Also in this issue:

• “Shocking” Gas Gun Experiments
• Mining Data for Gems of Information
• Probing Matter with New Light Source
About the Cover

This month’s S&TR features a report on Livermore’s contributions to the Department of Energy’s Russian programs. Through these programs, which began shortly after the dissolution of the Soviet Union, the U.S. attempts to assist Russia and the newly independent states in preventing nuclear proliferation. The Laboratory’s efforts focus on reducing the former Soviet Union’s nuclear weapons stockpile, controlling and safeguarding the nuclear materials produced during the Cold War, and finding productive nonweapons work for former Soviet weapons scientists. Shown on the cover is one aspect of the Russian programs—reducing the weapons stockpile. The article on Livermore’s work for the Russian programs begins on p. 4.

About the Review

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

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Abstracts
Alternative fuel tank gets Lab assist

Lawrence Livermore researchers are assisting in the development of a sturdy, ultralight fuel tank for use in alternative hydrogen-powered transportation.

The Laboratory is working with the Advanced Technology Center for IMPCO Technologies Inc. of Irvine, California. The Department of Energy has awarded IMPCO a $2.6-million contract to produce a set of tanks for colorless, odorless, pollution-free hydrogen, one of several alternative fuels competing for mass commercialization. Hydrogen gas can be used to fuel an internal combustion engine similar to conventional engines, or it can be combined with oxygen to generate electricity for fuel-cell-powered vehicles.

Fred Mitlitsky, program manager for Energy Storage and Propulsion Systems at Livermore, says that the Laboratory has studied hydrogen storage and propulsion systems for about eight years and “is close to being able to deliver certified tanks at the specified weight limits.” According to Mitlitsky, tank weight is one of the many critical factors in the marketability of hydrogen gas as a fuel source for cars. He adds that tanks to be produced by the Laboratory–private sector partnership will probably be made from a lightweight carbon-fiber material with plastic liners.

The goal of the year-long partnership is to build prototype tanks in which the hydrogen gas within the tank contributes just 7.5 to 8.5 percent of the weight of the filled tank.

Neel Strosh, director of fuel storage for IMPCO, says that hydrogen gas “has very low energy compared with gasoline,” and a challenge in designing tanks is to compress more gas into the tanks.

Because hydrogen gas is flammable, the safety standards for the tanks are extremely high. According to Strosh, conventional gasoline tanks are thin and flimsy compared with the robust hydrogen fuel tanks being developed. Strosh also notes that the cost of hydrogen fuel is high now but could become competitive with gasoline if hydrogen becomes more widely used.

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Nuclear smuggling prevention system tested

Two Laboratory researchers recently traveled to Pacific Northwest National Laboratory in eastern Washington State to join colleagues from Department of Energy headquarters, other DOE laboratories, the U.S. State Department, and Russia in developing methods and equipment to prevent nuclear material from being smuggled on trains. The effort was part of DOE’s Second Line of Defense program, which helps Russia combat illicit trafficking in nuclear materials and technology across its nearly 20,000 kilometers of land border.

Arden Dougan and Dan Archer from the Nonproliferation, Arms Control, and International Security Directorate represented Lawrence Livermore. Russian agencies included the Customs Service and Aspect, an organization affiliated with the Joint Institute for Nuclear Research at Dubna.

The researchers evaluated a Russian detector system developed by Aspect. The detector serves a function similar to that of an airport metal detector. It is designed to find the telltale radiation signals of fissile nuclear material in standing and moving trains.

As a deployed system, this detection equipment must be technically reliable and capable of finding nuclear materials wherever they may be on a train moving at varying speeds. The system must be able to detect radiation from materials that may be shielded by ordinary metal parts on the train and to distinguish between sometimes faint radioactivity signals and naturally occurring background radioactivity that can vary with elevation and geology. The detector and its software must also function in the Russian environment, where temperatures can range from –60 to +120°F. And they must be user-friendly.

Livermore scientists have already helped install radiation detectors in key locations such as Astrakhan, the principal Russian gateway to Iran, and Sheremetyevo, the main international airport in Moscow. They also joined in surveying and establishing priorities for future sites for similar detectors and helped train and certify Russian inspectors in the use of these detector systems.

These Second Line of Defense efforts dovetail with DOE’s many other programs to help reduce the threat of proliferation worldwide.

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The end of the Soviet era dramatically altered the political landscape. In less than a year, President Reagan’s “Evil Empire” disintegrated, and for the first time in history, Russia was not ruled by an autocracy. However, the former Soviet republics had virtually no experience with constitutional government. Neither did they have the economic prosperity or political stability that are the foundation of Western-style democracy.

As Russia struggles to turn the idea of democracy into reality, we cannot forget that it is the only country with a nuclear weapons stockpile capable of annihilating the United States. Even though the Russian Duma ratified the bilateral Strategic Arms Reduction Treaty II in April 2000, stockpile reductions will take years to achieve. Clearly, we must continue to address the Russian nuclear reality. But instead of the Cold War approach of developing more nuclear weapons in response to the threat, today’s approach is one of engagement and assistance.

The U.S.–Russian programs grew out of reciprocal visits and collaborative experiments in the late 1980s by U.S. and Soviet scientists, coupled with forward-looking planning by the Department of Energy and its national laboratories. Over the past decade, DOE’s Russian programs have grown from a handful of informal lab-to-lab contracts to a portfolio of formal activities to reduce nuclear threats and prevent proliferation.

These programs are an integral component of our nation’s multilayered nonproliferation strategy. They address the heart of proliferation prevention—arms reduction, protection of weapons-usable nuclear materials, and nonproliferation of weapons know-how.

The arms-reduction programs are the largest effort (approaching a billion dollars per year). Conducted primarily by the Defense Department, they implement formal treaties and agreements aimed at reducing the number of delivery systems, weapons, and warheads and eliminating stockpiles of weapons-usable nuclear material (including material from dismantled warheads). Livermore is involved in work associated with the secure storage facility at Mayak, in monitoring the Highly Enriched Uranium (HEU) Purchase Agreement, and in joint activities for plutonium disposition.

Programs that address the threat posed by weapons-usable nuclear materials comprise the next level of effort (hundreds of millions of dollars annually). Conducted primarily by the Department of Energy, they address the threat posed by weapons, nuclear facilities, and infrastructure. Livermore is involved in work associated with the secure storage facility at Mayak, in monitoring the Highly Enriched Uranium (HEU) Purchase Agreement, and in joint activities for plutonium disposition.

Programs that address the threat posed by weapons-usable nuclear materials comprise the next level of effort (hundreds of millions of dollars a year). Vast quantities of nuclear materials are located, sometimes under less than adequate protection, at many sites across Russia. Together with our sister laboratories, we are working with the Russians to secure these materials in place and to prevent nuclear material from leaving Russia.

At the third level of effort (hundreds of millions of dollars annually) are programs that address the human aspect of nonproliferation. Lawrence Livermore was instrumental in initiating programs to engage former Soviet weapons scientists in nonweapons research, contributing to their decisions to remain in Russia rather than possibly emigrating to find employment with proliferators. Other programs provide assistance in creating commercially viable regional employment and market opportunities.

In the decade since these programs were initiated, the U.S. has become an even more effective partner with Russia as both countries develop a much more complete understanding of each other’s nuclear complex. Joint planning and execution of projects has led to increased trust between U.S. and Russian personnel. As a result, we are being granted access to increasingly sensitive aspects of the Russian nuclear enterprise, and previously inconceivable joint projects are being proposed by the Russians. The downside of this increased openness is the revelation that securing Russia’s at-risk nuclear materials and assisting in redirecting the Russian nuclear weapons complex are much larger undertakings than previously thought.

Views of the value of these Russian programs vary widely. In the U.S., the programs are either lauded as an unprecedented opportunity to gain access to Russia’s nuclear facilities and essential for national and global security or reviled as excessively expensive and ineffective welfare for Russia. Views in Russia are similarly wide-ranging, where the desire for economic assistance runs counter to fears of spying, exploitation, and loss of national prestige.

Despite rhetoric to the contrary, these programs are beginning to have a real effect in Russia. Large quantities of at-risk nuclear materials have been secured. Thousands of weapons workers are turning to peaceful projects. Transparency is coming into once-dark corners of the Soviet nuclear enterprise. Most important, a foundation of trust has been laid between the U.S. nuclear laboratories and their Russian counterparts—trust that can help address both nations’ vital security concerns, today and in the future.

Wayne Shotts is Associate Director, Nonproliferation, Arms Control, and International Security.
To some observers, the end of the Cold War and sudden collapse of the Soviet Union posed a more dangerous situation than the Cold War itself. The problem was economic and political instability in a region laden with a large number of nuclear weapons, nuclear materials, and nuclear weapons scientists. With the collapse of centrally maintained controls, managing nuclear weapons, materials, and expertise to prevent their transfer to other nations or even terrorists became an urgent task for Russia and the other newly independent states—and an opportunity for the United States to provide assistance.

As Lawrence Livermore Director Bruce Tarter notes, “It is in the interest of the world and the U.S. to work with Russians to contain nuclear weapons, nuclear materials, and nuclear experts within the framework of a stable society.” The U.S. Department of Energy and its national laboratories have been given responsibility for developing programs with Russia’s Ministry of Atomic Energy (Minatom) and other agencies in the former Soviet Union.

Livermore’s Russian programs are concentrated in the Nonproliferation, Arms Control, and International Security (NAI) Directorate, specifically its Proliferation Prevention and Arms Control program. According to physicist William Dunlop, the program leader, Livermore’s Russian programs draw upon a wide range of Laboratory strengths, including nuclear materials characterization, radiation detection, forensic science, computer simulation, site security, weapons physics research, and design, testing, and dismantlement.

At nuclear materials storage facilities, weapons laboratories, remote customs sites, and airports and seaports across Russia and the other newly independent states, Livermore men and
women spend long weeks away from home helping to make nuclear materials and weapons know-how more secure. Despite occasional setbacks—and sometimes difficult negotiations—their progress is a testament to the strong professional relationships they have established with their colleagues in the former Soviet Union.

One telling mark of progress appeared in March when Lawrence Livermore signed the first contract between a DOE laboratory and a Russian nuclear weapons manufacturing plant. The partnership with the Avangard Foundation, an independent Russian business that is the commercial-projects-gathering arm of the Avangard production plant, contracts for the manufacture of kidney dialysis equipment in the closed city of Sarov. Until the 1990s, Western researchers were not allowed to visit the highly secure city; it and other cities like it dedicated to nuclear weapons activities were not even on maps.

Livermore’s Russian programs currently take one of two thrusts. The first is enhancing the protection, control, and accounting of weapons-useable nuclear materials and technologies. The second is helping to find new nonweapons job opportunities for the former Soviet weapons scientists. Taken together, these programs address two of the key proliferation concerns in Russia.

Countering Nuclear Theft

In 1993, the U.S. in partnership with the newly independent states formed a first line of defense against the theft of nuclear materials. The threat is particularly acute in Russia because the Russians have a large number of nuclear storage facilities and nuclear materials producers and exporters but lack an overall system to track or control these materials.

The Material Protection, Control, and Accounting program works with Minatom civil and weapons complexes, the independent Russian civil sector, the Russian nuclear navy, uranium and plutonium storage sites, and reactor and fuel facilities. The program protects against both insider and outsider theft with a host of physical security measures and systems to protect and monitor nuclear materials. Enhancements range from the installation of new fences and modern locks to sensitive radiation detection equipment and sophisticated alarm systems.

In analyzing a site, Livermore experts look for vulnerabilities such as inadequate access control systems and poorly protected building perimeters. For example, doors to vaults holding nuclear materials may have been secured using only wax-and-string seals to detect unauthorized entry. There may be no metal or radiation detectors at entrances to and exits from sensitive areas. Also, areas around facilities may be overgrown and poorly protected by fences and sensors.

Livermore project leader Scott McAllister notes that most U.S. principles, techniques, and tools for nuclear material protection, control, and accounting have been developed by or in conjunction with DOE national laboratories. Livermore personnel apply this longstanding expertise when working with their Russian colleagues. A Livermore employee visiting one of the upgraded sites in Russia would notice many similarities to the equipment and procedures currently used throughout the DOE complex. Examples include access control booths at building entrances, identification badges read by computerized systems to control access to high-security areas, and metal and nuclear material detectors to check people entering and leaving...
facilities containing nuclear material. “We’re helping the Russians update their old system of ‘guards, guns, and gates’ with more sophisticated technical systems,” McAllister says.

Livermore-aided upgrades are currently in place at many of the more than 300 buildings located at over 50 sites included in the program. These sites include some of the most important nuclear institutes in Russia, such as the All-Russian Scientific Research Institute of Technical Physics in Snezhinsk (formerly known as Chelyabinsk-70), a facility similar to Los Alamos or Livermore.

Livermore people also work with the Northern and Pacific fleets of the Russian Navy to strengthen the protection of highly enriched reactor fuel for nuclear-powered vessels. This work involves direct interactions with the Russian Ministry of Defense to characterize the sites, define the necessary improvements, and help implement upgrades, a situation that would have been inconceivable only 10 years ago. Livermore also manages development and implementation of the Federal Information System project, a comprehensive system for tracking Russia’s nuclear material inventory.

A Second Line of Defense

The Russian Federation State Customs Committee must deal with 20,000 kilometers of border to 14 nations, including Iran and North Korea. However, authorities have insufficient funds for equipping customs sites with modern technology to detect illicit nuclear materials trafficking. Since 1997, DOE’s Second Line of Defense program has been providing an additional layer of assurance by helping to protect the most important customs control sites and border points in Russia. Says Livermore project manager Jeff Richardson, “We’re establishing one more layer of defense that did not exist until very recently.”

The program supports the development and installation of Russian-manufactured nuclear detection equipment and provides better training for front-line customs officers. Livermore’s capabilities in radiation detection and forensic science are central to these efforts; a team of Russian customs officials and other government representatives visited Livermore in November 1998 and December 1999 for a series of workshops on preventing the smuggling of nuclear materials.

The program has already achieved several key milestones. In 1998, a U.S.–Russian team led by Los Alamos National Laboratory equipped Moscow’s Sheremetyvo International Airport with radiation detection equipment, including pedestrian portal monitors for departing passengers. The ceremony commissioning the equipment was part of the U.S.–Russia presidential summit in September 1998. Future airport upgrades will include a cargo monitoring system, a system for improved detection of shielded nuclear materials, and technical training for customs officers.

Also completed in 1998 was the Livermore effort to install pedestrian and vehicle monitoring portals at Astrakhan, a major seaport on the Caspian Sea for shipments to Iran and

(a) Livermore scientists and engineers helped to design a hardened annex to an existing Russian nuclear material storage bunker. (b) Upgraded facilities often include such modern systems as access control booths.
beyond. The following year, systems for monitoring rail cars were installed, and the development of new training programs began.

The Second Line of Defense has surveyed customs inspection posts at Vladivostok, Vostochniy, Olya, Rostov, and Novorossiysk—all cities situated along Russia’s southern and eastern borders—for future equipment upgrades. In 1999, Livermore completed a study prioritizing the remaining customs points and border posts, including those on the Black Sea and the Caspian Sea and those bordering North Korea and Kazakhstan.

In addition, Livermore experts in cooperation with Russian Customs Academy colleagues are developing a training program for customs officers. Under this program, Russian technical experts will instruct students and inspectors on how to use radiation portal monitors and handheld detectors, how to spot anomalies in export documents and manifests, and how to examine containers that might hide nuclear material.

Richardson says a particular technical challenge is detecting and identifying weak nuclear radiation sources such as highly enriched uranium. This year saw the initial development of Russian equipment employing what is known as active neutron interrogation. The equipment will bombard suspected cargoes with neutrons to detect illicit highly enriched uranium shipments.

**Warheads Pose Challenges**

Ironically, the success of nuclear arms reduction agreements has compounded the problem of monitoring nuclear materials. Both Russia and the U.S. are dismantling thousands of nuclear warheads. In April 2000, Russia’s Duma ratified the Strategic Arms Reduction Treaty (START) II that cuts each side’s strategic nuclear arsenal to between 3,000 and 3,500 warheads, down from the 6,000 level under START I. (The U.S. Senate ratified START II in 1996.) Future treaties could present several challenges to the West, such as verifying that warheads are in fact being dismantled, that the dismantlement is irreversible, and that the nuclear materials separated from the weapons are accounted for and secure.

Many of Livermore’s warhead dismantlement activities support the 1997 Helsinki summit accords. Presidents Clinton and Yeltsin declared that each country would remove 50 metric tons of plutonium from its nuclear weapons program and ensure that the material could never again be used in weapons. The June 2000 U.S.–Russian Moscow summit builds upon the Helsinki agreements by specifying the plans, schedules, and methods for making 34 metric tons of plutonium inaccessible for use in nuclear weapons. The International Atomic Energy Association (IAEA) is expected to have responsibilities for monitoring this plutonium. Livermore experts are helping to establish the U.S.–Russian–IAEA inspection system for the plutonium that is scheduled to be stored at the Mayak facility in the Ural Mountains. The U.S. is providing $400 million in goods and services toward construction of this storage facility, which is scheduled for completion in 2003. The U.S. has proposed using advanced detection systems that will verify, without revealing classified information, that the plutonium arriving at Mayak came from dismantled nuclear weapons. Jim Morgan, leader of Livermore’s Radiation Technology Group, says that the detection system

(a) Cars and (b) trains leaving and entering Astrakhan on the Caspian Sea are monitored for nuclear materials.
will be demonstrated to Russian experts at Los Alamos National Laboratory this fall. The meeting will be a follow-up to a joint workshop that was held at Livermore in 1997 to demonstrate high-resolution gamma-ray spectrometry for analyzing weapons-grade plutonium.

Livermore scientists also participate in DOE’s Lab-to-Lab Warhead Dismantlement Transparency program. This effort encourages Russian and American dismantlement experts to discuss ways to improve transparency through measures increasing confidence that agreed-to actions are taking place. Livermore is responsible for developing transparency measures for the conversion in Russia of 500 metric tons of highly enriched uranium from dismantled nuclear warheads to low-enrichment uranium. The U.S. is purchasing the converted uranium to fuel its civil nuclear power reactors. The highly enriched uranium effort is currently managed by Livermore’s Energy Programs Directorate in close cooperation with the NAI Directorate.

Livermore experts are also involved in negotiations with Russia to convert its three remaining weapons-grade plutonium production reactors to civil use (the U.S. has ceased producing weapons-grade plutonium). In return, the U.S. is allowed to monitor the 14 metric tons of weapons-grade plutonium oxide produced at the reactors from January 1, 1997, until the reactors are converted.

Disposing of Plutonium

Russia has long considered weapons-grade plutonium recovered from its intermediate products and wastes to be too important a national resource for permanent immobilization, which would ensure that it could never again be used for weapons. Their standard practice is to reprocess all plutonium-containing wastes and recycle the plutonium for their weapons program or as mixed oxide (MOX) fuel for reactors.

In contrast, the U.S. has decided on a dual-track approach. Relatively clean plutonium will be used for MOX reactor fuel, while impure plutonium will be immobilized. In the immobilization approach, plutonium is one constituent of a ceramic waste form, with a neutron-absorbing material added to the ceramic to prevent a nuclear chain reaction during long-term storage in a geologic repository. The plutonium-containing ceramic is sealed inside cans, the cans are placed in a stainless-steel canister, and the canister is filled with molten glass containing high-level defense wastes to further increase the plutonium’s inaccessibility.

Livermore scientists are leading the DOE program to develop U.S. immobilization technology. They have also been encouraging their Russian colleagues to consider immobilizing some of their plutonium. Russian scientists are familiar with the concept. Since 1995, Russian scientists have toured Livermore’s plutonium facility on six occasions (most recently in July 2000) to learn more about immobilization techniques.

Led by engineer Les Jardine, a Laboratory team has successfully encouraged Minatom officials to proceed with research and development, engineering, and system analysis for immobilizing a portion of its plutonium inventory. This plutonium would come from materials, residues, and wastes with concentrations higher than 200 parts per million. “We showed the Russians that it makes more economic sense to immobilize rather than reprocess some of their plutonium,” says Livermore’s Lee MacLean.

The current objective is to develop a Russian capability for industrial-scale immobilization of plutonium by 2005. Over 30 contracts have been placed with Russian institutes. The contracts include engineering feasibility studies at the Krasnoyarsk and Mayak industrial sites and research efforts at Russian scientific institutes to develop glass and ceramic immobilization forms. Russian and U.S. scientists have also defined the nonproliferation safeguards needed to prevent terrorists from retrieving the plutonium from its immobilized form.

In May, Lawrence Livermore received a plutonium oxide saltwasher it had purchased from the Russian Scientific Research Institute of Atomic Reactors. Once adapted to U.S. electrical
standards, the machine will be tested at Livermore’s plutonium facility, where it is expected to provide a more efficient method for preparing U.S. plutonium for immobilization.

According to Jardine, the equipment “shows that their technical people are extremely competent and are capable of efficiently handling plutonium fissile materials.”

Test Ban Treaty Collaborations
Livermore scientists are involved in a host of interactions with Russia in the context of the Comprehensive Test Ban Treaty (CTBT). Livermore teams support the U.S.–Russian CTBT Monitoring and Verification Working Group and collaborate on research projects related to the treaty, including on-site inspection measures.

Although not yet ratified by all participants, the treaty, which forbids all nuclear detonations, creates an international monitoring network to search for evidence of clandestine nuclear explosions. Livermore and Russian scientists are documenting how regional geology would affect the transmission of seismic signals from low-yield underground nuclear tests. They are also working to differentiate the seismic signals of a clandestine underground nuclear test from those of a mining blast or earthquake.

An allied effort is the On-Site Inspection program, which supports the CTBT Preparatory Commission in Vienna by defining the technologies, procedures, and equipment that would guide on-site inspections. Under terms of the treaty, a nation suspecting another of conducting a nuclear test may request an on-site inspection to determine the nature of an ambiguous event. The inspections must be conducted quickly in order to collect information about short-lived phenomena, such as seismic aftershocks, that are produced by an underground nuclear explosion.

A major milestone occurred in October 1998 when a joint on-site inspection exercise was conducted at Snezhinsk, Russia. The exercise played out the first 15 days of a hypothetical on-site inspection. In the exercise, separate U.S. and Russian inspection teams analyzed simulated data from visual, seismic, and radionuclide sources.

A second exercise was successfully completed in April 2000, again in Snezhinsk. Livermore geologist Jerry Sweeney says that this exercise was even more cooperative than the first because inspection teams were composed of both Russians and Americans. “The exercise was valuable because we saw how an international inspection team might function,” he says.

Livermore is also collaborating on several CTBT-related research projects sponsored by the International Science and Technology Center. One project is investigating electromagnetic signals accompanying underground chemical explosions as a way to enhance the discrimination between chemical and nuclear explosions.

Another project is using powerful mechanical seismic vibrators to produce 1- to 8-hertz waves that can be detected at distances of up to 500 kilometers. The goal is to determine if the semiportable vibrators (essentially a railroad tank car placed on end, combined with an air bladder to shift water at a given frequency) can cost-effectively substitute for large explosion sources that are commonly used to calibrate regional CTBT monitoring stations.

Keeping Expertise at Home
Two DOE programs, the Initiatives for Proliferation Prevention and the

Livermore’s Mark Bronson (left) and Les Jardine examine the Russian-designed and built plutonium oxide saltwasher that is being tested for use in the U.S. plutonium disposition program.
Nuclear Cities Initiative, focus on preventing the movement of technical knowledge and expertise from the former Soviet nuclear weapon complex to other nations or terrorist organizations. Both programs attempt to develop self-sustaining nonweapons-related work for former nuclear scientists, engineers, and technicians and introduce the basic principles of market economics and Western business practices.

Founded in 1994, the Initiatives for Proliferation Prevention (IPP) promotes collaborative projects among DOE’s national laboratories, U.S. industry partners, and 170 institutes in the newly independent states. The goal is to attract investment by U.S. companies that will lead to self-sustaining business ventures and provide long-term employment opportunities for former Soviet weapons workers.

The approach involves three steps. First, Livermore works with weapons scientists and institutes to identify and evaluate the commercial potential of research and development activities at the institutes. Second, partnerships are formed with U.S. industry, and DOE shares the investment costs. During the final phase, U.S. industry and the institutes continue the commercial relationship without DOE participation.

Project leader Ted Saito says that Lawrence Livermore’s longstanding knowledge of those institutes, its people, and their capabilities makes the Laboratory an excellent facilitator for U.S. companies. Livermore scientists and engineers bridge communication gaps and contribute to the evaluation of technical and economic potential by U.S. companies that consider creating ventures with Russian partners.

About 1,100 scientists from the former Soviet Union have been or are currently working on Lawrence Livermore IPP projects in the areas of materials science and manufacturing, optics and lasers, environmental remediation, biotechnology, computation, instrumentation, petroleum geology, and software development. Many individuals at research institutes make use of telecommunications capability installed through Livermore contracts to communicate with their U.S. colleagues and the outside world.

Saito cites a promising candidate for full-scale commercialization that involves aluminum–lithium alloys and thin-walled superplastic forming, a manufacturing technique used extensively by the Russian military. Livermore materials experts are working with Boeing to evaluate the technology’s commercial potential for several components of interest to their commercial aircraft and launch vehicle business. Livermore experts are also working with industry to evaluate the cost-effectiveness of automotive wheels formed in a single hydroprocessing operation from ultrahigh-strength aluminum alloys.

Don Lesuer, a Livermore engineer, is helping to commercialize these
Russian manufacturing techniques. He says, “The Russians are sharp technical people and their processes offer a lot to Western companies.” He notes, however, that collaborations with U.S. industry must overcome a weak Russian business infrastructure and export controls that make shipping materials in and out of Russia difficult.

Nuclear Cities Focus

Whereas the IPP focuses on commercial developments with institutes in several countries of the former Soviet Union, the Nuclear Cities Initiative (NCI), formed in 1999, is helping former weapons experts in Russia’s 10 closed nuclear cities make the transition to civilian employment. The closed cities (where Soviet nuclear weapons were designed and manufactured) were completely supported by the old Soviet system. Because of economic hardship throughout Russia, these cities currently receive little government support. What’s more, their nuclear institutes are being downsized by Minatom.

The program’s initial focus is on three cities: Sarov, Snezhinsk, and Zheleznogorsk. Livermore is concentrating much of its efforts at Snezhinsk, home to Russia’s second nuclear weapons design laboratory and sister city to Livermore, California.

Livermore experts are working to create jobs by helping to form new businesses or enhance existing industries, including medical technologies and optical-fiber production. “The goal is to develop business approaches that have a reasonable chance of success with a modest NCI investment,” says Livermore NCI leader Paul Herman.

A parallel goal is to create businesses that meet the needs of the global marketplace. Success requires the active participation of foreign industrial partners, for whom Livermore provides an important link to Russians cut off from current trade practices in democratic countries.
The well-publicized contract to begin production of kidney dialysis equipment is only one of several success stories as the program gains momentum. Livermore also signed two NCI contracts in Moscow last March. The first is for developing explosive charges for oil well casings to allow oil to flow effectively at selected depths. The second is for manufacturing a type of multiple mode optical fiber that is used in local area networks.

Livermore and the All-Russian Research Institute of Technical Physics have also agreed to form an open computer center at Snezhinsk for commercial software contracts for Western companies.

Building on the sister-city relationship, teams of Laboratory scientists and potential private-sector partners have visited Snezhinsk to explore new health-care business proposals. Possible areas of research include remote electrocardiograms, x-ray tomography, laser surgery, ultrasound for kidney stones and prostate treatment, ultraviolet blood treatment, and neutron cancer therapy.

California Representative Ellen Tauscher visited Snezhinsk in August 1999 to explore ways in which Laboratory and business leaders in the greater San Francisco Bay Area could help Russia’s closed cities create sustainable jobs. “People here in Russia acknowledge that the way for Russia to emerge as an economic force is to build on the shoulders of these very talented and experienced scientists,” she says.

The Right Thing to Do

By engaging thousands of former Soviet weapon scientists and enhancing security at dozens of nuclear materials facilities, Livermore programs have made important progress in helping to prevent nuclear proliferation. Dunlop says that much of that progress has been built upon strong professional relationships with colleagues in the former Soviet Union. In nurturing increasing and effective dialogue with scientists and government officials, Livermore people are also helping to develop the more open atmosphere that is the hallmark of a democratic society.

The Russian Programs Assessment Committee, headed by former Air Force Secretary Thomas Reed, was given the task of reviewing the effectiveness of Livermore’s Russian programs. “The Russian programs at Lawrence Livermore National Laboratory are the right things to do,” the committee reported in its May 2000 report. “The possibility of nuclear weapons, materials, and expertise leaking out of Russian government control is one of the most horrifying threats facing mankind today. In working to contain that threat, Lawrence Livermore National Laboratory is earning the respect of the national security community.”

The committee concludes that “these programs are beginning to have an impact in Russia. Materials have been secured, nuclear experts are turning to peaceful work, and transparency is coming slowly into once-dark corners of the Soviet nuclear empire. More importantly, however, these programs have created a foundation of trust between the U.S. weapons laboratories and their Russian counterparts that can help address both nations’ vital national security concerns in the future.”

—Arnie Heller

Key Words: All-Russian Research Institute of Technical Physics; Avangard Foundation; Comprehensive Test Ban Treaty (CTBT); highly enriched uranium; Initiatives for Proliferation Prevention (IPP); Mayak, Minatom; mixed oxide (MOX) fuel; Nuclear Cities Initiative (NCI); Material Protection, Control, and Accounting program; Proliferation Prevention and Arms Control program; plutonium; Sarov; Snezhinsk; Strategic Arms Reduction Treaty (START); warhead dismantlement.

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About the Scientist

WILLIAM DUNLOP received his B.A. from the University of Pennsylvania in 1967 and his M.S. and Ph.D in physics from the University of California at Los Angeles in 1968 and 1971, respectively. He joined Lawrence Livermore in 1972 as a physicist in the Special Projects program. From 1976 to 1985, he served as project manager and, later, program manager of various missile and weapons projects. Then for five years, he was a division leader overseeing work on thermonuclear weapons development.

Dunlop became interested in arms control work in 1979 when he was part of the U.S. delegation to the Conference on Disarmament in Geneva. In 1988 and 1989, he was a member of the U.S. delegation to the nuclear testing talks in Geneva. And from 1994 through 1995, Dunlop served as technical advisor to the U.S. Ambassador to the Geneva Conference on Disarmament, during which the Comprehensive Test Ban Treaty was negotiated. In 1990, he became leader of Livermore’s Arms Control and Treaty Verification program (recently renamed the Proliferation Prevention and Arms Control program).
Livermore’s big gas gun creates shock waves that are millions of times atmospheric pressure at Earth’s surface.

Take a small car cruising down the highway at 90 kilometers per hour and put its kinetic energy into something the size of an ice cube. That’s the energy of the small projectile screaming down the barrel of Livermore’s gas gun at 8 kilometers per second—three quarters of the velocity needed to escape Earth’s gravity. When the projectile hits its target, the pressure of the resulting shock wave is over 600 gigapascals, 6 million times the pressure of air at Earth’s surface. You don’t want to be on the receiving end of that.

These extraordinarily high pressures, created experimentally by the gas gun, occur during explosions, the detonation of nuclear weapons, in inertial fusion experiments, or when a large meteorite hits Earth. These pressures are also a way of life at the core of our own planet and inside the giant planets of our solar system. The high pressures of a shock wave make materials denser and heat them to thousands of degrees.

Livermore’s early shock physics experiments were designed so that scientists could learn what happens to gases, fluids, and solids when they are exposed to shock waves. In the days when Livermore was designing new weapons, better data about materials at high pressures led to improved output from weapon design codes and simulation models so that they better replicated the results of experiments.

Today, the Department of Energy’s science-based Stockpile Stewardship Program demands that researchers be able not just to match the results of experiments but actually to predict in detail the behavior of stockpiled nuclear weapons. This mission puts a premium on understanding the basic underlying science. Knowing the properties of weapon materials is critical to understanding every weapon component and its ongoing performance. Yet even after several decades of working with,
say, the byproducts of high explosives, weapons scientists are still missing much information. The byproducts are disarmingly simple—water, carbon dioxide, and nitrogen. But at high pressures, densities, and temperatures, their behavior is often anything but simple. Experiments that reveal their fundamental nature are essential to predicting their behavior and, by extension, the performance of the overall weapon.

Livermore is one of just a few institutions in the world with a major shock physics experimental program. Notes physicist Neil Holmes, who leads the shock physics program at Livermore, “Each of the three DOE weapons laboratories has its areas of expertise, and the physics of shocked fluids and condensed matter is one of ours. Although gas-gun experiments have been under way since the early 1970s, there is still so much we need to learn.”

He goes on to say, “What started as strictly weapons research has broadened considerably. Experiments about the properties of iron under shock conditions tell us about the center of our own planet where iron exists under high pressures and temperatures. We have also applied data about hydrogen and other molecular fluids such as water to understanding the giant planets in our solar system. For example, the interiors of Uranus and Neptune are made up mostly of complex molecular fluid under high pressures and temperatures. The molecules that make up the fluid are the same molecules as those of the detonation products of high explosives. Our experiments are like sending a probe deep inside those planets.”

Under shock conditions, it is also possible to induce novel configurations that give materials entirely new properties. It was theorized in 1935 that under extremely high pressures, hydrogen would become a metal at room temperature. The effort continues today to find the predicted solid metallic hydrogen. In 1994, however, a team of Livermore researchers produced fluid metallic hydrogen using shock compression. Suddenly, fluid hydrogen was a conductor rather than an insulator (S&TR, September 1996, pp. 12–18). Still other experiments at Livermore are using lasers and pulsed power to induce even higher pressures than the gas gun can achieve. And then there is the diamond anvil cell, which exerts high pressures but not shock waves. The diamond anvil cell operates slowly, allowing careful observation over many hours or days of how a material responds to pressure. This is in contrast to the gas gun, whose shock experiments are over in a millionth of a second or less. (See the box on p. 15 for information on how the gas gun works.)

Measuring Change
All materials change phase if pressure and temperature change enough. We all know about water, which is in the gas phase—steam—at high temperature and in the solid phase—ice—at low temperature. What may be less well known is that as pressures increase, different kinds of ice form. All materials have a phase diagram that shows how its phases change as pressure and temperature change, as shown in the top figure to the left.

A shock wave can change the phase of a material, vaporizing a solid, for example. When a shock wave hits a target, it travels in the target material with a supersonic velocity, taking it to a new state with higher density, temperature, and pressure.

The shock wave is used to find the relationship between the target’s pressure, density, and temperature, which together constitute the material’s equation of state. Experiments to determine the equation of state of various materials have formed the basis of Livermore’s shock physics program for years, and these data are input into weapon simulations.

In shock physics experiments, a curve known as the Hugoniot is a valuable tool for analyzing a material’s equation of state. If a material with a defined initial pressure, density, and energy is subjected to a series of compression experiments of varying shock strengths, a set of new compression states can be plotted. The resulting curve is the material’s Hugoniot. Every material has a unique

A phase diagram for a hypothetical material shows how the material changes as temperature and density (a function of pressure) change.

This is the Hugoniot curve for a hypothetical target material. The pressure (P) and density (D) of a target before impact are P₀ and D₀. When the target is hit and compressed, its pressure and density increase to P and D. A series of compression experiments of varying shock strengths will result in the curve shown.
Hugoniot curve. The Hugoniot can be determined absolutely through experiments that need to measure only distance and time—that is, velocity.

In the last 10 years, the shock physics program has expanded to include experiments to measure such transport properties as electrical and thermal conductivity as well as sound velocity in shocked materials. The optical properties of the shocked target—the light emitted during an experiment—are also being studied. This additional information is needed to understand the physical processes occurring in a shocked sample.

How Hot Is Hot?
Conservation of momentum, mass, and energy are implicit in Hugoniot curves, but the curves provide no direct way to derive temperature at high pressures. Even after 20 years of study, scientists still do not agree on the melting temperature of iron at pressures above 100 gigapascals (1 gigapascal equals 10,000 times atmospheric pressure at Earth’s surface). Recall that temperature is a critical variable in a material’s equation of state.

Temperatures in a gas-gun experiment can reach as high as 7,000 kelvin, which contrasts with the relatively cool 5,800 kelvin at the surface of the Sun. The only way now to measure such high temperatures during an experiment is with optical pyrometry. A pyrometer measures the radiance—a combination of brightness and color—of the shocked sample. A simple calculation then translates radiance to temperature. That sounds good in theory, but the reality is not so easy.

All measurements of shocked metals and other opaque materials must be taken through a window. A window made of a strong material preserves the surface of the sample at high pressure while allowing light from the sample to pass through to a fiber-optic detector. “But,” notes Holmes, “at very high temperatures, the window can absorb light and emit its own light, and the window’s presence changes the final state of the sample.” Researchers are just beginning to be able to account for the effects of the window on overall radiance and hence on measured temperature.

Physicist Dave Hare is studying the properties of window materials. Lithium fluoride has been used as a window material for gas-gun experiments for many years. For many experiments, it is fine. But for planetary studies and some other types of experiments, the window material needs to be stiffer (harder to compress) to be an effective window in gas-gun experiments. Most of Hare’s research centers around sapphire, another window material used for many

<table>
<thead>
<tr>
<th>Inside Livermore’s Gas Gun</th>
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<td>Livermore’s shock physics group has three two-stage gas guns—one 20 meters long and two about 6 meters long. The larger one is faster and is used for the highest pressure experiments. Both consist of three major parts: a breech containing gunpowder; a pump tube filled with a light gas, typically hydrogen; and a barrel for guiding a high-velocity projectile to the target. When the projectile hits the target, the impact produces a high-pressure shock wave. The guns are driven in two stages, first with gunpowder and then with a light gas such as hydrogen, helium, or nitrogen. The smaller guns can also be used as a single-stage gun driven only by gas.</td>
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<td>Hot gases from the burning gunpowder drive a heavy piston down the pump tube, compressing hydrogen gas. This gas, the second-stage driving medium, is compressed before the gas breaks the rupture valve. The gas then accelerates a 15-gram projectile down the barrel to a muzzle velocity of up to 8 kilometers per second.</td>
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<td>Hydrogen is used as the second-stage driving gas because it produces the highest projectile velocities, ranging from 4 to 8 kilometers per second. When hydrogen is used as a single-stage gun, the velocities of the smaller guns range from 100 meters per second to 1 kilometer per second. Velocities are determined by carefully selecting the gun firing parameters: the type and amount of gunpowder, the driving gas (helium and nitrogen are used for velocities below 4 kilometers per second), the pressure required to open the rupture valve, the diameter of the barrel, and the mass of the projectile.</td>
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<td>A wide range of diagnostic equipment is available to study the shocked targets to measure equations of state, thermal and electrical conductivity, wave profiles, optical pyrometry, and spectroscopy.</td>
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Lawrence Livermore National Laboratory
years by Livermore researchers. “Sapphire should be a great window,” he says. “It is dense and stiff, and its optical transparency at room temperature and pressure is excellent. But at shock pressures above 200 gigapascals, its transparency degrades too much for it to be useful. I’ve been trying to figure out why.”

In one series of experiments, Hare has found that the orientation of the sapphire crystal relative to the direction of the shock wave makes a big difference in determining its light emissions when shocked. Besides providing an understanding of how sapphire stands up to strong shock waves, these data also help to show how strong materials are deformed by shock waves.

Measuring thermal conductivities under high-pressure conditions is not easy. But thermal conductivity measurements of window and sample materials are crucial to deriving accurate temperatures of the sample’s interior. While the pyrometer measures the sample’s surface temperature, the interior temperature is the real subject of concern. Because the sample and the window are usually at different temperatures when shocked, heat can flow from the hot sample to the colder window, altering the temperature that the pyrometer measures. Once the thermal conductivity of the window and the sample are known, experimenters can correct their data to derive a more accurate temperature of the sample’s interior.

Physicist Jeff Nguyen is tackling another area that is critical to converting radiance data to temperature. In these calculations, emissivity—which measures how effectively a hot body radiates energy—is assumed to be constant at all pressures and wavelengths. Physicists have known that this is not in fact the case but have had no way to determine the precise changes with pressure. According to Nguyen, “To say that emissivity at high pressures is not well understood is an understatement. Right now, there are virtually no data on emissivity at high pressures.”

Emissivity measurements at ambient pressures and high temperatures have been done routinely. But no definitive theoretical or experimental work has been done at high pressure, especially at the pressures produced by shock compression.

Nguyen’s emissivity experiments of sample materials under shock conditions were performed on metals such as aluminum, copper, and iron. In the experiments, a laser was reflected off a metal target that was shocked, and Nguyen measured the change in the light’s polarization as the metal underwent shock compression. These experiments were the first of their kind. The results are expected to have a major effect on the study of phase diagrams.

“Our goal,” says Holmes, “is to do a shock experiment and know accurately what the temperature inside a sample is. Temperature is a fundamental property. It is, after all, the ‘thermo’ in thermodynamic. But first, we need to know enough about window properties, the emissivity of metals, and the conductivity of windows and metals to separate the sample’s radiance from the window’s.”

**Inside Planets**

For a brief moment, shock-compression experiments can reproduce the conditions under which some materials spend their entire lives. Iron in Earth’s core is one example, and the interiors of the giant planets are

This cut-away view of an experiment to measure sound velocities in iron shows the level of complexity in target design. Although not seen in detail here, the target baseplate has seven steps. Its surfaces are diamond-turned, and the thickness of the steps is precisely measured. The gap between the iron and the window is filled with bromoform that emits light whose intensity is dependent on the shock it receives. Light emitted from each of the steps is focused into specific optical fibers that send the light into 14 different recording channels. The electrical pins in the gap between the target and the window trigger the instruments that measure the sound velocity through the iron.
another. By reproducing the relevant high pressures, densities, and temperatures with the gas gun, Livermore researchers can reach deep inside the planets where most of the mass is. Convection puts this mass in motion, creating strong magnetic fields that scientists want to understand.

Duplicating the innards of giant planets often requires achieving isentropic or at least quasi-isentropic conditions—that is, constant or near constant entropy. Entropy is a measure of the disorder in a system and relates the total heat in a material to its temperature. In the planets and stars, pressure and temperature increase with depth, but entropy does not change. “A quasi-isentropic experiment comes as close as we can get in the laboratory to duplicating these conditions,” says Holmes.

When stiff plates—stiffer than the target material—are added to the gas-gun experiment, the shock wave will reverberate between them. This is known as a “ring-up” experiment. While a shock experiment always changes the entropy, each repeating shock is weak, and the change in entropy is small. So by compressing the target material with a series of weak shocks rather than one strong one, the overall change in entropy is smaller and hence quasi-isentropic.

Researchers have found that just a single bounce, called a double-shock experiment, will also produce planetary conditions. Quasi-isentropic experiments, which are at lower temperature and higher density than double-shock experiments, are appropriate for experiments seeking information about the makeup of large planets. Duplicating the conditions at Earth’s core can be achieved with single-shock experiments.

In the hydrogen experiments, liquid deuterium (an isotope of hydrogen with one proton and one neutron in the nucleus) could not be metallized by a single shock. Only when deuterium was compressed to higher densities using a reverberating, quasi-isentropic shock did it become metallic. Many scientists surmise that fluid metallic hydrogen exists deep inside Jupiter and Saturn.

To study the core of our own planet, Nguyen worked on a series of experiments with iron samples to determine the melting pressure at Earth’s core. Geophysicists combine Nguyen’s results with those from other experiments to build the melting curve for iron. From this melt line, they can determine the temperatures at the boundaries between the core and the mantle and between the inner solid core and outer liquid core.

In single-shock experiments at shock pressures up to about 400 gigapascals, Nguyen measured sound velocities, which change with changes in pressure and temperature. When a material melts, its sound velocity decreases abruptly by 10 to 15 percent. Nguyen found such a decrease in iron near 220 gigapascals, indicating melting. Other metals exhibit a similar drop in sound velocity at the solid–liquid phase change.

What they have not found is just as significant. Twenty years ago, a similar sound velocity experiment suggested an additional solid–solid phase transition at 200 gigapascals, potentially complicating the iron phase diagram. Nguyen’s results simplify the iron phase diagram and prove lower temperatures at the core boundaries than previously thought. These results are also important given the lack of agreement in the scientific community about the melting point for iron at high pressures.

Physicist Ricky Chau and his colleagues are studying the interiors of...
Experiments will test whether metallic lithium will become a nonmetal and hence no longer a conductor of electricity at high pressures. Researchers expect to find what is shown in this model, where lithium ions pair with each other (red), and the valence, or conduction, electrons become localized and nonconducting in the interstitial space (blue). (The image is used by permission of J. B. Neaton and N. W. Ashcroft, Cornell University.)

The giant planets Uranus and Neptune. These planets are thought to have a three-layer structure: a small rocky core; a thick layer of “ice” composed of water, methane, and ammonia comprising two-thirds of the planetary mass; and an outer atmosphere of molecular hydrogen and helium. The ice is actually a warm, dense fluid with pressures ranging from 30 to 600 gigapascals and temperatures from 2,500 to 7,000 kelvin. The ring-up method takes temperatures and pressures to those closely matching the interior.

These experiments study the electrical conductivity of the planetary ices. The goal is to use changes in the electrical conductivity to reveal the state of the interior fluids. For example, the convection of conducting fluids deep inside the giant planets is a reasonable explanation for the generation of the strong planetary magnetic fields. To understand the complex magnetic fields, we must measure the electrical conductivity of the planetary fluids.

Using electrodes attached to the gas-gun target, Chau and his coworkers measured the electrical conductivity of water, which they found to be a relative poor conductor. Physicist Marina Bastea has also examined oxygen, which, like hydrogen, is thought to become a metal at high pressures. Team members are currently studying nitrogen and will be studying methane later this year.

Conductors and Insulators

When Livermore scientists used a quasi-isentropic experiment to produce metallic hydrogen in 1994, they were operating on an assumption basic to high-pressure physics—namely, that all materials will become conductive beyond a certain pressure threshold. Now, Livermore physicists Marina Bastea and Bill Nellis have begun working to produce the opposite phenomenon: using pressure to induce a metal (conductor) to become an insulator. Their studies on metallic lithium could provide the first experimental evidence that this phenomenon is possible.

The theory is that the pairing of atoms of the same element has a strong effect on the electrical properties of low-atomic-number elements such as lithium. Bastea and Nellis hope to find that under high pressures, monatomic lithium metal (Li) will change into a state in which lithium atoms pair with each other (Li₂). The conduction electrons in the monatomic metal will become localized and nonconducting as the monatomic lithium metal transforms into a diatomic lithium insulator.

The earlier Livermore experiments showed that hydrogen changes from an insulator to a metal at 140 gigapascals. Monatomic lithium is predicted to become nonmetallic diatomic lithium at 100 gigapascals. So what will lithium hydride, a combination of these two elements, do at elevated pressure?

Lithium and lithium hydride are ideal test cases for the fundamental physics that takes place in highly compressed, condensed matter. They are also relevant for understanding newly discovered astrophysical objects such as brown dwarfs. Both materials have a wide range of technological applications, from high-performance batteries to fuel cells.

More Pioneering Work

Holmes and his team have begun experimenting with new materials for windows such as gallium–gadolinium–garnet, which is twice as dense as sapphire, almost like steel. If it proves to be a good electrical insulator in quasi-isentropic experiments, it will allow researchers to reach much higher densities and pressures in experiments than are now possible.

Livermore is also producing some of the first quantum molecular dynamic models of materials under shock conditions. Scientists believe that under high pressures and temperatures, all materials will disassociate and come...
back together quickly. Using Livermore’s substantial computational capability, physicist Giulia Galli has modeled the behavior of water under high pressures, calculating where the oxygen and hydrogen atoms are and how hydrogen bonding occurs.

Weapon materials such as uranium, plutonium, and other actinides have not yet been studied directly under shock conditions. But beginning in 2001, a new gas gun in a nested confinement system at the Nevada Test Site will change that. The recently completed Joint Actinide Shock Physics Experimental Research (JASPER) facility is specifically designed to study the behavior of actinides and other hazardous materials under high pressures, temperatures, and strain rates, approximating the conditions experienced in nuclear weapons. Data from the JASPER experiments will be used to determine equations of state and to validate computer models of material response for weapons applications.

Basic science is at the core of the DOE’s Stockpile Stewardship Program, and a full picture of how materials behave when they are shocked is a critical component. Being able to predict material behavior with full confidence is still some time off. In the meantime, look out—another gas-gun experiment is set to go.

—Katie Walter

Key Words: equations of state, Joint Actinide Shock Physics Experimental Research (JASPER) facility, planetary physics, shock physics, stockpile stewardship, two-stage light-gas gun.

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About the Scientist

NEIL HOLMES received a B.S. in physics from the California Institute of Technology in 1970 and a Ph.D. from Stanford University in 1977. He joined the Inertial Confinement Fusion program in 1977 and, in 1978, moved to the Shock Physics Group in the Physics Directorate, becoming group leader in 1984. He also holds leadership positions in the Physical Data Research program and is chief scientist for JASPER, a new experimental facility at the Nevada Test Site devoted to shock-wave studies of plutonium at high pressures.

Holmes initially worked on laser-driven shock-wave experiments; most of his current work uses the gas guns. His current research interests include time-resolved spectroscopy of transparent solids and molecular fluids, the thermodynamic properties of materials at extreme conditions, and nonequilibrium phenomena in shock-loaded materials. He is a fellow of the American Physical Society and recently completed a term as national chair of the American Physical Society’s Topical Group on Shock Waves in Condensed Matter. Holmes is a two-time recipient of a Department of Energy Award of Excellence.
Mining Data for Gems of Information

MINING is an arduous, time-consuming business. Sometimes, tons of material must be excavated to uncover ounces of precious metals or gems. The computational equivalent of old-fashioned, down-in-the-dirt mining is data mining. Whether the search is for metals or information, the task is similar. In data mining, trillions of bytes of data must be sifted to find a handful of precious numbers or images.

As computers grow in speed, number-crunching capabilities, and memory, scientific researchers are edging into data overload as they try to find meaningful ways to interpret data sets holding more information than the U.S. Library of Congress. According to Livermore computer scientist Chandrika Kamath, “The problem has its roots in the many advances in technology that allow scientists to gather data from experiments, simulations, and observations in ever-increasing quantities,” says Kamath. “In many scientific areas, the data sets are so enormous and complex that it is no longer practical for individual researchers to explore and analyze them by hand. When the sets get so large, useful information is easily overlooked, and the data cannot be fully utilized.”

To address this problem, Kamath and a small team of Livermore researchers are developing Sapphire—a semiautomated, flexible data-mining software infrastructure. Sapphire shows great promise in helping scientific researchers plow through enormous data sets to turn up information that will help them better understand the world around us, from the makeup of the universe to atomic interactions. Sapphire is funded by the Laboratory Directed Research and Development program and the Department of Energy’s Accelerated Strategic Computing Initiative (ASCI).

Data mining is not a new field. In the commercial world, it is used to detect credit card fraud and computer network intrusions; reveal consumer buying patterns; recognize faces, eyes, or fingerprints; and analyze optical characters. At Lawrence Livermore, the terascale computing environment created by ASCI as well as the prolific use of several different types of sensors have created great interest in large-scale, scientific data-mining efforts such as Sapphire. Kamath and her team envision that Sapphire will be applicable to a variety of scientific endeavors, including assuring the safety and
reliability of the nation’s nuclear weapons, nonproliferation and arms control, climate modeling, astrophysics, and the human genome effort.

Data Mining Step by Step

Data mining starts with the raw data, which usually takes the form of simulation data, observed signals, or images. These data are preprocessed using various techniques such as sampling, multiresolution analysis, denoising, feature extraction, and normalization. (See the box at the left.)

Once the data are preprocessed or “transformed,” pattern-recognition software is used to look for patterns. Patterns are defined as an ordering that contains some underlying structure. The results are processed back into a form—usually images or numbers—familiar to the scientific experts who then can examine and interpret the results.

To be truly useful, data-mining techniques must be scalable. “In other words,” says Kamath, “when the problem increases in size, we don’t want the mining time to increase proportionally. Making the end-to-end process scalable can be very challenging, because it’s not just a matter of scaling each step but of scaling the process as a whole. For instance, the raw data set may be 100 terabytes, and as the data move through the data-mining process, the process decreases the data set size in ways we cannot predict. By the end of the process, we may have a resulting data set that’s only a few megabytes in size.”

To test and refine their algorithms, Sapphire researchers teamed up with Laboratory astrophysicists who were examining data from the FIRST (Faint Images of the Radio...
Once preprocessing is complete, the transformed data are input to pattern-recognition software. Two types of general pattern-recognition techniques used in data mining are classification and clustering. In classification, the algorithms “learn” a function that allows a researcher to map a data item into one of several predefined classes. In clustering, the algorithms work to identify a finite set of categories or clusters to describe the data. There are several different algorithms for classification and clustering, and frequently, both types of pattern recognition can be used within an application.

Once patterns are identified and translated by the Sapphire software back into a usable format, the results are examined by an expert. “We consider data mining to be a semiautomatic process because a human is involved in each step of the entire discovery process,” explains Kamath. “The process is both iterative and interactive.”

Gems Uncovered

Kamath and her team are pleased with how the data-mining algorithms tested out on the bent-double research—as are the astrophysicists. “Using our algorithms on the FIRST data, we identified a bent double previously overlooked by the astrophysicists in their manual search,” said Kamath.

The data-mining algorithms in Sapphire are modular and easy to use in a variety of scientific applications and across diverse computer platforms. The beta release of this software to Lawrence Livermore users is scheduled for late 2000.

“We’re also looking at what can be done to apply complex pattern recognition algorithms to data as they are being gathered,” says Kamath. “For example, if one is looking for transient events—asteroids in astrophysics data or fraud in business transactions—the processing must keep up with the rate at which new data are acquired.”

—Ann Parker

Key Words: Accelerated Strategic Computing Initiative (ASCI), data mining, Faint Images of the Radio Sky at Twenty Centimeters (FIRST), pattern recognition, Sapphire.

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More information about Sapphire can be found at www.llnl.gov/casc/sapphire/sapphire_home.html.
X-RAYS are handy for examining all kinds of materials, from our bones and lungs to high explosives and other ingredients in a nuclear weapon. If the x rays are intense enough and come in short enough pulses, they can supply information about the dynamic processes in many forms of condensed matter, such as solid materials, liquid crystals, and extremely dense plasmas. Using the Linac Coherent Light Source (LCLS)—an x-ray machine with unprecedented brilliance being considered for construction at the Stanford Linear Accelerator Center—researchers will be able to measure, for the first time, melting, recrystallization, and light-induced structural change on time scales down to a quadrillionth of a second.

The extraordinarily bright, short pulses of the LCLS have the potential to open new areas of science that are unimaginable given current scientific knowledge. The LCLS will make visible dynamic processes that can only be guessed at now. Upon completion in 2004, the new facility is certain to help solve problems in ultrahigh-energy-density physics, structural biology, fundamental quantum electrodynamics, warm dense matter, and high-field atomic physics, among others. The extreme brightness of the LCLS also means that results will be available much faster than before and will offer a level of detail that has been impossible to obtain with existing tools.

“For decades, we have studied nonlinear phenomena at optical wavelengths,” says physicist Art Toor, who is leading the Livermore work on the LCLS. “But we’ve never had the tools to study nonlinear multiphoton processes in the x-ray region. That is tremendously exciting and opens the door to whole new regimes of research in physics, biology, and chemistry.”

Protein crystallography, used to study the structure of proteins, is just one example of the research techniques that will benefit from the new x-ray source. Livermore and other biological research facilities use third-generation light sources to obtain images of molecules in a process that takes many hours of exposure time for each image. The shorter, brighter pulses of the LCLS will produce enough flux to image a molecule in a single pulse.

Livermore is part of the collaboration that is conducting research and development leading to this fourth generation light source. The LCLS is the next step beyond third-generation synchrotron radiation light sources, such as the Advanced Light Source at Lawrence Berkeley National Laboratory and the Advanced Photon Source at Argonne National Laboratory and the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory.
National Laboratory. Third-generation light sources rely on storage rings where electrons traveling at nearly the speed of light are forced into a circular path by magnets. When the electrons pass through a magnetic structure called an undulator, they emit soft x rays that shine down beamlines to experimental stations.

The LCLS, in contrast, will use a linear accelerator rather than a circular one. It will also be home to the first x-ray free-electron laser, made possible by recent progress in undulator technology and in forming high-brightness, short-duration electron bunches in accelerators. The light from the LCLS will come in wavelengths smaller than the size of an atom. These hard x rays can be superior to longer-wavelength soft x rays for studying matter. The laser light will be fully coherent across the beam and 10 billion times brighter than the x-ray beams produced at the Advanced Light Source and its third-generation cousins. (Brightness is a measure of photon density, as shown in the figure on p. 23). The pulses will also be 100 times shorter than those of today’s machines.

The Key to Success

The LCLS will be built around the portion of the Stanford Linear Accelerator that is not being used by the B Factory. (See S&TR, “The B Factory and the Big Bang,” January/February 1997, pp. 4–13.)

Its first major component is the photoinjector, which produces tiny bunches of electrons traveling at almost the speed of light. Next is a 1,000-meter-long linear accelerator that pushes the electrons’ energies up to 14 gigaelectronvolts. Compressors along the accelerator path reduce the length of each bunch by a factor of 30 to increase their peak current. Then the electrons enter an undulator, a vacuum chamber just 5 millimeters across and about 125 meters long that is lined with 7,000 magnets arranged in alternating poles. In this narrow channel, the magnetic fields push and pull on the electron bunches, causing them to emit x rays that in turn force the electrons into even tinier microbunches that release x-ray photons in a bright, coherent beam. Optical devices beyond the undulator manipulate the direction, size, energy, and duration of the x-ray beam and carry it to whatever experiment is under way.

Key to making this machine work is the low emittance of the electron beam injected into the accelerator. Emittance is a function of the diameter and divergence of a beam. A small beam with a wide spread has been easy to achieve, but a small beam with narrow spread has typically been difficult to produce. New photoinjector technology can produce a narrow, bright beam of electrons with emittance several times lower than previously achieved.

When the accelerated beam enters the undulator, interaction with the magnetic fields there causes x rays to appear. As the electron bunches move down the undulator,
for the LCLS a real challenge. We also are designing optical systems to accommodate a variety of experiments. Some require submicrometer focus at very high intensity, others require only coherence, and still others require illuminating large areas at much lower light levels.”

A critical element in the optical system that Livermore scientists are working on is the absorption cell, which intercepts the beam after it leaves the undulator. The cell attenuates the beam’s power to levels manageable with conventional optics and provides a transition to power densities that match the needs of the various experiments. The cell can also completely remove the free-electron laser light for experiments that use only the spontaneous radiation. Both the spontaneous and coherent x radiation pass through an ultrahigh-vacuum system to the experimental areas, which may ultimately be as much as a kilometer away. Shielding will protect personnel and experiments from bremsstrahlung, the gamma radiation that results from high-energy electrons interacting with matter.

This work is opening new territory. Virtually no information exists now on the interaction of extremely high levels of hard x rays with matter. If the Department of Energy approves construction of the LCLS, the beginning of testing and experimentation in 2004 will herald a brave new world in physics.

—Katie Walter

Key Words: free-electron laser, Linac Coherent Light Source (LCLS), linear accelerator, Stanford Linear Accelerator Center.

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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

<table>
<thead>
<tr>
<th>Patent issued to</th>
<th>Patent title, number, and date of issue</th>
<th>Summary of disclosure</th>
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<tr>
<td>Howard Nathel</td>
<td>Multiple-Wavelength Spectroscopic Quantitation of Light-Absorbing Species in Scattering Media U.S. Patent 6,015,969 January 18, 2000</td>
<td>An oxygen concentration measurement system for blood hemoglobin comprising a multiple-wavelength, low-coherence optical light source that is coupled by single-mode fibers through a splitter and combiner and focused on both a target tissue sample and a reference mirror. Reflections from both the reference mirror and from the depths of the target tissue sample are carried back and mixed to produce interference fringes in the splitter and combiner. The distance traversed by both reflections is the same. The tissue sample reflections must emanate from a depth sufficient to provide light attenuation information dependent on the oxygen in the tissue’s blood hemoglobin. Two wavelengths of light are used to obtain concentrations. The method can be used to measure total hemoglobin concentration or total blood volume in tissue. In conjunction with oxygen saturation measurements from pulse oximetry, it can be used to absolutely quantify oxyhemoglobin in tissue. The apparatus and method provide a general means for absolute quantitation of an absorber dispersed in a highly scattering medium.</td>
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<tr>
<td>Harry E. Cartland</td>
<td>Method for Forming a Bladder for Fluid Storage Vessels U.S. Patent 6,017,600 January 25, 2000</td>
<td>A lightweight, low-permeability liner for graphite–epoxy compressed-gas storage vessels. The liner is composed of polymers that may or may not be coated with a thin layer of a low-permeability material such as silver, gold, or aluminum. It is deposited on a thin polymeric layer of substrate and formed into a closed bladder using torispherical or near-torispherical endcaps, with or without bosses therein. A high-strength-to-weight material, such as a graphite–epoxy shell, is formed about the torisphere to withstand the storage pressure forces. The polymeric substrate may be laminated on one or both sides with additional layers of polymeric film. The liner may be formed to a desired configuration using a dissolvable mandrel or by inflation techniques, and the edges of the film sealed by heat sealing. The liner may be used in almost any type of gas storage system and is particularly applicable for hydrogen gas mixtures, oxygen used for vehicles, fuel cells or regenerative fuel cell applications, high-altitude solar-powered aircraft, hybrid energy-storage propulsion systems, lunar–Mars space applications, and other applications requiring high cycle life.</td>
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<td>Billy W. Colston, Jr.</td>
<td>Cone Penetrometer Fiber-Optic Raman Spectroscopy Probe Assembly U.S. Patent 6,018,389 January 25, 2000</td>
<td>A chemically and mechanically robust optical Raman spectroscopy probe assembly that can be incorporated in a cone penetrometer (CPT) for subsurface deployment. This assembly consists of an optical Raman probe and a penetrometer-compatible optical probe housing. The probe is intended for in situ chemical analysis of chemical constituents in the surrounding environment. The probe is optically linked by fiber optics to the light source and the detection system at the surface. A built-in broadband light source provides a strobe method for direct measurement of sample optical density. A mechanically stable sapphire window is sealed directly in the sidewall of the housing using a metallic, chemically resistant hermetic seal design. This window permits transmission of the interrogation light beam and the resultant signal. The spectroscopy probe assembly is capable of accepting Raman, laser-induced fluorescence, reflectance, and other optical probes with collimated output for CPT deployment.</td>
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<tr>
<td>Matthew J. Everett</td>
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<td>Jeffrey N. Roe</td>
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<td>Fred Mitlitsky</td>
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<td>Blake Myers</td>
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<td>Frank Magnotta</td>
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<td>Kevin R. Kyle</td>
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<tr>
<td>Steven B. Brown</td>
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Summary of disclosure

Low-work-function, stable compound clusters are generated by coevaporation of a solid semiconductor (silicon) and alkali metal (cesium) elements in an oxygen environment. The compound clusters are easily patterned during deposition on substrate surfaces using a conventional photoresist technique. The cluster size distribution is narrow, with a peak range of angstroms to nanometers, depending on the oxygen pressure and the silicon source temperature. Tests have shown that when deposited on a carbon substrate, compound clusters contain the desired low-work-function property and are stable up to 600°C. When the plate containing the patterned cluster is used as a cathode baseplate and a faceplate covered with phosphor is used as an anode, a positive bias can be applied to the faceplate to easily extract electrons and obtain illumination.

A catheter-based device for generating ultrasound excitation in biological tissue. Pulsed laser light is guided through an optical fiber to provide the energy for producing the acoustic vibrations. The optical energy is deposited in a water-based absorbing fluid (such as saline, a thrombolytic agent, blood, or a thrombus) and generates an acoustic impulse in the fluid through thermoelastic and/or thermodynamic mechanisms. By pulsing the laser at a repetition rate varying from 10 hertz to 100 kilohertz, an ultrasonic radiation field can be established locally in the medium. This method of producing ultrasonic vibrations can be used in vivo for the treatment of stroke-related conditions in humans, particularly for dissolving thrombuses or treating vasospasm. The catheter can also incorporate thrombolytic drug treatments as an adjunct therapy and can be operated with ultrasonic detection equipment for imaging and feedback control and with optical sensors for characterizing thrombus type and consistency.

A method for detecting and isolating a target sequence in a sample of nucleic acids. It uses a bifunctional probe capable of hybridizing to the target sequence. The probe includes a detectable marker and a complexing agent that can bind with a second complexing agent. A kit that uses this method for detecting a target sequence in a sample of nucleic acids is also provided.

The Evaluated Teletherapy Source Library is a system of hardware and software for maintaining a library of useful phase space descriptions (PSDs) of teletherapy sources used in radiation therapy for cancer treatment. The PSDs are designed to be used by PEREGRINE, the all-particle Monte Carlo dose-calculation system. The library also stores other information such as monitor unit factors for use with the PSDs, results of PEREGRINE calculations using the PSDs, clinical calibration measurements, and geometry descriptions sufficient for calculational purposes. The library can also be a repository for the Monte Carlo simulation history files from which the generic PSDs are derived.
Becky Failor, a division leader in the Hazards Control Department at Livermore, has received a Distinguished Alumni award from her undergraduate alma mater, Oakland University in Michigan.

Failor currently leads Environment, Safety, and Health Team 3. The Oakland University award cited Failor for her technical and professional accomplishments and for her work with the university over the years, including bringing university students to the Laboratory for summer internships and keeping the university apprised of DOE’s surplus equipment list.

The Joint Conflict and Tactical Simulation (JCATS) computer code developed by the Laboratory for combat simulation was honored recently by an award from the Defense Department’s Defense Modeling and Simulation Office. Developers Mike Uzelac, Hal Brand, Greg Bowers, and Tom Kelleher traveled to Virginia to receive the award. Faith Shimamoto led the development team, which is part of the Laboratory’s Proliferation Detection and Defense Systems Division led by Alan Spero.

First released in 1998, JCATS can simulate large-scale battles and small group operations in rural and urban areas. A second version with increased capabilities was released in October 1999. JCATS development in recent years has been sponsored by the Defense Department’s Joint Warfighting Center. Particularly effective in simulating conflicts in urban settings, the code has been used in training exercises such as the Urban Warrior Advanced Warfighting Experiment in the San Francisco Bay Area in March of 1999 and to support actual military operations in places such as Panama, the Persian Gulf, and Bosnia. (See S&TR, January/February 2000, pp. 4–11, for details about JCATS’s capabilities and deployment.)

JCATS is widely used throughout the government to address a variety of security concerns. Commenting on the effectiveness of the code, Chris Christenson of the Institute for Defense Analysis, a Defense Department contractor for studies and analysis, found “JCATS to be, hands-down, the model of choice for small unit urban operations. Nothing else comes close.”

A system that assays containers of radioactive waste safely, accurately, and nonintrusively has garnered a prestigious R&D 100 Award for Lawrence Livermore National Laboratory and its commercial partner, Bio-Imaging Research, Inc.

Developed by a team of engineers and physicists headed by Livermore’s Patrick Roberson and Harry Martz, the Waste Inspection Tomography for Non-Destructive Assay (WIT-NDA) system combines computed tomography and gamma-ray spectroscopy to accurately quantify all detectable gamma rays emitted from waste containers. The WIT-NDA is part of the Waste Inspection Tomography system, a product of Bio-Imaging Research (BIR). The BIR system provides nondestructive examination and assay of radioactive waste and has been on the market since August 1999.

“What makes this system unique is that, to use it, we don’t need to open the container, we don’t need to know what specific waste is inside, and we don’t have to calibrate the system to a specific waste,” explains Roberson.

Patents and Awards

(continued from p. 27)

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<tr>
<td>Russell Hudyma</td>
<td>High Numerical Aperture Ring Field</td>
<td>An all-reflective optical system for a projection photolithography</td>
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<td>Projection System for Extreme</td>
<td>camera, including a source of extreme ultraviolet radiation, a wafer, and</td>
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<td>Ultraviolet Lithography</td>
<td>a mask to be imaged on the wafer. The optical system is composed of a</td>
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<td>U.S. Patent 6,033,079 March 7, 2000</td>
<td>first concave mirror, a second mirror, a third convex mirror, a fourth</td>
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<td>concave mirror, a fifth convex mirror, and a sixth concave mirror. The</td>
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<td>system is configured so that five of the six mirrors receive a chief ray at</td>
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<td>an incidence angle less than substantially 12 degrees, and each of the six</td>
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<td>mirrors receives a chief ray at an incidence angle of less than</td>
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<td>substantially 15 degrees. Four of the six reflecting surfaces have an</td>
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<td>aspheric departure of less than substantially 14 micrometers. Each of the</td>
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<td>six reflecting surfaces have an aspheric departure of less than 16 micrometers.</td>
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Awards

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Lawrence Livermore National Laboratory
Preventing Nuclear Proliferation: The Post-Cold War Challenge

At nuclear materials storage facilities, weapons laboratories, remote customs sites, and airports and seaports across Russia and the other newly independent states of the former Soviet Union, Livermore employees are helping to make nuclear materials and weapons know-how more secure. Livermore’s Russian programs are concentrated in the Nonproliferation, Arms Control, and International Security Directorate, specifically its Proliferation Prevention and Arms Control program. Russian programs have two thrusts. The first is enhancing the protection, control, and accounting of weapons-usable nuclear materials. The second is helping to find nonweapons job opportunities for the former Soviet weapons scientists. The overall effort draws upon a wide range of Laboratory strengths, including nuclear materials characterization, radiation detection, forensic science, computer simulation, site security, and weapons physics, design, testing, and dismantlement.

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“Shocking” Gas-Gun Experiments

Livermore’s gas guns create shock waves that may be millions of times atmospheric pressure at the surface of Earth. Experiments with powerful shock waves were originally designed to help researchers understand how materials in nuclear and conventional weapons respond during detonation. Now, under the Department of Energy’s Stockpile Stewardship Program, researchers must be able to not only model but also predict the behavior and performance of stockpiled weapons. This mission requires a basic understanding of the behavior of a variety of materials. Of particular interest is developing the capability to accurately measure temperature in materials at extremely high pressures, which requires new experimental capabilities and approaches. Other experiments are duplicating, for a brief moment, the extreme pressures inside Earth and the giant planets of our solar system. Over the course of this work, Livermore has produced some of the first quantum molecular dynamic models of materials under shock conditions. In 2001, the Joint Actinide Shock Physics Experimental Research (JASPER) facility will come on line at the Nevada Test Site, allowing scientists to study uranium, plutonium, and other actinide materials under shock conditions.

Contact:
Neil Holmes (925) 422-7213 (holmes4@llnl.gov).

Also in October

• An assay system that can accurately identify the contents of sealed radioactive waste drums has won an R&D 100 Award.

• Researchers discovered a quartzlike carbon dioxide when they conducted experiments to obtain data for modeling high-explosive detonations.

• Sol-gel chemistry is being researched as a new method for making energetic materials such as explosives.