric insulator surrounding the center conductor and connecting the center conductor to this conductive surface. The advantages of removing the electric fields from the weaker dielectric region to a stronger area are to improve reliability, increase component life and operating levels, reduce noise and losses, and allow for a smaller, compact design. This electric field control approach is currently possible on many existing products at a modest cost. Several techniques are available to provide the level of electric field control needed. Choosing the optimum technique depends on material, size, and surface accessibility. The simplest deposition method uses a standard electroless plating technique, but other metallization techniques include vapor and energetic deposition, plasma spraying, conductive painting, and other controlled coating methods.

Detection and Quantitation of Single Nucleotide Polymorphisms, DNA Sequence Variations, DNA Mutations, DNA Damage and DNA Mismatches

Sandra L. McCutchen-Maloney
U.S. Patent 6,340,566 B1
January 22, 2002
DNA mutation binding proteins alone and as chimeric proteins with nucleases are used with solid supports to detect DNA sequence variations, DNA mutations, and single nucleotide polymorphisms. The solid supports may be flow cytometry beads, DNA chips, glass slides, or DNA dipsticks. DNA molecules are coupled to solid supports to form DNA-support complexes. Labeled DNA is used with unlabeled DNA mutation binding proteins, such as TthMutS, to detect DNA sequence variations, DNA mutations, and single nucleotide-length polymorphisms by binding, which gives an increase in signal. Unlabeled DNA is used with labeled chimeras to detect DNA sequence variations, DNA mutations, and single nucleotide-length polymorphisms by nuclease activity of the chimera, which gives a decrease in signal.

Printed Circuit Board for a CCD Camera Head

Alan D. Conder
U.S. Patent 6,341,067 B1
January 22, 2002
A charge-coupled device (CCD) camera head that can replace film for digital imaging of visible light, ultraviolet radiation, and soft to penetrating x rays, such as within a target chamber where laser-produced plasmas are studied. The camera head is small, can operate both in and out of a vacuum environment, and is versatile. The CCD camera head uses PC boards with an internal heat sink connected to the chassis for heat dissipation, which allows for close (0.1-centimeter, for example) stacking of the PC boards. Integration of this CCD camera head into existing instrumentation provides a substantial enhancement of diagnostic capabilities for studying high-energy-density plasmas, for a variety of military, industrial, and medical imaging applications.

Fissile Material Detector

Alexander I. Ivanov, Vladislav I. Lushchikov, Evgeny P. Shabalin, Nikita G. Mazny, Michael M. Khvastunov, Mark Rowland
U.S. Patent 6,341,150 B1
January 22, 2002
A detector for fissile materials that provides for integrity monitoring of fissile materials and can be used for nondestructive assay to confirm the presence of stable fissile material in items. The detector has a sample cavity large enough to enable assay of large items of arbitrary configuration, uses neutron sources fabricated in spatially extended shapes mounted on the endcaps of the sample cavity, and incorporates a thermal neutron filter insert with reflector properties. The electronics module includes a neutron multiplicity coincidence counter.

Awards

Abbie Warrick, an Engineering Directorate employee and member of the Extreme Ultraviolet Lithography program, has received an **International SEMATECH Corporate Excellence Award**.

The award is the highest presented by SEMATECH and recognizes exceptional performance, achievement, and innovation in contributing to the semiconductor industry. International SEMATECH is a consortium of semiconductor companies collaborating on research and development for semiconductor manufacturing technology.

Warrick received the award in December 2001 at SEMATECH's facilities in Austin, Texas, where she is wrapping up a two-year assignment as part of the consortium's Advanced Defect Detection project. The award recognizes work performed by Warrick and project teammates Amy Engbrecht and Rick Jarvis of Advanced Micro Devices in helping produce programmed defect reference wafers. These silicon wafers are like those used to print computer chips, except they contain intentional defects and are used to test the inspection tools that chip manufacturers use to spot defects during computer chip production.

Abstracts

Quantum Simulations Tell the Atomic-Level Story

Simulations of quantum molecular dynamics make it possible for the first time to get an accurate look at what happens to individual atoms and molecules during the course of a high-pressure experiment. Such simulations are supplying some of the first information about deceptively simple materials such as water and hydrogen. Recent simulations of shocked liquid hydrogen, the largest ab initio simulations to date on the ASCI White computers, sought to locate reasons for differences found during two sets of high-pressure experiments on deuterium. Other simulations examined water at ambient conditions and under static pressures up to 30 gigapascals. While water molecules dissociate just once every 11 hours at ambient pressures and temperatures, dissociation occurs once every billionth of a second at 30 gigapascals. The same dissociation process occurs under both sets of conditions: two water molecules become hydroxide and hydronium. The smallest part of the DNA backbone has also been modeled, as have a mustard-based drug for treating cancer and silicon quantum dots that may be used in biosensors to detect chemical warfare agents.

Contact:
Giulia Galli (925) 423-4223 (galli@llnl.gov).

Forensic Science Center Maximizes the Tiniest Clue

Founded in 1991, the Laboratory's Forensic Science Center (FSC) offers a comprehensive range of analytical expertise to counter terrorism, aid domestic law enforcement, and verify compliance with international treaties and agreements. The center is among the best of its kind for collecting and analyzing virtually any kind of evidence, some of it no larger than a few billionths of a gram. The center's approach to forensic analysis maximizes the information that can be obtained from extremely small samples of explosives residue, dust particles, hair strands, blood stains, radioactive isotopes, drugs, chemicals, and clothing fibers. Many projects have required FSC scientists to develop new analytical tools and forensic techniques as well as unique sampling procedures. Several new portable instruments have been developed for analysis in the field. FSC has also played a pivotal role in several well-publicized criminal investigations.

Contact:
Brian Andresen (925) 422-0903 (andresen1@llnl.gov).

Coming Next Month

A Virtual Telescope Scans the Skies

Livermore's massively parallel computing capabilities and its store of knowledge on stellar physics, structure, and evolution come together in the three-dimensional stellar code called Djehuty.

Also in May

- ***The atomic force microscope has been adapted for studying soft materials and is useful in medical, dental, and earth sciences applications.***

- ***50th Anniversary Highlight: Physics is where it all started and is still at the core of much of the Laboratory's work.***

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