Science & Technology REVIEW

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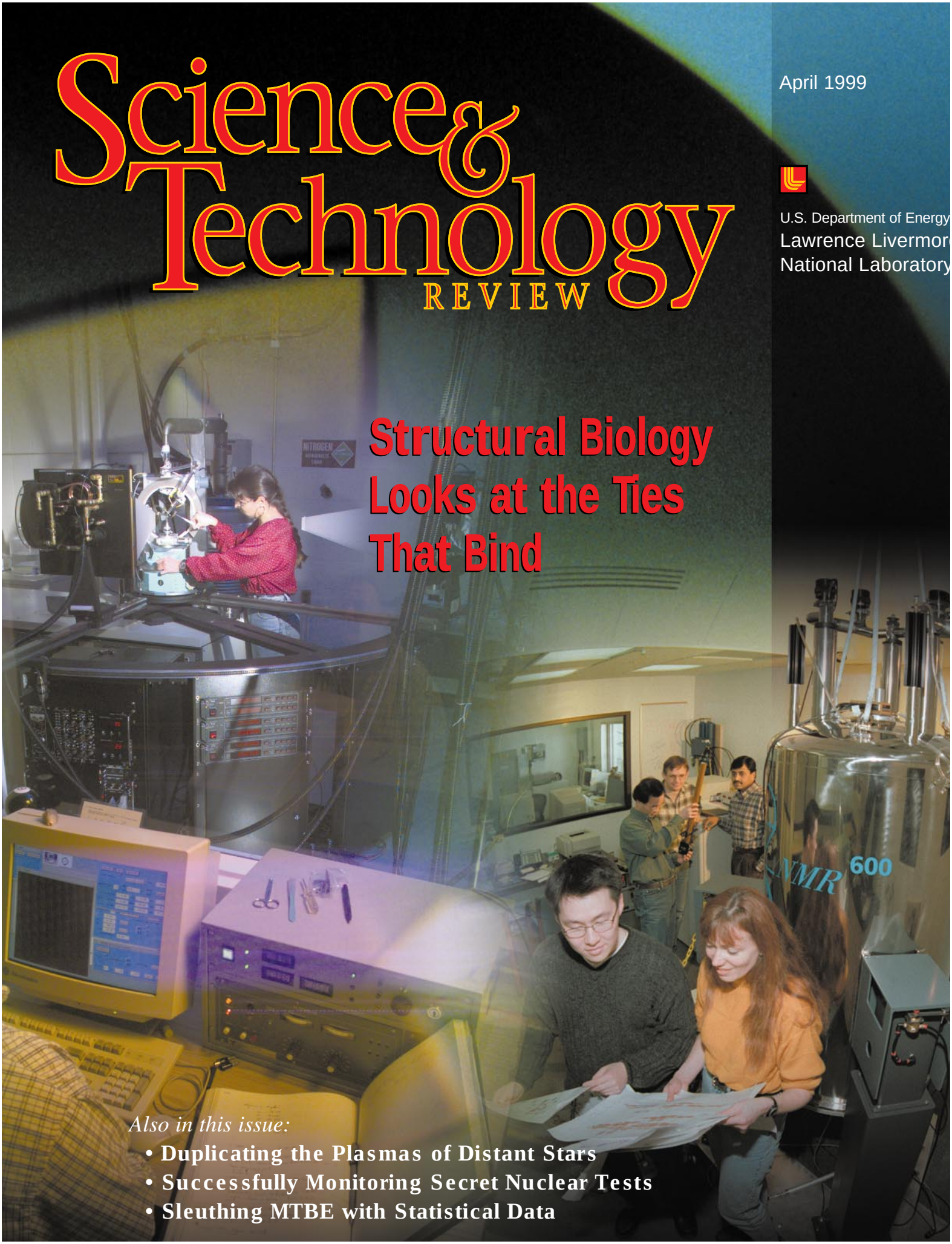

Structural Biology Looks at the Ties That Bind

Also in this issue:

- **Duplicating the Plasmas of Distant Stars**
- **Successfully Monitoring Secret Nuclear Tests**
- **Sleuthing MTBE with Statistical Data**

About the Cover

As an outgrowth of its work on the Human Genome Project, Livermore's Biology and Biotechnology Research Program Directorate is developing a structural biology capability. This capability promises rich rewards for discovering the mechanistic causes and cure of diseases. The two methods for determining the structure of individual biomolecules are x-ray crystallography and nuclear magnetic resonance spectroscopy, pictured respectively at the left and right on this month's cover. The story of Livermore's growing capabilities and accomplishments in the field of structural biology begins on p. 4.

Cover design: Ray Marazzi

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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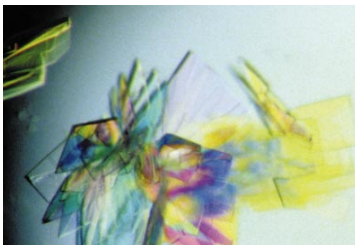

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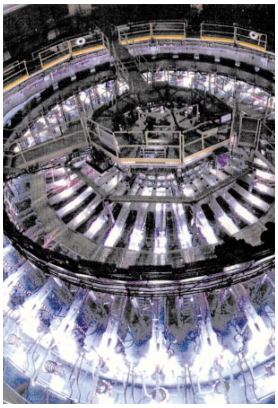

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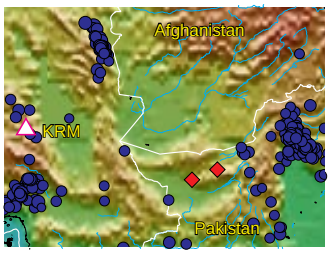

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NIF laser glass-making facility opens

The National Ignition Facility (NIF) reached another major milestone in late January, but it was not achieved at the Lawrence Livermore construction site. It came with the opening of Hoya Corporation's laser glass-manufacturing facility in Fremont, California. Constructed at a cost of $12 million, the 32,000-square-foot facility will provide neodymium-doped laser amplification glass for NIF and for the French government's Laser Megajoule (LMJ) project currently under construction in Bordeaux, France.

The Hoya facility will manufacture the some 3,000 ultrahigh-quality glass slabs required by NIF. Produced at the rate of about 10 per day, each 790- by 440-millimeter, violet-hued slab will weigh more than 100 pounds and be capable of amplifying laser energy by 14 percent.

According to Mike Campbell, Associate Director of Laser Programs at Livermore, these glass slabs are "the heart of the laser," its "single most essential component."

NIF will be the world's largest optical instrument with 192 laser beams, each 40 centimeters in diameter, focused on a tiny fusion target. NIF experiments are designed to produce fusion ignition in the laboratory for the first time in history, creating temperatures and pressures similar to those found in the sun and some stars and in exploding nuclear weapons. These experiments will help the U.S. ensure the safety and reliability of its nuclear weapons without nuclear tests. They will also demonstrate the scientific feasibility of fusion energy and contribute to scientific understanding in astrophysics and other basic sciences.

The Hoya facility's 45 employees, most from the Fremont area, will produce more than $50 million of laser glass over the next 10 years for the NIF and LMJ projects.

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Lab helps capture first gamma burst images

Using a robotic camera, designed in part at Lawrence Livermore, astronomers recently captured images for the first time of visible light from a gamma-ray burst, a mysterious deep-space eruption more powerful than the energy of 10 million billion stars. These bursts occur with no warning and last so briefly that they previously could not be captured on film.

The burst that occurred in the early morning of January 23 was, however, a different story. The gamma-ray-burst detectors of the Burst and Transient Source Experiment on board NASA's orbiting Compton Gamma Ray Observatory detected the beginning of a bright and relatively long-lived gamma-ray burst, which lasted a total of 110 seconds. Onboard computers determined its rough location and radioed the position to the Gamma Ray Burst Coordinates Network (GCN) based at Goddard Space Flight Center in Maryland, which immediately forwarded it to observatories throughout the world.

Just 22 seconds later, the Robotic Optical Transient Search Experiment (ROTSE) in Los Alamos, New Mexico, took images of the patch of sky where the burst was reported.

The data acquisition system used to process the information from the ROTSE collaboration's telescope camera was designed by ROTSE participants Stuart Marshall, an astrophysicist at Livermore's Institute of Geophysics and Planetary Physics, and Robert Kehoe of the University of Michigan.

Although the camera's response time was longer than the normal 10 seconds, Marshall was delighted with the results. "I never expected we'd see anything this bright," he marveled.

Astronomers are not certain what produces gamma-ray bursts, but possible causes include the merger of two neutron stars, two black holes, or a neutron star and a black hole or the explosion of a hypernova, believed to be a type of supernova or exploding star.

"This is the Holy Grail for the [GCN]," said Scott Barthelmy, the astronomer who developed and runs the network at Goddard. "Optical telescopes had seen the afterglow of a burst, but never the burst itself. This observation will help us understand the physical processes behind the bursting."

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Lab–Russian collaboration creates new element

Nuclear physicists from Lawrence Livermore working in collaboration with a team of Russian scientists from the Joint Institute for Nuclear Research in Dubna, Russia, have announced the creation of a new ultraheavy element—element 114. Using isotopes provided by Livermore, the Russian–U.S. team bombarded a plutonium-244 target with calcium-48 atoms to create the new element.

The excitement generated by the discovery stems largely from the stability of the new element, the nucleus of which is believed to consist of 114 protons and 184 neutrons. Unlike other manufactured heavy elements, element 114 is relatively long-lived, surviving for 30 seconds—as opposed to mere microseconds—before decaying. And some of element 114's decay particles lived for an unheard-of 16.5 minutes.

The significance of element 114's long life is the support it gives to the theory that the more densely packed the nucleus of heavy elements, the more stable they are. This stability should make it easier for scientists to study the chemical properties of these manufactured elements to see if they match those of more familiar, naturally occurring elements.

The Livermore team, which includes John Wild, Ronald Laugheed, Kenton Moody, Nancy Stoyer, and Mark Stoyer, is working with their Russian collaborators, led by Yuri Oganessian and Vladimir Utyonkov, to confirm element 114's creation and prepare a formal report on their experimental results.

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Is There Life after the Human Genome Project?

WE are in the midst of revolution in the biological sciences. While the 20th century has been termed the century of physics, heavily dominated by the advent and rise of computers and telecommunications, the 21st century may well be the century of biology and medicine. The foundation for this change is the science of genomics, which began in the mid-1980s and was accelerated by the huge success of the Human Genome Project.

At that time, some claimed that sequencing the human genome was a dream—that biotechnologies to support such an effort did not exist or were not sufficiently advanced. Times have changed, and the technologies are available. The pace of the human genome effort is accelerating. The original plan was to complete the sequence of the human genome by 2005. In the last year, that target completion date first changed to 2003 and is now 2001. Moreover, other species are beginning to be sequenced, including the mouse, plants, and microbes. Knowledge of these other species provides insight into human disease, crop improvement, bioremediation, and pathogen diagnostics.

The Human Genome Project primed the pump for this bioscience revolution. Today, bioscientists' visions are not focused on whether they can sequence the genome, but how fast they can do it, and how we as a species can capitalize on the information for the diagnosis, prevention, and treatment of disease. In other terms, we need to functionalize the sequence data. The successes of the genome project have generated a set of new bioscience visions with semantic descriptors such as functional genomics, proteomics, and structural genomics.

It must be remembered that the DNA sequence being determined is really a code. The code is read by complex molecular machinery in the cells of our body. The products of genes that are encoded in the DNA sequence are proteins. Proteins, themselves, are the engines of our body. They are responsible for our body's metabolism; they play a role in structure at the cellular, tissue, organ, and whole-body level; and they can protect us from, or even cause, some diseases. Understanding how proteins function is essential to understanding how biological systems work. Protein function can be investigated several ways—by biochemical methods, genetic approaches, or structural and computational analysis. All approaches are complementary and generally necessary to characterize the biological function of a single protein.

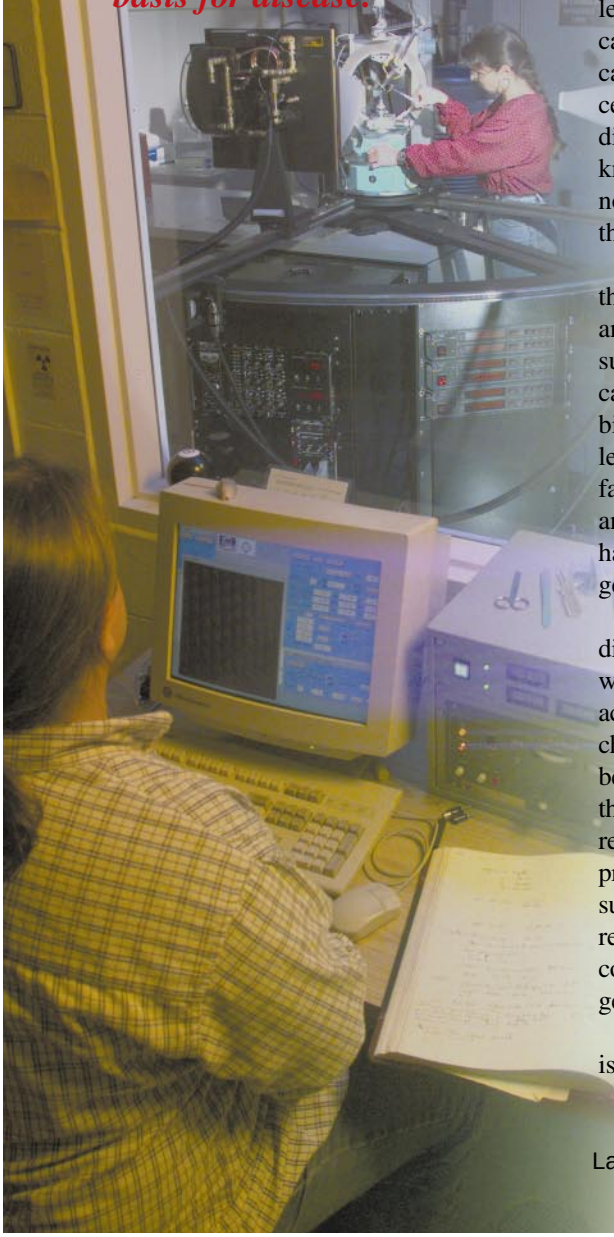
The article beginning on p. 4 describes one of Livermore's approaches to and accomplishments in protein structure analysis, that is, using crystallographic and diffractometry techniques to determine the three-dimensional structure of proteins at the atomic level. Once a three-dimensional structure is determined, computational methods can be used to model function and potentially to design drugs or inhibitors that interact with the protein to either enhance or modify its function. The Department of Energy and its national laboratories are bringing unique, multidisciplinary physical, engineering, and computational resources to bear on these efforts.

While the world is still dealing with unraveling the structure and function of proteins one at a time, each of which might take years of research, it is clear that this one-by-one approach is not sufficient to deal with the expected 100,000 or so proteins in the human genome. The challenge to the scientists is to find ways to multiplex protein functional analysis, just as DNA sequencing has been multiplexed. Then myriad proteins can be researched in parallel. So the answer to the question "Is there life after the human genome project?" is not only yes, but a resounding yes.

■ Tony Carrano is Associate Director, Biology and Biotechnology Program.

Structural Biology Looks at the Ties That Bind

Experts in biochemistry, genetics, physical chemistry, and computational modeling are working together to understand the mechanistic basis for disease.



NOT so many years ago, no one knew how cancer and many other diseases occurred. Over time, scientists learned that smoking can cause lung cancer, overexposure to sunlight can cause skin cancer, eating too much of certain types of foods may lead to heart disease, and so on. But even when they knew what caused disease, they still did not know how the change took effect in the body.

It has only been in the last 10 years that researchers at Lawrence Livermore and elsewhere have discerned that subtle, permanent alterations to DNA cause changes in proteins and other biological molecules, sometimes leading to cancer and other diseases. In fact, the very act of living—of eating and breathing—can expose DNA to harmful agents that result in damage to genes and ultimately to proteins.

Humans produce as many as 100,000 different protein molecules, each of which is a long, folded chain of amino acids. Proteins activate essential chemical reactions, carry messages between cells, fight infections, control the growth and differentiation of cells, regulate the activity of genes, and provide structural and mechanical support. They also provide the motion required in cell division, muscle contraction, and cell propulsion, and they generate and transmit nerve impulses.

The link between proteins and DNA is strong: the amino-acid sequence of each protein is specified by a unique DNA base sequence in the coding region of a single gene. Mutations in the DNA sequence may be caused by small molecules, called chemical mutagens, that appear everywhere in our environment and bind to the DNA bases. Changes resulting from mutations in the DNA base sequence of a gene can produce proteins that function abnormally and result in disease.

Scientists have known that changes in genes resulted in the production of proteins that did not function properly. But they had to know the specific structure of these proteins before they could make the technical advances needed to detect human disease and cancer successfully and design new drugs and treatment therapies. While amino-acid sequences of more than 20,000 proteins have been deposited in data banks that are available to medical researchers, complete three-dimensional structures have been identified for less than 5 percent of them.

The Need for a Closer Look

The impetus for Lawrence Livermore's Biology and Biotechnology Research Program (BBRP) Directorate to establish a structural biology capability was its work on the human genome, especially DNA repair processes and DNA damage.

Proteins known as DNA repair enzymes constantly scan the genome for

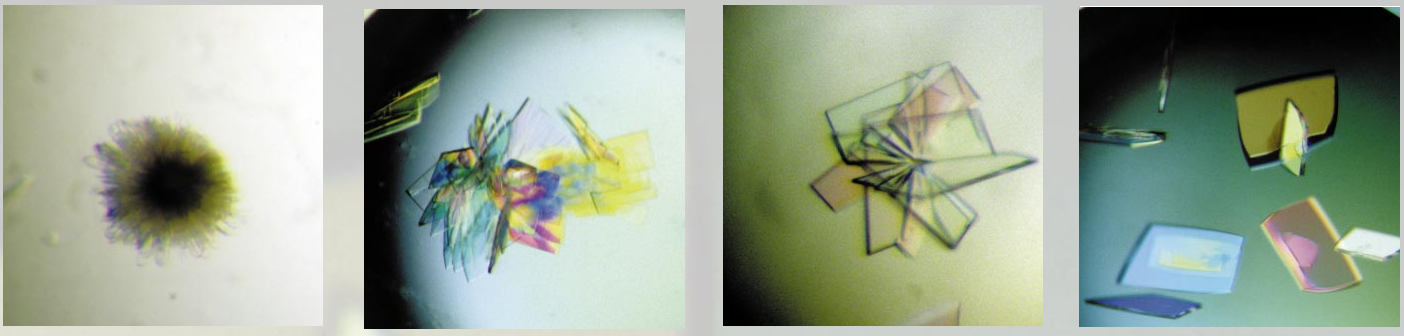


Figure 1. This series of images shows the gradual improvement in crystal quality as crystals of a benign portion of the tetanus toxin are grown under varying crystallization conditions. In the photograph on the opposite page, Mark Knapp and Sabine Ringhoffer collect data from a crystal like those on the far right above for use in Livermore's structural biology research efforts.

damage, remove the defective region of the molecule, and resynthesize the missing segments of DNA. But sometimes, the repair process stops working, or damage may be too great for the repair process to overcome. Unrepaired DNA damage eventually produces mutations that may trigger the growth of malignant tumors. Livermore scientists under Larry Thompson had been researching this repair process for 20 years. At the same time, Andy Wyrobek, Jim Felton, and others were studying DNA damage itself, in sperm and from food mutagens.[1] They had learned, for instance, that eating certain foods may cause mutations in DNA, changes that could later give rise to cancers.

Biochemist Rod Balhorn, who has spearheaded much of the structural biology work at Livermore, says, "After almost 15 years of research, both groups knew that they needed more information." They required a better look at the proteins responsible for DNA repair to figure out precisely how they recognize, bind to, and replace damaged segments of the DNA molecule.

Thus, in the mid-1990s, with funding from the Department of Energy's Laboratory Directed Research and Development Program, BBRP began developing a structural biology capability. They brought in experts in x-ray crystallography and nuclear magnetic resonance spectroscopy, which are the only methods for obtaining high-resolution, three-dimensional information about individual molecules. Bernhard Rupp set up an x-ray crystallography laboratory, while Monique Cosman established a laboratory for nuclear magnetic resonance spectroscopy. Their teams began providing experimental data on protein structures, some of which are used by another new group under Mike Colvin that performs molecular modeling. Yet another new group led by Krzysztof Fidelis specializes in predicting the structure of proteins from information about the amino-acid sequences that are encoded in DNA.

Today, under the leadership of Jim Felton, these groups support a number of projects at BBRP. Some of them are a continuation of previous work, including identifying how chemical mutagens damage and perturb the structure and function of DNA as well as characterizing the structure of proteins that recognize and repair DNA damage. A newer project with the Gladstone Institute of San Francisco is identifying how mutations in proteins involved in lipid (fat) metabolism and plaque formations in the brain relate to cardiovascular and neurogenerative diseases, especially Alzheimer's disease. The results of these and other studies are helping scientists understand why particular individuals are susceptible to cancer and certain diseases and how DNA repair proteins interact with and repair damaged DNA.

Another project is part of the Laboratory's work to reduce the threat of biological weapons. Scientists in BBRP are working to obtain high-resolution structure and function information for tetanus and botulinum toxins, which belong to the same family of bacterial toxins. Structural information is playing an important role in the development of antidotes, detection systems, and other countermeasures for minimizing the threat of exposure to biological warfare agents.

Examining in 3-D

X-ray crystallography and nuclear magnetic resonance spectroscopy operate in very different ways, but both can determine the locations of the individual atoms that make up a biomolecule.

X-ray crystallography exploits the fact that x rays are scattered by the electron cloud around each atom in a crystallized molecule. Based on the diffraction pattern obtained from the assembly of molecules or atoms in the crystal, the electron density of the crystal's individual components can be reconstructed, resulting in a very accurate model of the crystallized protein's molecular structure.

Rock crystals or crystals of salt or sugar are hard objects because of their regular atomic structure. Protein molecules have irregular, folded shapes and produce fragile, soft crystals that resemble tiny jelly cubes (Figure 1).

Their fragility makes them sensitive to environmental variations and to radiation, including x rays. Flash-cooling to almost the temperature of liquid nitrogen (–196°C) eliminates their sensitivity to radiation.

Protein x-ray crystallography of large molecules has been around for 50 years, but advances are being made all the time to achieve higher and higher resolutions (Figure 2). Because the highest resolution data come from the highest power x-ray sources, Rupp and his team have used such DOE accelerators as the Advanced Light Source at Lawrence Berkeley National Laboratory to achieve the highest possible resolutions. Work is also under way at Livermore to develop advanced computational methods for processing the data collected by x-ray diffraction.

Nuclear magnetic resonance (NMR) spectroscopy involves the interaction of the magnetic "moment" of each atom's nucleus with an external magnetic field. When a molecule is placed in a magnetic field, the field will align the spins of the nuclei either parallel or antiparallel to the field, with each spin having a discrete energy level. Transitions can be induced between high- and low-energy states by the application of a radio-frequency perturbation, and a resonance signal for each spin can be detected. Because the chemical environment significantly modifies the properties of a nucleus, the position of an NMR signal can provide information about the structure and dynamics of a molecule.

Series of radio-frequency pulses and delays are designed to manipulate the nuclear spins and their interactions with neighboring spins. In this way, NMR spectra are generated containing information about the distance and angles between nuclei that are separated in space and/or through chemical bonds (Figure 3).

The two methods complement one another, providing different kinds of information to researchers. X-ray crystallography works with solid materials and results in very fine detail of molecules that are frozen in time. NMR spectroscopy, on the other hand, uses molecules in solution, which means that they are in motion. Spectral data is averaged to give information on the movement of atoms in the molecules in relation to one another.

Both x-ray crystallography and NMR require considerable time to reduce experimental data to usable structural information. After successful growth of a crystal, x-ray diffraction patterns can often be obtained in less than a week, but the actual definition of molecular structure from these data may require several years of effort. Similarly, the NMR spectra needed to identify the structure of a small protein can be obtained in a few weeks, but many months may be required to analyze and assign the data before the structure can be calculated.

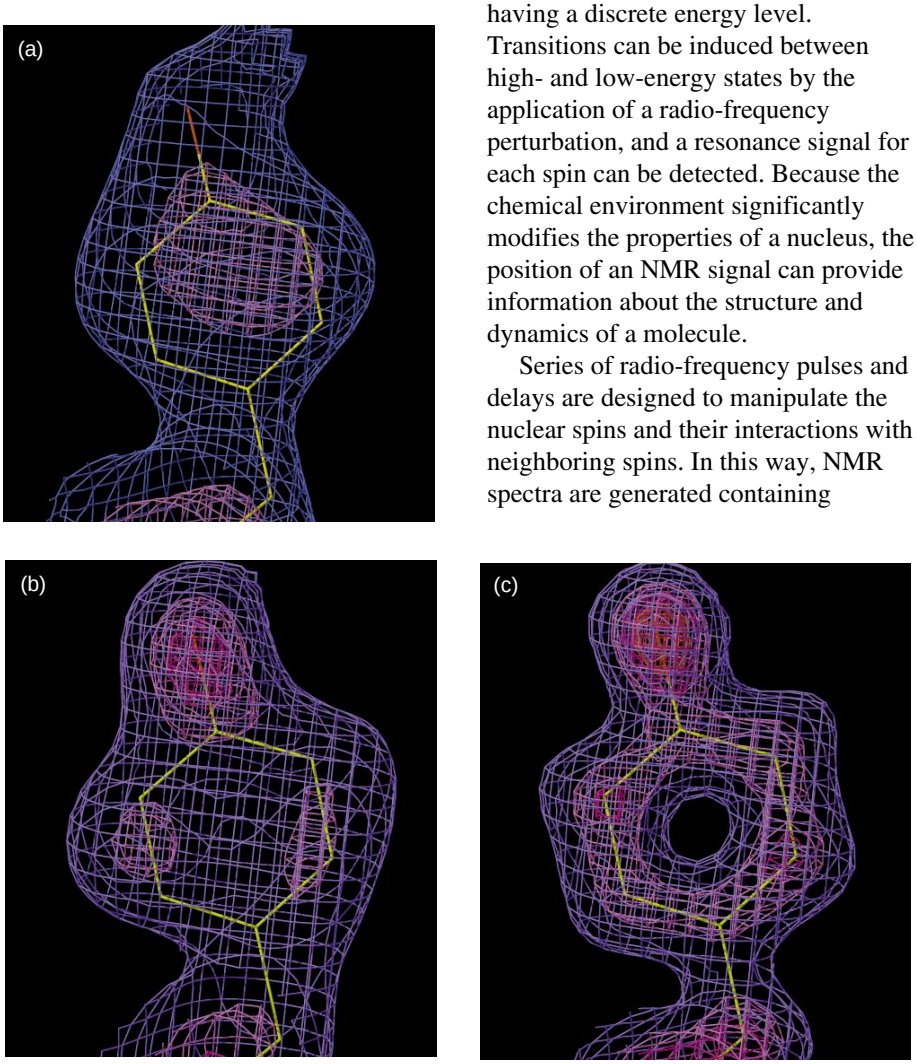


Figure 2. Images of the electron density of a molecule at three resolutions—(a) 3 angstroms, (b) 2 angstroms, and (c) 1.1 angstroms. The higher the resolution, the more accurate the model of the molecule.

Predicting Structure

Because of the time requirements for determining protein structure with x-ray crystallography and NMR, computational modeling and simulation methods have been used for many years to augment experimental efforts. Because these techniques are so computationally intensive, they have benefited enormously from the recent dramatic increase in computer performance—in particular, the development of massively parallel computers—and concomitant software developments. Using these computer advances, scientists can today model much larger molecular systems than before.

Mike Colvin's computational biochemistry effort makes use of two primary modeling methods: quantum

chemistry (based on fundamental quantum mechanics) and empirically based molecular dynamics models.

Modeling with quantum chemistry allows the calculation of extremely accurate chemical structures and reaction energies. Until recently, this method was limited to small, simple molecules, but compounds with up to several dozen atoms can now be studied on inexpensive personal computers, while massively parallel computers are used for compounds with up to several hundred atoms. Molecular dynamics simulations involve much larger molecules, typically with tens of thousands of atoms. The two methods work together to constantly refine the model. Quantum chemical calculations are used to generate force fields and atomic charges for molecular dynamics simulations, which in turn are used to determine local structural constraints that are used in accurate quantum chemical-energy calculations.

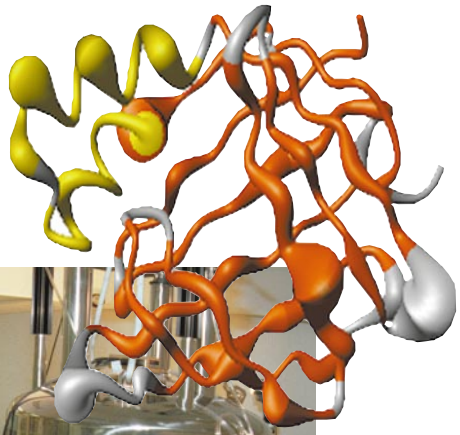
Together, molecular dynamics and quantum chemistry are being used by Colvin's group to study a number of biological problems, including the mechanisms of enzymes that repair damaged DNA as well as drugs that bind to the DNA of cancer cells. The molecular dynamics simulations are used to determine the large-scale changes in the DNA helix due to damage or drug binding. Then, quantum chemical simulations are applied to smaller segments of the modified DNA to give more accurate energies and structural properties (Figure 4).

Krzysztof Fidelis and his colleagues are taking an entirely different tack to predict protein structure. Their approach works with whole proteins, which can involve tens of thousands of atoms. Furthermore, the method uses the sequence of amino acids and its environment in the protein as a starting point.

Two predictive techniques—comparative modeling and fold recognition—operate on the proven assumption that similar amino-acid sequences will produce similar protein structures. With these methods, predicting the structure of an unknown protein would include a visit via computer to data banks containing information on known protein structures.

A third technique that Livermore has not yet used starts closer to ground zero: it combines sequence data with known physical and chemical properties of individual amino acids to predict the structure of the complete protein. Says Fidelis, "If scientists can predict even small structures with this method, it means they really know something about protein structure."

In 1994, Lawrence Livermore, together with researchers at the University of Maryland and Sandia National Laboratories, established an international organization for the prediction of protein structures. Today, Livermore is home to the Protein Structure Prediction Center, which acts as a clearing house for an ongoing



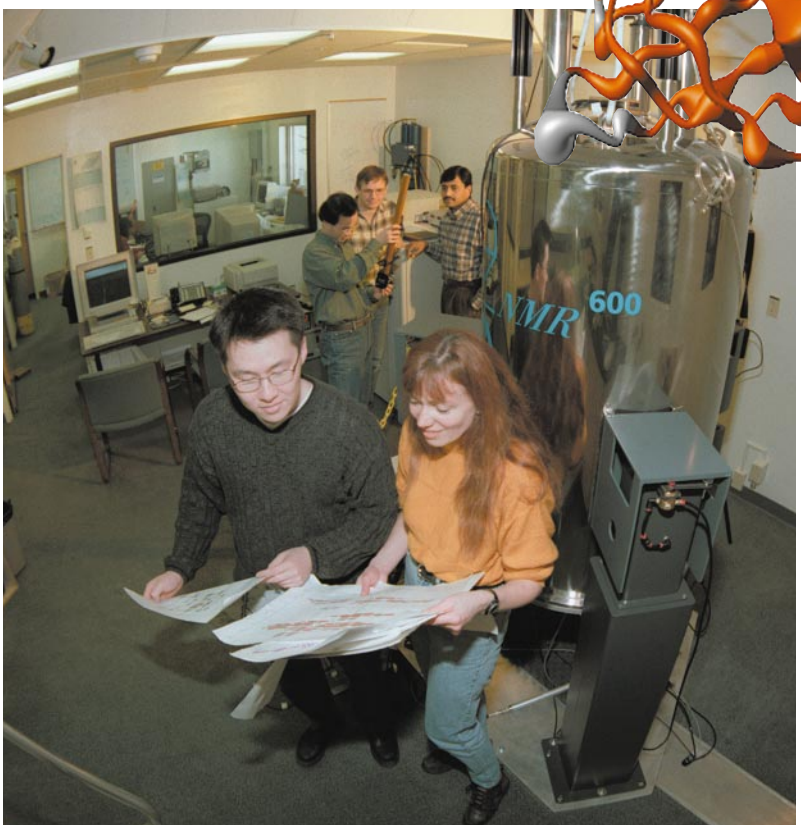


Figure 3. Monique Cosman at work with her team in Livermore's nuclear magnetic resonance (NMR) laboratory. Team members are Steve Chan (foreground) and (background, left to right) Kin Yan, Kevin Thornton, and Viswanathan Krishnan. (Inset) A solution-state, three-dimensional structure of a fatty acid binding protein as determined using NMR. The thickness of the lines provides information about the motions of the atoms in the molecule.

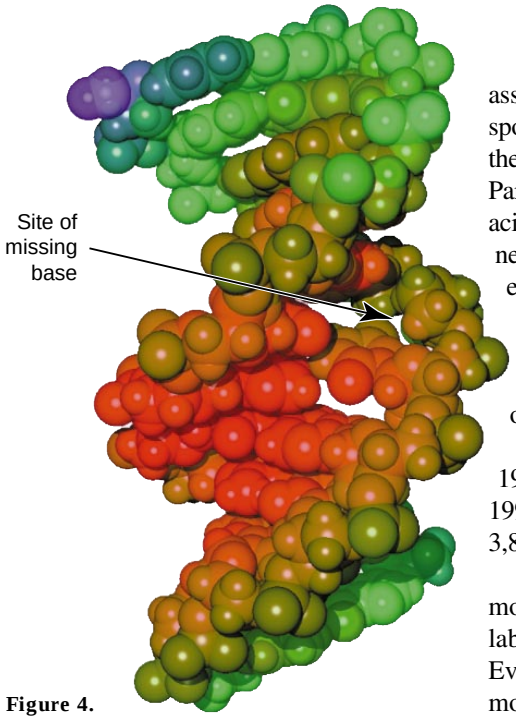


Figure 4.
Model of a DNA double helix with a base missing in the middle. This type of damage occurs by natural processes thousands of times each day in every cell in the body and must be repaired to maintain good health. Each atom in this simulation is colored according to the amount it moved during a molecular dynamics computer simulation (red moved least; blue moved most). The damage seems to affect the DNA flexibility and is thought to play a role in the repair of DNA.

assessment of prediction methods and sponsors a biennial conference to discuss the most successful methods. Participating researchers receive amino-acid sequence information for a set of new structures that have been determined either by x-ray crystallography or NMR spectroscopy but not yet released to public data banks. Later, predictions are compared to laboratory results, often with excellent results (Figure 5). This is clearly a growing effort. In 1994, there were 130 predictions; in 1996, 980 predictions; and in 1998, 3,800 predictions.

The strong dynamic between these modeling and predictive efforts and laboratory experimentation is evident. Even with the largest computers, modeling cannot stand entirely on its own. It needs validation from experimental results in an ongoing, iterative process that constantly refines modeling results and methods.

New Inhibitors for Toxins

A recent structural biology success story at Livermore involves the tetanus toxin, a member of a family of toxins that could be used by an aggressor or terrorists as biological warfare agents. BBRP's goal is to learn how to develop inhibitors for these toxins in case one of these bacteria is used in a biological attack.

Inhibitors are protective drugs that stop or slow the biological action of a toxin or other damaging molecule. Think of the protease inhibitors that patients with HIV receive. Inhibitors are weaker and easier to develop than antidotes, which reverse a toxin's damage after the fact. Inhibitors might be used if an exposure is anticipated, and they require constant dosing.

Tetanus is a paralytic disease caused by a neurotoxin produced by the anaerobic bacterium *Clostridium tetanii*. It is just one of a whole family of clostridial neurotoxins that are believed to have a similar cell invasion mechanism. All the deadly botulinum toxins belong to this family.

The tetanus toxin targets the membranes of the central and peripheral nervous systems to block the release of neurotransmitters, causing the nerve cells to fire constantly. The result is muscle rigidity—thus, the common name for tetanus, "lockjaw." An effective inhibitor for the tetanus toxin must stop the toxin from binding to cells in the nervous system.

Tetanus and other clostridium family toxins have two parts: the light chain, which contains the enzymatic portion of the toxin and is responsible for its toxic effects, and the heavy chain, which binds to the neuron and aids delivery of the light chain to the interior of the neuron. The heavy chain has two parts or domains. The binding domain binds to gangliosides, which are sugar-based recognition molecules on the nerve cell membrane. The translocation domain makes a pore in the cell through which the toxin may pass.

Considerable research at several institutions has established the propensity of the binding domain to bind to gangliosides. But what had not been determined was which part of it bound to the ganglioside.

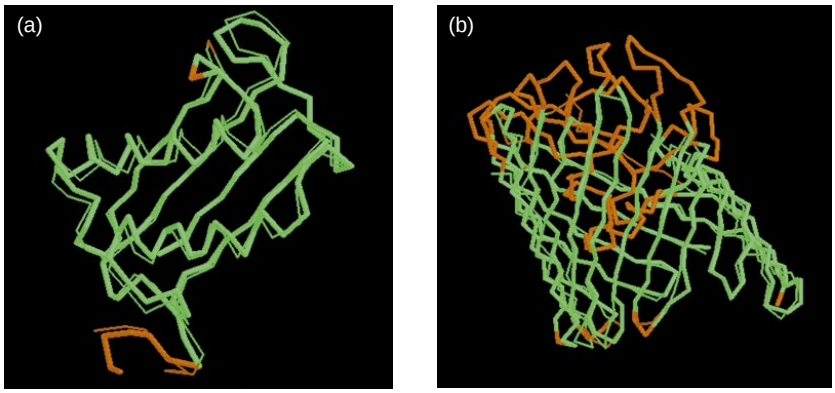


Figure 5. Comparison of the modeling prediction with the actual structure of two proteins, (a) human D-dopachrome tautomerase and (b) *C. aciodovorans* OMP32. The thick lines represent the structure as determined by x-ray crystallography, while the thin lines correspond to atoms in the prediction. Regions colored green are correctly predicted to 3.5 angstroms.

Knowing the precise site of binding and what the site looks like is important. For an inhibitor to be effective, it must bind at the same site, which means that its molecular structure must fit there as neatly as does the toxin's binding domain. If binding by the toxin can be blocked, penetration of the cell will be stopped.

A major accomplishment in 1998 was the high-resolution structure determination of the binding domain of the tetanus toxin by Livermore's x-ray crystallography group. (The three parts of the toxin can function separately, so it is possible to do this research without working with dangerous, intact toxins.)

With the high-resolution protein structure in hand, researchers on Colvin's computational biochemistry team collaborated with scientists at Sandia National Laboratories to computationally select compounds that might fit in the same binding site. They were able to quickly identify 30 compounds predicted to bind to the tetanus toxin protein from a database of 250,000 compounds (Figure 6).

Figure 6. High-resolution (1.56 angstroms) structure of the binding domain of tetanus toxin. This structure shows that this portion of the protein has two separate parts. One binds to sugars called gangliosides present on the surface of motor neurons. The function of the other is unknown.

Moving from those 30 possible compounds to an approved inhibitor drug will involve a long process that will likely take years. Rod Balhorn is currently testing the 30 compounds using mass spectrometry to see if they bind to the tetanus binding molecule. While the testing is incomplete, he and his colleagues have already discovered seven new molecules that will bind to the toxin. These compounds will be bound to the toxin, and the site of binding will be determined by x-ray diffraction or NMR spectroscopy. Armed with these data, a pharmaceutical company can then develop an inhibitor drug that is specific for this toxin.

The invasion mechanism of toxins might someday be put to another use entirely. The light chain, which carries the toxin, could be reengineered to remove the toxin portion of the molecule and add a drug. The formerly deadly protein could thus become a life-saving, drug-delivery vehicle. The drug might be designed to target specific cells, for example, cancer cells with anticancer drugs.

Experts Finding Solutions

With its strength in physical sciences and international recognition for work in genomics and DNA repair, Lawrence Livermore was ideally suited to develop capabilities in structural biology. Experts in biochemistry, genetics, physical chemistry, and computational modeling are working together to understand the mechanistic basis for disease. Molecular medicine is a new and rapidly evolving field and one in which Lawrence Livermore is beginning to play an important role.

—Katie Walter

Key Words: clostridium toxins, computational biochemistry, DNA repair, nuclear magnetic resonance spectroscopy, protein structure prediction, tetanus, x-ray crystallography.

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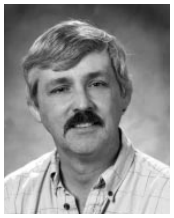
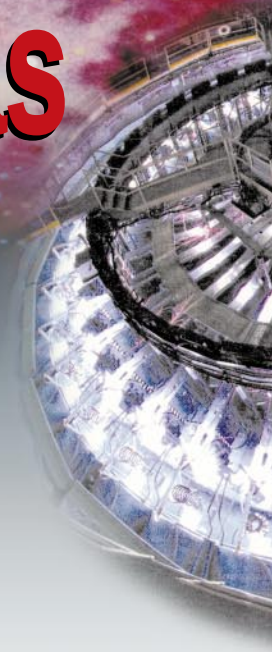
About the Scientist



ROD BALHORN is a senior biomedical scientist in Lawrence Livermore's Biology and Biotechnology Research Program (BBRP) Directorate. He joined the Laboratory in 1974 after receiving a B.S. in chemistry and a Ph.D. in biochemistry from the University of Iowa, where he was also a postdoctoral fellow. He was instrumental in initiating a structural biology capability at Livermore as a logical outgrowth of BBRP's human genome research into DNA damage and repair processes. He is the coauthor of numerous publications reporting advances in protein biochemistry, chromatin organization, and structural biology research and is currently working on the application of structural biology findings to the search for inhibitors of the deadly botulinum toxin.

Duplicating the Plasmas of Distant Stars



Groundbreaking Livermore experiments are strengthening our understanding of matter at extreme conditions. The results are aiding researchers in both astronomy and nuclear stockpile stewardship.

AT first glance, it might seem odd for weapons scientists to be looking to the stars for information and inspiration. However, the physical processes of stars have long been of interest to Lawrence Livermore researchers because the prime stellar energy mechanism, thermonuclear fusion, lies at the very heart of the Laboratory's national security mission.

For many years, Livermore researchers have played a major role in astrophysics by applying their expertise in high-energy-density physics and computer modeling of atomic processes. The astronomical community has benefited enormously from Livermore contributions, including the search for "dark matter" in the universe, laser guide star optics that sharpen terrestrial astronomical viewing, instruments to map the moon in unprecedented detail with the Clementine satellite, advanced x-ray spectrographs for U.S. and European spacecraft, and theoretical models of supernovae and other stars.

Livermore researchers are again breaking new ground, creating in the laboratory the same kinds of extremely hot plasmas (gases containing electrically charged particles) found in distant stars and comparing the results to models. The data from these experiments will help strengthen the theory of matter at extreme conditions. In turn, these models will help scientists gain a more complete understanding of the birth and evolution of stars, galaxies, and the universe itself.

Closer to home, the new experimental techniques, improved codes, and diagnostics developed for the tests are aiding stockpile stewardship, the Department of Energy's program to keep the nation's aging arsenal of nuclear weapons safe, secure, and reliable in the absence of underground nuclear testing. The expertise gained will also aid experiments on the National Ignition Facility (NIF), the giant laser now under construction at Livermore as a key stockpile stewardship facility.

"There's a tremendous amount of overlap between the kinds of physics involved in astrophysical systems and those in nuclear weapon systems," says Bill Goldstein, acting Associate Director of the Physics Directorate and leader of the Laboratory's effort to provide the most modern validated physics models for stockpile stewardship. Even when an astronomical process is not exactly duplicated by a nuclear weapon, studying the phenomenon is useful to ensuring that Livermore atomic models are versatile and valid in different environments, he says.

Many astrophysicists, Goldstein says, become weapon scientists because the fields involve similar physics. He also notes that the Accelerated Strategic Computing Initiative (ASCI), DOE's program to significantly advance computer simulations of nuclear weapon performance, has formed alliances with several universities to model supernovae in unprecedented detail.

Paul Springer, Livermore physicist and stellar plasma experiment leader, observes that the same computer models, as well as the same diagnostic equipment, are used for understanding atomic processes at work in both weapons and stars. Springer is a member of Livermore's High Energy Density and Space Technology Division, which studies the properties of matter at extreme conditions of density and temperature.

The division's work includes weapons physics experiments, diagnostic instrument development, advanced modeling codes, as well as theoretical, laboratory, and observational astrophysics. Aiding the research are numerous collaborations with other DOE national laboratories and astronomy departments of leading universities and observatories.

Figure 1. The Livermore experiments re-creating stellar plasmas were done at the 500-kilojoule Saturn accelerator at Sandia National Laboratories.

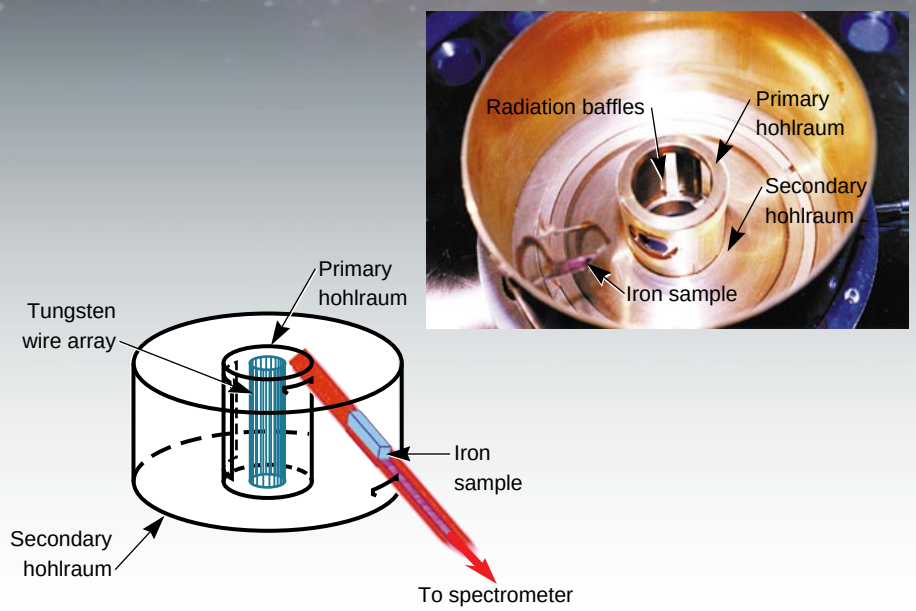


Figure 2. Schematic diagram and photograph of the apparatus used for laboratory astrophysics experiments.The stellar experiments confine an intense x-ray flux to a metal case (called a hohlraum) to improve the radiation's spatial uniformity and heat the case to temperatures exceeding 1 million degrees centigrade. Energy from the primary hohlraum flows through an adjustable baffle into a gold-plated secondary hohlraum, which in turn heats the 1- centimeter-long sample to create a plasma. The illumination of the target is analyzed by a spectrometer.

Focusing on Three Kinds of Stars

Springer's experimental program focuses on three classes of astronomical objects: cepheids (big pulsating stars), supernovae (the brightest objects in the universe), and stars that generate x rays through a process called accretion. A key aspect of the experiments is testing advanced Livermore atomic models—OPAL for the cepheid and supernova experiments, and LXSS for the x-ray tests. Unlike older codes that simplify atomic processes, these codes were built for accuracy and completeness.

Livermore experiments make use of the pulsed-power facilities at Sandia National Laboratories in Albuquerque, New Mexico. Until the completion of NIF in 2003, Sandia's facilities are unique in their ability to create the low-density plasmas typical of many star systems. Livermore researchers have used these facilities during the past two years for stockpile stewardship studies, such as determining the radiation effects on warhead components and testing three-dimensional computer codes that simulate nuclear weapon effects. Until Springer's experiments, the facilities had never been exploited for astrophysics research.

The cepheid and supernova experiments were conducted at Sandia's 500-kilojoule Saturn accelerator (Figure 1), while experiments duplicating x-ray objects' stellar plasmas are planned for Sandia's more powerful Z-Machine, rated at 2,000 kilojoules of energy. Diagnostic equipment for the experiments, including advanced spectrometers, is built at Livermore and transported to Sandia.

The Sandia machines use large banks of capacitors to build and store electrical charges, then simultaneously discharge them in a fraction of a second. The electrical pulse produces a powerful electromagnetic field. A circular array of fine tungsten wires, each a few micrometers in diameter, is ionized into a hot plasma by the compressive force of the electromagnetic field.

Implosion of the wire causes the release of hundreds of thousands of joules of x-ray energy. The intense x-ray energy is confined within a metal case (called a hohlraum), thereby enhancing the spatial uniformity of the radiation and heating the case to temperatures exceeding 1 million degrees centigrade. Energy from the primary hohlraum flows through an adjustable baffle into a gold-plated secondary hohlraum, which in turn heats a target to create a plasma. (Figure 2). This x-ray target "illumination" is captured and analyzed by a spectrometer. The data are then

compared to results predicted by the Livermore atomic models. The experiments thus serve to both validate the codes and refine them.

Springer notes that the experiments require months of preparation, both in the design of the experiment and in the selection and occasional manufacturing of diagnostic equipment. The experiments benefit from researchers' accumulated expertise in designing targets for Livermore lasers, diagnosing underground nuclear tests at the Nevada Test Site, and working with pulsed-power facilities.

Understanding Pulsating Stars

When massive stars evolve from blue supergiants to yellow supergiants, they can temporarily become extremely luminous pulsating stars called cepheid variables. There are only about 700 known cepheids in our galaxy; the best known is the North Star, Polaris.

What fascinates astronomers about cepheids is their regular variation in brightness, with periods ranging from 1 to 70 days. A longer pulsation period means an intrinsically brighter (hotter) star. Consequently, cepheids give astronomers a means of measuring distances to stars in other galaxies. If the pulsation period is known, its true luminosity can be deduced. By comparing the intrinsic brightness with the average brightness of the star, as seen from Earth, the actual distance to the star (and its parent galaxy) can be calculated. The technique is similar to judging the distance to a lighthouse at night based on its brightness as seen from a boat. In this way, cepheids serve as what astronomers term a "standard candle" for distances up to 60 million light years.

Accurately determining the star's intrinsic luminosity depends on energy transport models, or opacity (see the box at the right). Astronomical observations of cepheids had pointed to larger stellar masses than those predicted by the existing opacity model. In 1992, however, Livermore's OPAL opacity code resolved the quandary by including more accurately the opacity effects of elements heavier than helium (called "metals" by astronomers) such as iron. The new stellar models now calculate stellar masses in good agreement with the observations.

"We know now that cepheids pulsate because of the dominant role played by iron," says Springer. He compares the stars to a covered pot of water being heated that builds up heat and generates steam that lifts the lid, releasing the pressure. The lid falls back, and the process begins again. As cepheids contract, they become hotter because of iron ions blocking the transmission of

OPAL Tracks the Transfer of Energy

The physical properties of stars depend upon the transport of energy from their nuclear cores to their surface. Although energy can be transferred out from the center by conduction and convection, radiation transport is the most important mechanism. In turn, the transport of photons depends on the transparency of the intervening matter, termed the radiative opacity. Consequently, opacity plays a key role in determining the evolution, luminosity, and instabilities of stars and even the eventual fate of the universe.

Acquiring a better understanding of opacities is a key goal of the Department of Energy's Stockpile Stewardship Program to keep America's nuclear stockpile safe and reliable. Stellar opacity is involved primarily with lighter elements, while opacity of nuclear weapons plasmas focuses on heavier elements like uranium; yet, the physics in both cases is similar.

It is extremely difficult to measure plasma opacities directly; researchers must rely on a detailed computer model to calculate opacities. However, "Modeling opacity is one of the more difficult tasks in physics," says Livermore physicist Bill Goldstein. In addition to temperature, density, and composition of a plasma, opacity depends on the many atomic absorption processes possible within every ion. Ions continually jump from one energy state to another, each with its own characteristic spectral absorption line. (Iron, with its 26 electrons, can have literally millions of different energy states and corresponding spectral lines.)

Livermore physicists Forrest Rogers, Carlos Iglesias, and Brian Wilson built a new model of stellar opacity called OPAL. Cited more than 500 times in the past few years in astrophysical research papers, OPAL has had an enormous influence. It achieved widespread acceptance earlier in the decade when it helped to resolve longstanding quandaries concerning pulsating stars.

"OPAL is accurate, thorough, and has a proper consideration for physics," says Livermore physicist Paul Springer. "It avoids many of the approximations and simplifying assumptions used in earlier codes." In particular, the code accurately treats the myriad energy transitions in iron. The role of these transitions was previously overlooked in blocking radiation, says Iglesias. As a result, the new OPAL calculations show that iron, the most abundant heavy element in a star, can significantly impede radiation flow and therefore plays a huge role in the properties of a star.

Over the years, OPAL has been refined through experiments on Livermore's Nova laser, which gave the first measurement of the opacity of iron, and more recently, in experiments at Sandia National Laboratories in Albuquerque, which gave the first iron opacity measurements at stellar conditions.

heat. To release the heat, the cepheids expand, radiating the energy away and, in the process, becoming cooler and larger.

Given the complexity of stellar models, it was crucial to validate OPAL's model of cepheid opacities directly in the laboratory. In separate experiments, Livermore physicists Luiz Da Silva, Springer, and others had previously verified data and atomic models in OPAL using Livermore's Nova laser. Although these measurements provided opacity data at astrophysically relevant temperatures, these plasmas were too dense and too short-lived to simulate those of cepheids.

Springer turned to Sandia's 500-kilojoule Saturn facility to more accurately duplicate the plasmas. To achieve plasma equilibrium and meet the goal of 100 times lower density (10^{-4} grams per cubic centimeter), the iron foil target used on Nova was increased in length from 0.03 to 1.0 centimeter, and radiation fields lasting tens of nanoseconds (billionths of a second), some 10 times longer than was possible on Nova, were generated. In addition, a 10-fold improvement in spectral resolution was achieved using an advanced spectrometer built by Livermore engineer Grant Hill (Figure 3). The experiment provided the first direct test of stellar opacities, verifying OPAL's atomic model and helping to refine it.

Simulating Exploding Stars

Building upon the success of the cepheid experiments, Springer's team duplicated plasmas at the Saturn facility resembling those created by one of the most spectacular phenomena in the universe, supernovae. A longtime focus of Livermore interest, supernova explosions leave behind gaseous nebulae, neutron stars, or black holes, objects so dense that even light cannot escape their gravity. In addition, supernovae are believed to produce nearly all the elements in the universe heavier than helium, and their occurrences in or near clouds of cold, molecular gas may trigger the formation of stars.

The Livermore experiments produced a miniature, low-density, expanding (200 kilometers per second) plasma similar to those detected on supernovae. In both cases, the rapid expansion causes spectroscopic absorption lines to be blurred together, significantly complicating calculations of opacity. The experiments again verified OPAL's atomic model, this time for dealing with expanding plasmas, and provided data to benchmark all simulation codes used to model the transport of radiation through rapidly expanding plasma.

Springer's experiments were designed to approximate conditions in the expanding debris (ejecta) being blown off Type Ia supernovae. These explosions result from old, dead stars called white dwarfs, which have the mass of the sun but a size comparable to that of Earth. In most cases, the white dwarf consumes matter from an evolving companion star via a process called accretion, one of the dominant energy conversion processes in the universe. Once the white dwarf reaches a mass 1.4 times that of the sun, a thermonuclear explosion ensues that rips it apart, and the entire star is expelled at velocities reaching one-tenth the speed of light.

Type Ia supernovae have played a central role in recent results obtained by cosmologists attempting to determine the curvature of space. The results obtained so far, says Livermore astrophysicist Ron Eastman, point to the exciting possibility that in the distant

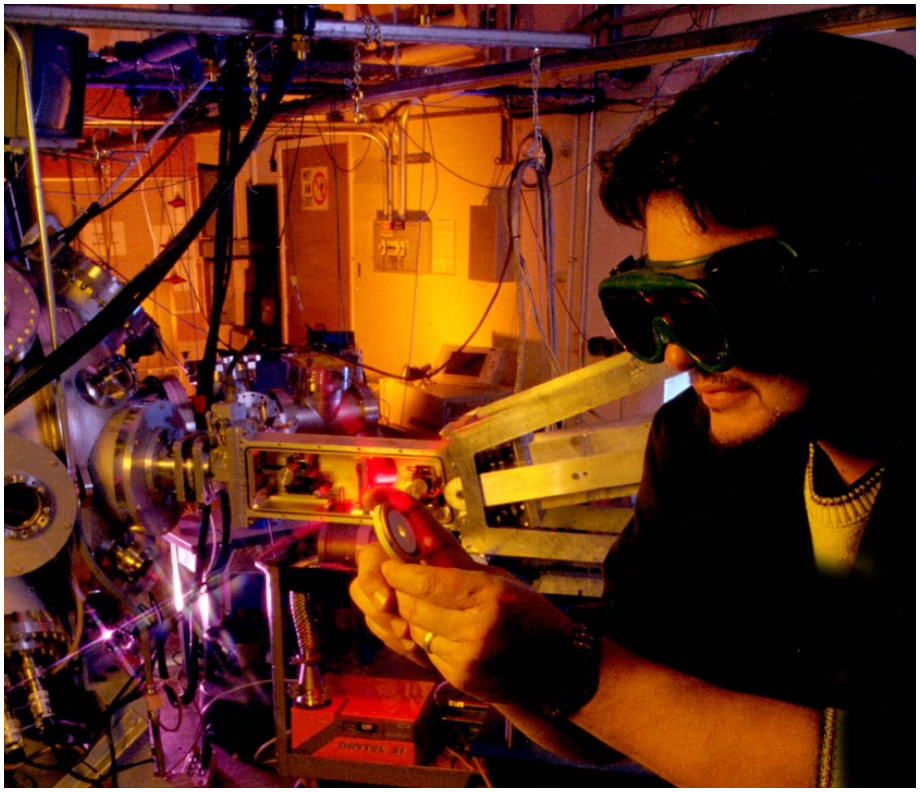


Figure 3. Livermore technician Jim Emig inspects a Livermore-designed spectrometer undergoing calibration with a laser-plasma x-ray monochrometer.

past, the universe expanded more slowly than it does today, implying perhaps the existence of a fifth, repulsive force in nature. But scientists still need to understand the relationship between a Type Ia's luminosity and its light curve shape (the way in which the supernova's brightness changes with time) (Figure 4) in order to rule out other, more mundane possibilities, such as supernovae in the distant past differing from much younger ones that exploded closer to Earth.

Some varieties, known as Type II supernovae, represent the evolutionary endpoint for a massive star, which spends 10 million years burning the hydrogen at its center to iron and then explodes violently in a series of events lasting only a fraction of a second. During the following two to three months, the amount of radiation released from the initial explosion rivals that emitted by the rest of the entire galaxy in which the supernova resides.

In recent years, supernovae have become a major tool for exploring the expansion rate and geometry of the universe. Because of their great luminosity, supernovae are visible at vast cosmological distances. By determining their intrinsic luminosity, astronomers can calculate their distance by measuring the apparent brightness measured through a telescope. And by measuring how fast the supernova and its host galaxy are receding from Earth, astronomers can measure the so-called Hubble constant, which relates recession speed to distance and characterizes the age of the universe.

Eastman and collaborators at Harvard University and Australia's Mount Stromlo Observatory have developed a method for determining the intrinsic luminosity of Type II supernovae explosions using computer models of the emitting gas and

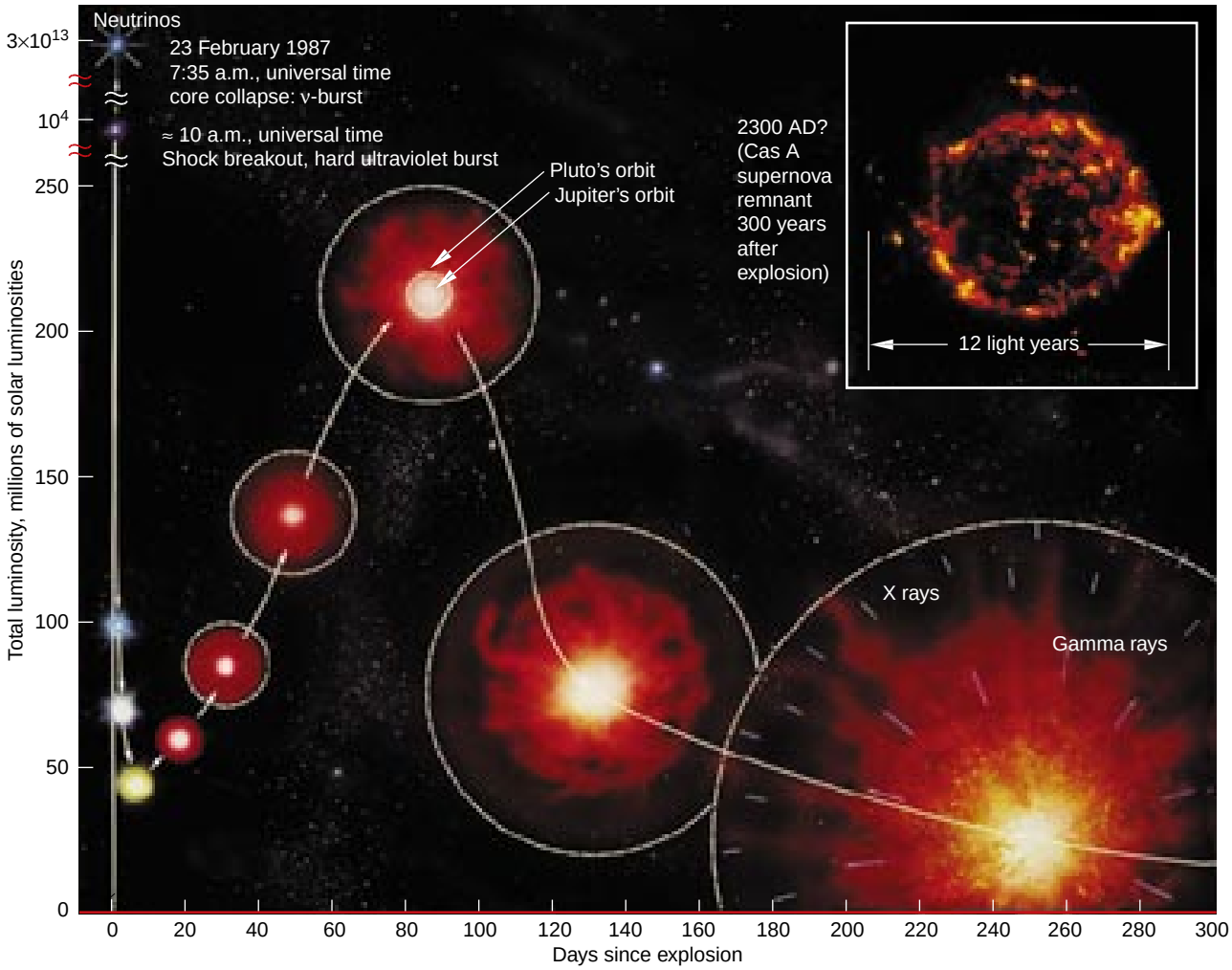


Figure 4. The light curve of a supernova (in this case one that exploded on February 23, 1987) is a measure of its luminosity over the months following its violent explosion. Analyses of light curves help cosmologists determine whether the universe's expansion is speeding up or slowing down.

telescope observations. Their expanding photosphere method is a powerful technique for determining the Hubble constant. Eastman and his colleagues plan to model Springer's experiment with the same code used to model Type II supernovae, thereby determining the accuracy of the code's predictions.

Says Eastman, "The ability to produce, in the laboratory, the same kind of plasma conditions that exist in supernovae will allow both atomic and computational theories to be accurately tested and will provide a firm, experimental foundation for its application to distant supernovae."

Probing the X-Ray Universe

The x-ray universe (wavelengths of 1 to 140 angstroms) features such exotic objects as supernova remnants, x-ray binaries, pulsars, active galaxies, and black holes (Figure 5). Notes Livermore physicist Mark Foord, "X-ray observations allow one to probe into extreme environments in the universe, like conditions found near black holes. We can't get this information from visible light or infrared astronomy."

X-ray spectroscopy, the study of the absorption and emission of x rays, yields significant data on chemical compositions, temperatures, and densities of stellar objects. Livermore has long established itself in the x-ray astronomy community with its expertise in modeling x-ray phenomena and building state-of-the-art diagnostic instruments. Achieving a better understanding of x-ray data is an important goal in stockpile stewardship studies.

With the launch of three major x-ray observatories scheduled to begin during 1999, the astrophysics community will be taking a big step toward understanding the x-ray universe. These spacecraft are NASA's Advanced X-Ray Astrophysics Facility (AXAF), the European Space Agency's X-Ray Multi-Mirror Mission (XMM), and the Japanese Space Science's Astro-E (Figure 6). Livermore researchers helped to build a spectrometer grating for the XMM, and they will be working with colleagues at NASA and U.S. and European universities to analyze data from the AXAF.

The new spacecraft will provide a more than 10-fold improvement in sensitivity and resolution and will send

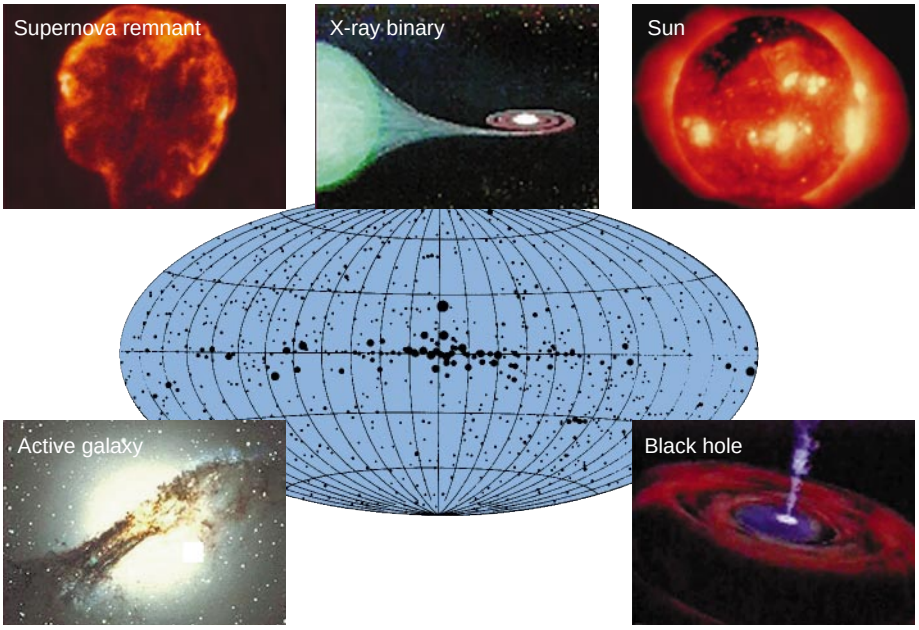


Figure 5. The x-ray universe includes exotic objects such as supernovae remnants, x-ray binaries, pulsars, active galaxies, and black holes.

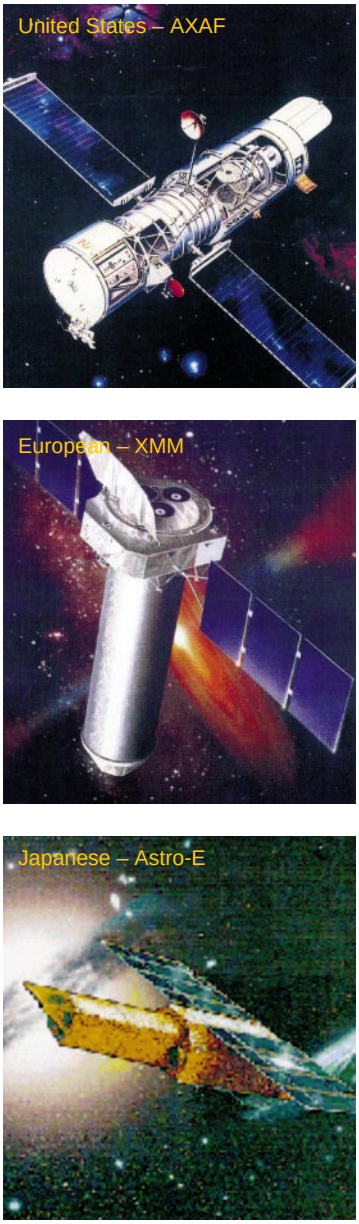


Figure 6. Data from three x-ray space telescopes will provide a more than 10-fold improvement in sensitivity and resolution.

back a wealth of new information about the x-ray universe akin to that about visible light radiation provided by NASA's Hubble Telescope. "The level of detail contained in these data will provide a major challenge to our analytical capabilities," says Livermore astrophysicist Duane Liedahl, because current computer models often yield widely different interpretations of data from x-ray satellites. The cause, as with the predecessors to OPAL, is oversimplified treatments of atomic structure.

In response to the need for a more detailed and comprehensive model of x-ray phenomena, Liedahl and coworkers Kevin Fournier and Christopher Mauche have developed the Livermore X-Ray Spectral Synthesizer (LXSS) (Figure 7). "We've been working on the model since 1990 in anticipation of these launches," Liedahl says. "We expect that LXSS will play a key role in analyzing the new x-ray satellite data."

This code was designed to interpret data from what astrophysicists call accretion disks. One such x-ray source is a binary star system, in which the higher mass star eventually becomes a compact object, either a white dwarf star, a neutron star, or a black hole. The lower mass star may be so close to the compact star that its outer atmosphere begins to heat up and fall onto the compact star. This reaction generates x-rays that photoionize the gas surrounding the binary system. When the ionized gas transitions back to a more favorable energy state, it generates x rays, which are picked up by astronomical observatories.

Data from LXSS have been successfully tested in laboratory experiments, but the experiments could not realistically duplicate the plasma conditions found in accretion-powered x-ray sources. By using Sandia's new Z-Machine, Livermore researchers plan, for the first time, to create plasmas photoionized with x rays, characterize them, and compare the results to those predicted by LXSS. The Livermore experiments, planned for this summer, will use the Z-Machine's x rays to study the photoionization of iron, an important element that is key to understanding the energy balance in many astrophysical x-ray sources.

Explains Foord, "In accretion-powered objects, like binary stars and active galaxies, the x rays are responsible for ionizing the surrounding gas. In typical laboratory experiments, ionization occurs because of electron collisions, a fundamentally different process. Until now, we have not had facilities that could create the sufficient x-ray fluxes needed to reach astrophysical conditions." He says that calculations using Livermore's LASNEX code indicate Z-Machine's radiation fluxes will photoionize samples into astrophysically relevant regimes.

Liedahl notes that LXSS will be used on NIF experiments to help characterize plasmas created by the giant laser. "We intend to keep building on the code to make it as versatile as possible," he says. (See also the December 1997 *Science & Technology Review*, "Marrying Astrophysics with the Earth," p. 21.)

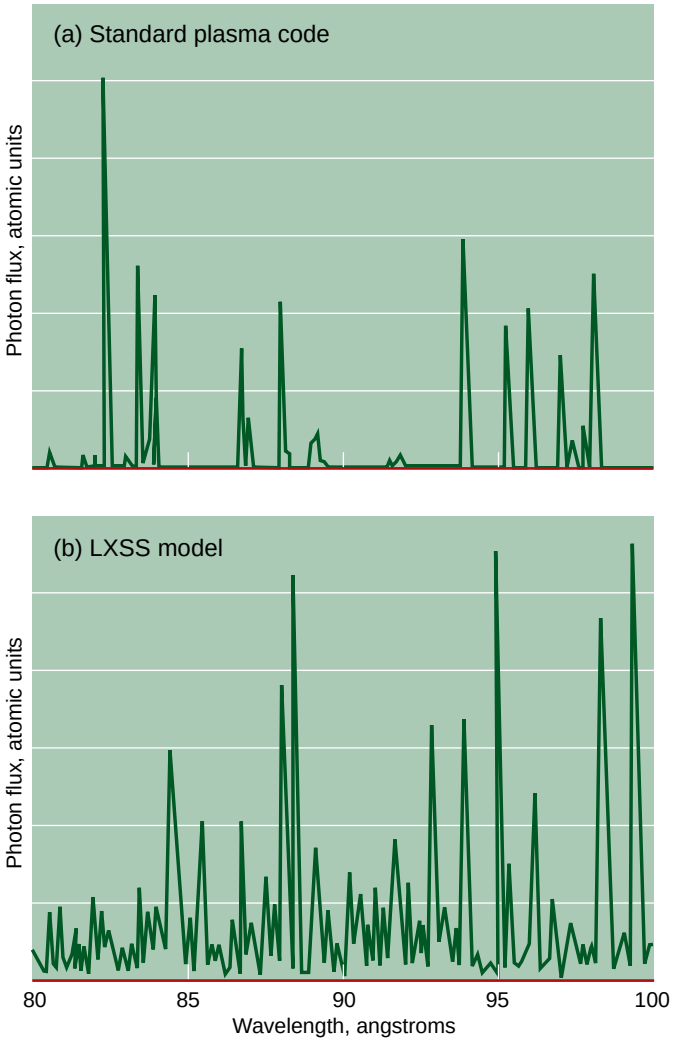


Figure 7. By more accurately predicting the details of intensity (photon flux) versus wavelength, the Livermore X-Ray Spectral Synthesizer (LXSS) code will analyze data from the space telescopes in a far more thorough manner than existing codes.

Deepening Our Understanding

The experiments re-creating stellar plasmas are sure to have a lasting effect on a variety of research communities. For astrophysicists, the experiments are validating codes and deepening the understanding of stars to help answer the most basic questions about the nature and evolution of the universe.

For DOE's Stockpile Stewardship Program, the experiments are strengthening fundamental knowledge of atomic processes in extreme environments and providing greater confidence in the computational tools needed to maintain America's nuclear forces. Greater understanding of opacity, for example, will help guide experiments planned on NIF for both stockpile stewardship and inertial confinement fusion.

"We'll be using the same people, facilities, and equipment on NIF that we use for the pulsed-power experiments," says Springer. He notes that NIF will be able to duplicate the stellar regimes created at Sandia's facilities—"and so much more."

Springer also points out that the Laboratory's astrophysical research is attractive to individuals considering a career at Livermore. For example, Robert Heeter, a postdoctoral physicist from Princeton University, will be leading the x-ray experiment effort this summer as part of the new Lawrence Livermore Fellowship Program to attract promising recent graduates.

At least for the next few years, the skies will continue to be an important source of data as well as inspiration for Livermore researchers.

—Arnie Heller

Key Words: accretion, Accelerated Strategic Computing Initiative (ASCI), Advanced X-Ray Astrophysics Facility (AXAF), Astro-E, astrophysics, binary star, cepheids, hohlraum, Hubble constant, iron, Livermore X-Ray Spectral Synthesizer (LXSS), National Ignition Facility (NIF), Nova, OPAL code, opacity, plasmas, Saturn facility, Stockpile Stewardship Program, supernovae, white dwarf, x-ray astronomy, X-Ray Multi-Mirror Mission (XMM), x-ray spectroscopy, Z-Machine.

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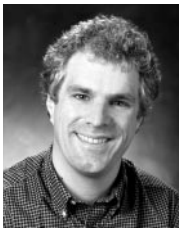
About the Scientist



PAUL SPRINGER holds a B.S. in physics from the University of California at San Diego and a Ph.D. in nuclear physics from Princeton University. He joined Lawrence Livermore in 1984 as a physicist in the Nuclear Chemistry Division while working on his thesis project, a measurement of the neutrino mass. He is currently leader of the Experiments Group and associate Physical Database Research Program leader in V Division of the Physics Directorate. He is the author or coauthor of many journal articles and presentations on high-energy-density plasma physics research. He has received numerous honors and awards, including the Department of Energy's Weapons Recognition of Excellence Award in 1994 and 1997 and a 1994 and 1996 Distinguished Achievement Award from the Physics and Space Technology Directorate. Current research interests include high-temperature plasmas, atomic processes in plasmas, astrophysics, x-ray spectroscopy, atomic physics, and neutrino physics.

Seismic Monitoring Techniques Put to a Test

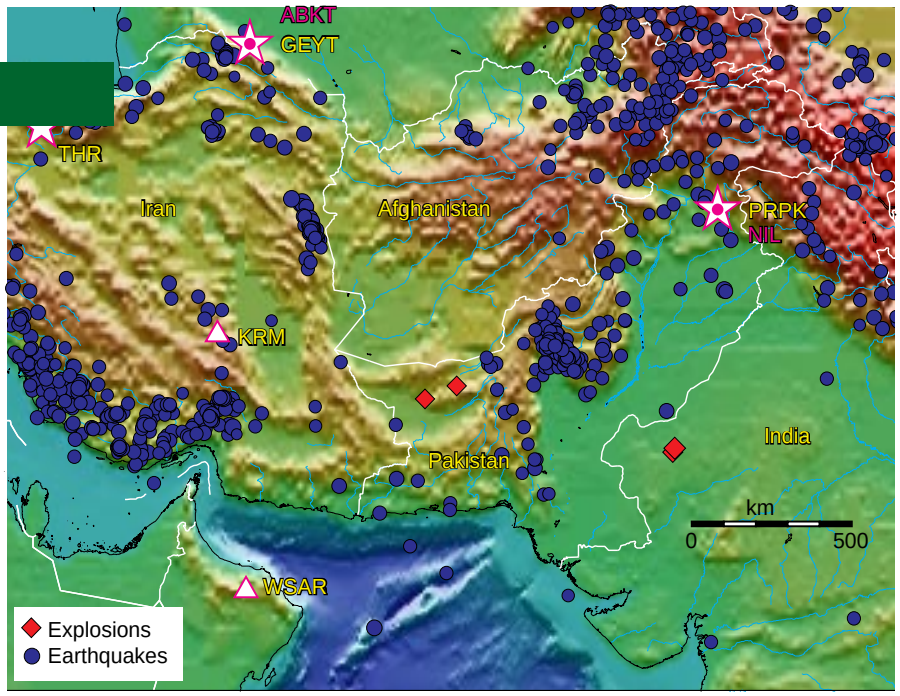


Figure 1. Topographic map showing the locations of the Indian nuclear tests in 1974 and on May 11 and 13, 1998, the Pakistani nuclear tests on May 28 and 30, 1998, and earthquakes recorded in the region between 1995 and 1997. Also shown are the planned locations of the International Monitoring System's primary (stars) and auxiliary (triangles) seismic stations and the Incorporated Research Institutions for Seismology's stations closely collocated at Alibek, Turkmenistan (ABKT), and Nilore, Pakistan (NIL).

WHEN the world received the news of the Indian and Pakistani clandestine underground nuclear tests last May, a team of Livermore researchers used the events to validate several seismic methods they have developed over the past decade to monitor the Comprehensive Test Ban Treaty (CTBT). Using data recorded worldwide by a host of seismic monitoring stations, the team successfully differentiated the nuclear blasts from typical regional earthquakes, characterized the yields of the tests, and noted inconsistencies between the announced test yields and the seismic data. In all, the seismic signals from the nuclear tests provided important new data to help calibrate seismic stations in a critically important region of the world.

The CTBT has been signed by 152 nations, although not by India or Pakistan. The treaty provides for an International Monitoring System (IMS) of automated seismic stations, many of them still to be installed, to record any evidence of clandestine nuclear explosions. These stations transmit data via satellite to the International Data Center in Vienna, Austria, which in turn distributes them to national data centers around the world. Figure 1 shows the location of existing seismic stations in the Southwest Asia area, planned IMS seismic stations, the seismically determined locations of the recent tests by India and Pakistan, and locations of some recent earthquakes in the region.

The U.S. Department of Energy is supporting the U.S. National Data Center (USNDC) at Patrick Air Force Base, Florida, as it prepares to monitor the treaty. As part of DOE's effort, teams at Livermore and Los Alamost have been working to improve ways to seismically characterize clandestine underground nuclear explosions and differentiate them from other sources of seismicity, such as earthquakes and mining explosions. Much of Livermore's work has centered on developing regional discriminants, which are characteristic features of a seismic waveform (for example, the peak amplitude at a particular frequency, within a specific time frame) recorded at distances less than 2,000 kilometers away. These discriminants are used to differentiate between explosions and other types of seismic sources. (See the September 1998 *Science & Technology Review*, "Forensic Seismology Supports the Comprehensive Test Ban Treaty," pp. 4–11.)

India's nuclear test took place on May 11 and 13, 1998, followed by Pakistan's on May 28 and 30, 1998. None of the planned IMS seismic stations in the region was installed at the time of the tests. Fortunately, stations belonging to IRIS (Incorporated Research Institutions for Seismology), a consortium of U.S. universities, were operating. Two of those stations, called ABKT, in Alibek, Turkmenistan (one of the former Soviet republics), and NIL, in Nilore, Pakistan, were near the sites of two proposed IMS stations GEYT and PRPK. While ABKT data were not available, NIL records of the Indian tests, some 740 kilometers away, were available through the Internet within a few hours, as were data provided by IRIS for other stations throughout the world. The NIL station was turned off during the Pakistan tests, so the data were unavailable.

As part of their calibration work for the USNDC, the Livermore seismologists had already collected and analyzed data recorded by NIL and other seismic stations from more than 200 regional earthquakes between 1995 to 1997 in Iran, Afghanistan, Pakistan, western India, and the surrounding

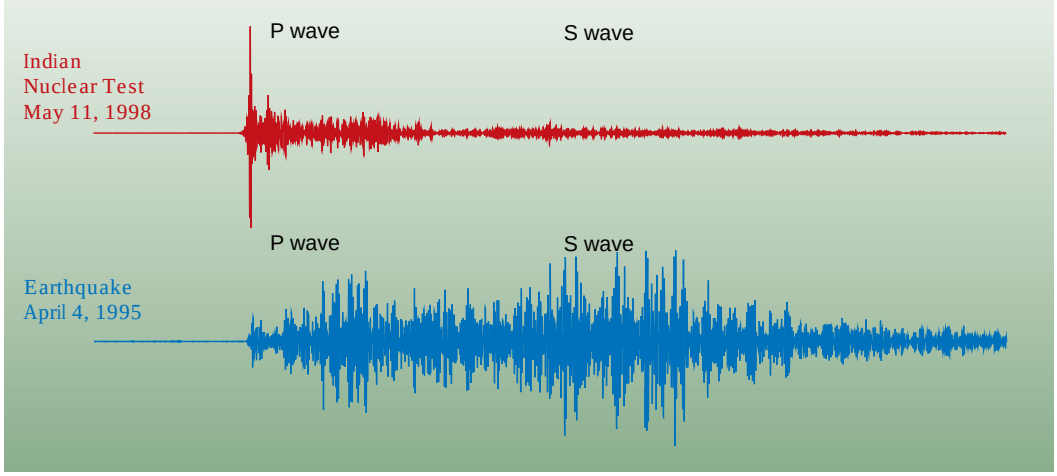


Figure 2. Seismograms of the Indian nuclear test (top) and a representative nearby earthquake (bottom) recorded at the seismic station at Nilore, Pakistan. These seismic signatures for an explosion and earthquake are typical and clearly distinguish one from the other.

region. Within hours of the announcement of the May 11, 1998, Indian tests, Livermore seismologists were comparing its seismogram with those from nearby earthquakes.

As seen in Figure 2, the seismogram from a representative earthquake clearly differs from that of the May 11 test. Livermore-refined discriminants based on P and S waves were strongly indicative of an explosion, not an earthquake or other seismic source, at all frequencies tested (0.5 to 8 hertz). Livermore seismologist Bill Walter explains that the differences in seismic P- and S-wave energy provide one method of discriminating explosions from earthquakes. Seismic P waves are compressional waves, similar to sound waves in the air. Shear (S) waves are transverse waves, like those that propagate along a rope when one end is shaken. Because underground explosions are spherically symmetric disturbances, they radiate seismic P waves efficiently. In contrast, earthquakes result from sliding or rupture along a buried fault surface and strongly excite the transverse motions of S waves. Thus, we expect that explosions will show strong P waves and weak S waves and that earthquakes will show weak P waves and strong S waves, as seen in Figure 2.

According to Walter, one way to quantify this difference is by determining the ratio of P-wave to S-wave energy measured from the seismograms. Explosions should have higher P/S ratios than earthquakes, but the frequency at which the best separation occurs varies by region and station. Figure 3 shows the P/S ratio for the May 11 Indian test and for earthquakes shown in Figure 1. The measurements in Figure 3 were made at four different frequencies. The Indian test has a higher P/S ratio than the earthquakes, as expected.

India reported that its nuclear testing on May 11, 1998, was composed of three almost simultaneous explosions with yields of 45, 15, and 0.2 kilotons and that the two larger tests were separated by about a kilometer. According to Walter, the team's examination of regional data recorded at NIL and at teleseismic stations thousands of kilometers away did not reveal obvious signs of multiple shots. The U.S. Geological Survey reported a teleseismic magnitude of mb 5.2 (mb is the bodywave magnitude and is roughly related to the Richter scale). Assuming simultaneous detonation of the three tests and using published magnitude–yield formulas for a stable region, the announced total yield of 55 to 60 kilotons appears to be at least three times larger than the yield indicated by the seismic data.

Livermore researchers then compared the seismogram from the May 11, 1998, tests with India's May 18, 1974, single test (its only previous nuclear test) using data from stations in Canada and Scotland that recorded both events. The 1974 test generated a clearly detected teleseismic signal with an mb of 4.9. Because India declared the 1974 explosion a "peaceful nuclear explosion," some information about it was reported, such as the fact that it was a single explosion at a depth of 107 meters. However, Indian scientists and officials stated a large range in the yield estimate—4 to 12 kilotons.

Figure 4 shows the seismograms from the 1974 and 1998 tests using data from the Canadian station (for ease of comparison, the 1974 test's amplitude is doubled to match that of the 1998 test.) The two seismic waveforms show remarkable similarity.

Several interpretations of the seismic observations are possible. According to Livermore seismologist Arthur Rodgers, if the three 1998 shots were indeed detonated nearly simultaneously and separated by less than a few kilometers, "We would probably see just one large shot in the seismic waves." Rodgers also says that the second and third shots could have been so small compared to the first that they were overwhelmed in the seismogram. Also, a cavity or substantial amount of porous material near the explosive site could, if present, have reduced the coupling of energy into seismic waves, thereby significantly reducing the seismic magnitude of all three tests. Finally, it is possible that the yield announced by the Indian scientists was simply three to six times too large.

On May 13, India announced two additional low-yield tests totaling 800 tons. The Livermore team examined data

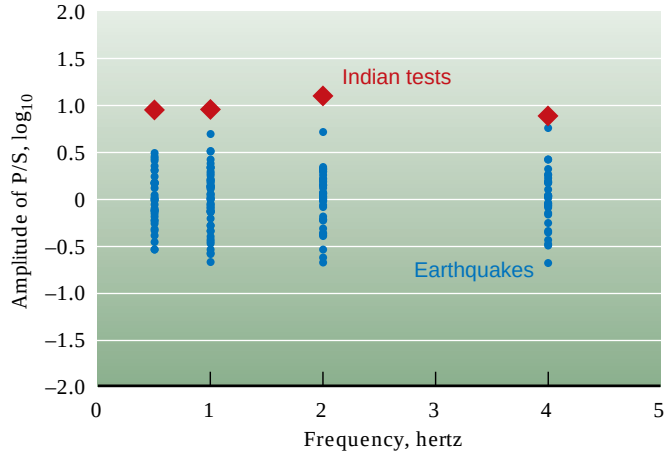


Figure 3. P-to-S amplitude ratios versus frequency for the Indian nuclear test (diamonds) and nearby earthquakes (circles). Note that the P- to S-wave ratios are higher for the Indian test than for the earthquakes.

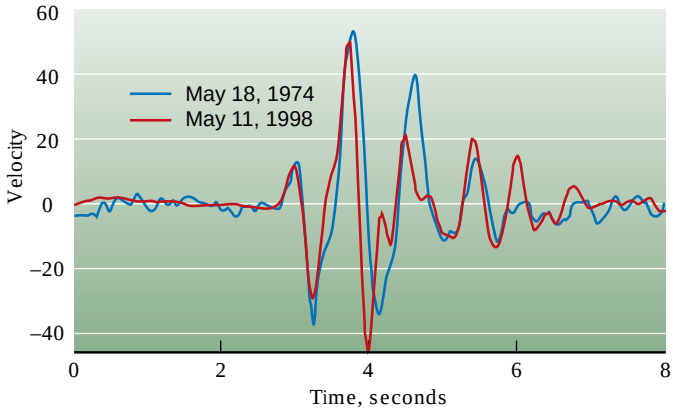


Figure 4. Signals from the 1974 and 1998 Indian underground nuclear tests recorded in northern Canada. (To make the similarities more apparent, the amplitude of the May 18, 1974, data has been doubled.)

provided by the NIL station, but none showed any obvious seismic signal. Using the largest amplitude of the background earth noise around the time of the test as an upper bound for the signals from the event, the Livermore researchers determined that the event must have produced an mb of less than 2.8. The two tests were said to be conducted in a sand dune, which might poorly couple the explosive energy into seismic waves and thus reduce the strength of any recorded seismic signal. Adjusting for this geologic condition, says Walter, a signal should have been observable at NIL if the yield was 100 tons or more.

Walter says that the nuclear tests in India provided valuable data in a region with only a single previous nuclear test. This data will be used to help calibrate the CTBT monitoring network.

The data from the Indian tests will also improve scientists' understanding of the physical basis of the regional discriminants developed at Livermore. As a result of the tests, the discriminants may be applied with greater confidence to much lower yield explosions than the Indian tests and in South Asia and other regions where no nuclear test data are available to calibrate nearby monitoring stations.

The Livermore team plans to conduct more research to further characterize the May events as additional seismic data and information on emplacement conditions become available from Indian and Pakistani officials and scientists. In the meantime, researchers are hopeful that their detailed analysis of the nuclear tests, done without the forthcoming IMS stations, shows that the planned international network will indeed be effective in detecting and identifying clandestine nuclear tests.

—Arnie Heller

Key Words: Comprehensive Test Ban Treaty (CTBT), discriminants, U. S. National Data Center (USNDC), nuclear test.

For further reading:

W. R. Walter, A. J. Rodgers, K. Mayeda, S. Myers, M. Pasyanos, and M. Denny, *Preliminary Regional Seismic Analysis of Nuclear Explosions and Earthquakes in Southwest Asia*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-130745, July 1998.

For further information contact Bill Walter (925) 423-8777 (bwalter@llnl.gov) or Arthur Rodgers (925) 423-5018 (rodgers7@llnl.gov). Information on DOE's overall CTBT program may be found at www.ctbt.rnd.doe.gov.

Sleuthing MTBE with Statistical Data

METHYL tertiary-butyl ether, more commonly known as MTBE, is a chemical Janus. It benefits air quality by making gasoline burn cleaner, thus reducing automobile emissions. But it can also find its way into groundwater supplies and give drinking water an unpleasant taste and odor. At present, more than 20 public drinking water wells in California have ceased water production for this reason. Worse yet, the health effects of MTBE are uncertain—the U.S. Environmental Protection Agency currently classifies MTBE as a possible human carcinogen.

Since 1992, MTBE has been the compound of choice for U.S. oil refineries required by the federal Clean Air Act to add an oxygenate to gasoline to help reduce air pollution. However, some MTBE has appeared in drinking water wells throughout the U.S. This discovery has sparked a national controversy between the need to reduce air pollution (especially in heavily populated areas) and the necessity to safeguard precious water resources from contamination. In an effort to resolve this controversy, the U.S. Environmental Protection Agency (EPA) formed a 14-member panel of MTBE experts from government, the oil industry, academia, regulatory agencies, and environmental groups to explore the environmental and public health effects of MTBE and make policy recommendations by July 1999.

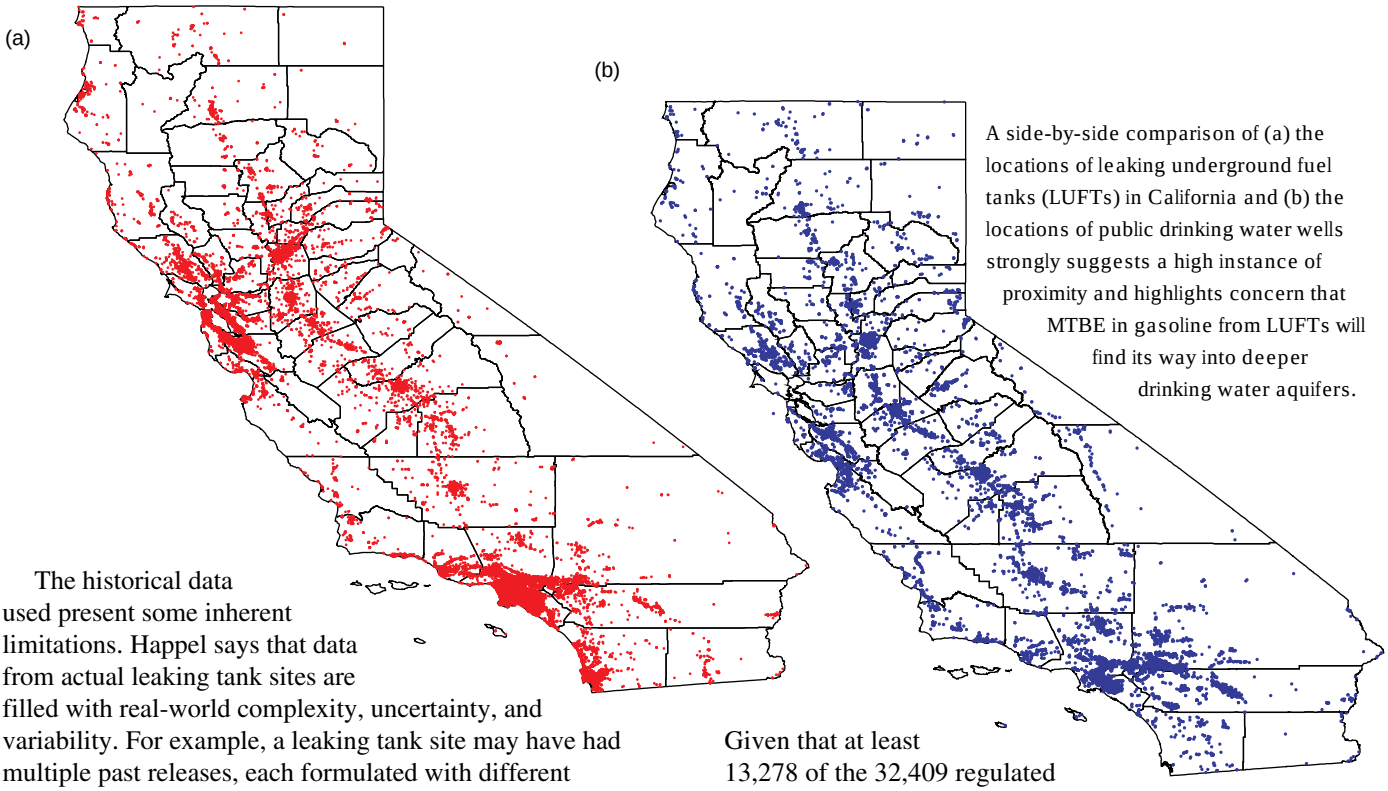
Anne Happel, an environmental scientist at Lawrence Livermore, is a member of this EPA blue-ribbon panel. She leads a multidisciplinary team in the Environmental Restoration Division studying MTBE contamination of groundwater from leaking underground fuel tanks (LUFTs) throughout California. The team's goal is to help water quality regulators, public health specialists, and MTBE users understand more about how MTBE enters and behaves in groundwater so they can better manage its use, prevent harm to humans, and protect limited groundwater resources. The team has estimated how often MTBE escapes into groundwater through gasoline release and traced the behavior of MTBE in groundwater. The team is currently designing a data management system to target LUFTs most in need of remediation because of the risk they present to drinking water sources. The database will allow those responsible for water quality to better manage the cleanup of leaking tank sites and strategically protect drinking water from MTBE.

The study results to date have provided the project sponsors—the California State Water Resources Control Board, the U.S. Department of Energy, and the Western States Petroleum Association—with fundamental information for effective management of California's groundwater resources. They will also be used to help make legislative decisions and set policy regarding MTBE's use as a gasoline additive in California and nationwide.

Analyzing Field Data

Scientists know that MTBE behaves differently in groundwater from other petroleum products such as benzene. Unlike petroleum hydrocarbons, it is highly water soluble, not easily adsorbed to soil, and resists biodegradation. Thus, with widespread use, MTBE has the potential to occur in high concentrations in groundwater, travel far from leak sources, and accumulate to become a hazard on a regional scale.

To investigate these potentialities, the Livermore project team designed a study of MTBE subsurface plumes based on statistical analysis of historical data from California LUFT sites. Researchers investigated data collected at leaking tank sites throughout California to gain insight into MTBE movement from actual gasoline releases. They examined the frequency of MTBE contamination of groundwater at LUFT sites and public water wells throughout California and analyzed the behavior (mobility and attenuation) of MTBE plumes as compared to benzene plumes at LUFT sites.



A side-by-side comparison of (a) the locations of leaking underground fuel tanks (LUFTs) in California and (b) the locations of public drinking water wells strongly suggests a high instance of proximity and highlights concern that MTBE in gasoline from LUFTs will find its way into deeper drinking water aquifers.

The historical data used present some inherent limitations. Happel says that data from actual leaking tank sites are filled with real-world complexity, uncertainty, and variability. For example, a leaking tank site may have had multiple past releases, each formulated with different quantities of MTBE; the ages of the releases are also unknown; and estimates of their volume are uncertain.

When natural variability is added into the analyses—for example, MTBE transport can vary in different geologies, or it can fluctuate because of the elevation and gradient of the groundwater surface—it is easy to see that data from these sparsely monitored individual sites are less than ideal for precise, quantitative contaminant transport research, which relies on data from large, heavily monitored sites. The project team overcame some of these limitations by treating data from a large number of sites as a statistical population. Similar to an epidemiological survey, this approach allowed them to deduce general trends in the behavior of MTBE and other petroleum hydrocarbons.

The first data analyzed were from 236 LUFT sites located in 24 counties where groundwater had been monitored for MTBE prior to the beginning of 1996, earlier than legally required. The Livermore team began by assessing how well standard Environmental Protection Agency analytical methods (EPA 8020 and EPA 8260) performed for detection and quantification of MTBE in groundwater samples in the presence of dissolved gasoline. This evaluation enabled the team to quantify the margin of error in the historical data collected using the EPA methods so that the data could be interpreted, presented, and used with appropriate caveats and qualification.

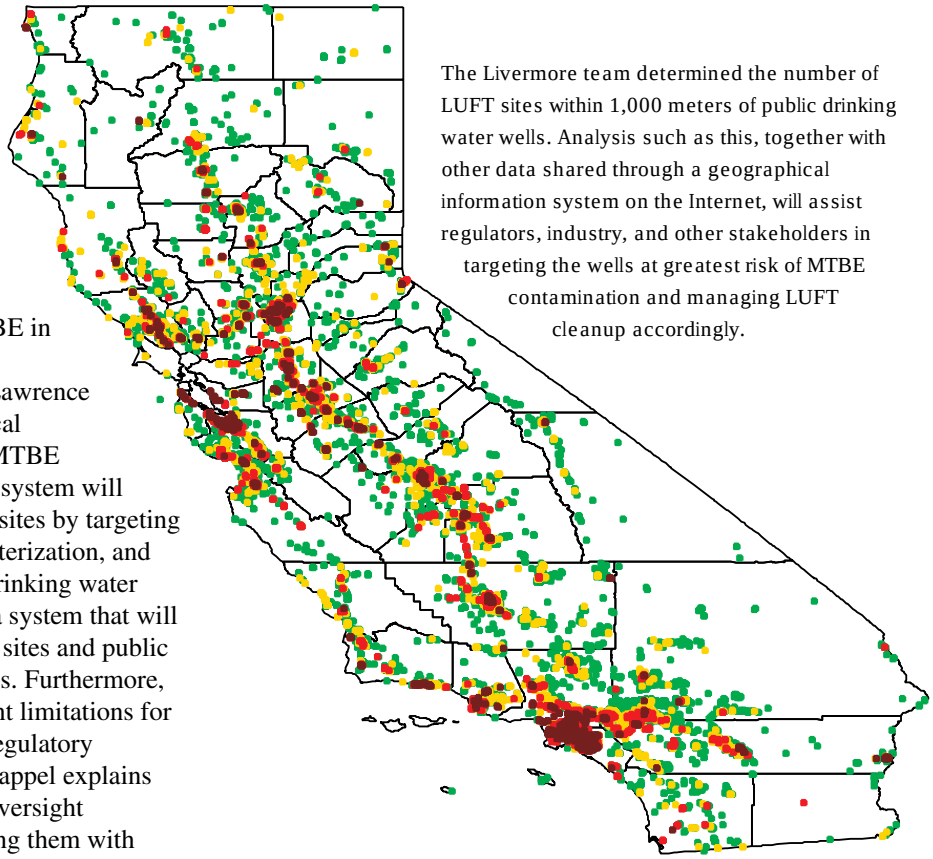
The project team found that the groundwater of 78 percent of these 236 sites contained detectable levels of MTBE. Given that at least 13,278 of the 32,409 regulated LUFT sites are known to have contaminated groundwater, the project team inferred that more than 10,000 LUFTs may have released MTBE into groundwater. These conclusions are consistent with recent work in which data were collected from over 4,000 sites throughout California.

The Conclusions They Reached

While the inferred 10,000 sources of MTBE contamination were the focus of journalistic reporting on MTBE problems, that number was an estimate of the extent of contamination and only one of the findings from the overall investigation. The project team also measured MTBE plume lengths and compared them with the lengths of benzene plumes—benzene is currently the petroleum compound of greatest regulatory concern—to determine the overall plume migration of the two compounds. Finally, team members analyzed the behavior of MTBE groundwater plumes over time. They were fortunate to obtain MTBE data for 29 sites in San Diego County collected since the beginning of 1992 by an oil company that had analyzed for MTBE while sampling for other hydrocarbons.

The team's work confirmed and quantified what other informal, piecemeal studies had hypothesized, namely, that MTBE is a frequent and widespread contaminant in shallow groundwater throughout California, that MTBE plumes are more mobile than hydrocarbon plumes, and that MTBE may attenuate primarily through dispersion because it resists biodegradation.

Put together, these conclusions point to a compound that may progressively accumulate until it contaminates groundwater resources on a regional scale. The team's findings substantiate the need for MTBE regulation and help provide the initial regulatory boundaries.



The Livermore team determined the number of LUFT sites within 1,000 meters of public drinking water wells. Analysis such as this, together with other data shared through a geographical information system on the Internet, will assist regulators, industry, and other stakeholders in targeting the wells at greatest risk of MTBE contamination and managing LUFT cleanup accordingly.

Public drinking water wells
- More than 10 LUFT sites within 1 km
- 4–9 LUFT sites within 1 km
- 1–3 LUFT sites within 1 km
- No LUFT sites within 1 km

More Insights to Come

Given the widespread distribution of MTBE in groundwater at leaking tank sites throughout California, the State Water Board is asking Lawrence Livermore to develop a statewide geographical information system to manage the threat of MTBE contamination to public water supplies. This system will allow regulators for the first time to "triage" sites by targeting manpower and resources for analysis, characterization, and remediation of leaking tank sites closest to drinking water supplies. The Livermore team has designed a system that will provide detailed information on leaking tank sites and public water supplies to multiple regulatory agencies. Furthermore, access over the Internet will overcome current limitations for obtaining and sharing data among multiple regulatory agencies, industry, and other stakeholders. Happel explains that the goal is to give all interested parties oversight management of leaking tank sites by providing them with access to LUFT data and on-line tools to analyze the data. "We believe that this system has the potential to dramatically transform the way regulators and industry make cleanup decisions and establish priorities for managing cleanup."

The team also will be performing more studies of MTBE biodegradation. All the while, it will be leveraging information and technologies from other projects in Livermore's Environmental Restoration Division to further its MTBE work. The team's insights will be valuable contributions to revising MTBE regulations.

—Gloria Wilt

Key Words: gasoline releases, geographical information system, groundwater, leaking underground fuel tanks (LUFTs), methyl tertiary-butyl ether (MTBE), statistical analysis, water quality.

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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

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Oliver T. Strand Robert J. Deri Michael D. Pocha	**Microminiature Optical Waveguide and Method for Fabrication** U.S. Patent 5,846,694 December 8, 1998	A method for manufacturing low-cost, nearly circular cross-section optical waveguides. A thin layer of material that a molten waveguide material (polymer or doped silica) will wet is deposited on a substrate that the waveguide material cannot wet or coat and is patterned to describe the desired surface-contact path pedestals for a waveguide. A resist material is deposited and excess is removed to form pattern marks. The waveguide material is etched away to form waveguide precursors, and the masks are removed. Heat is applied to reflow the waveguide precursors into near-circular cross-section waveguides that sit on top of the pedestals. The waveguide material naturally forms nearly circular cross sections because of surface tension effects. After cooling, the waveguides maintain the round shape. If the width and length are the same, spherical ball lenses are formed. Alternatively, the pedestals can be patterned to taper along their lengths on the surface of the substrate, causing the waveguides to assume a conical taper after heat has caused them to reflow.
Richard F. Post	**Passive Magnetic Bearing Element with Minimal Power Losses** U.S. Patent 5,847,480 December 8, 1998	Systems employing passive magnetic bearing elements having minimal power losses. These include stabilizing elements employing periodic magnet arrays and inductively loaded circuits that improve the elements disclosed in U.S. Patent No. 5,495,221, "Dynamically Stable Magnetic Suspension/Bearing System." The improvements increase the magnitude of the force derivative, while reducing the power dissipated during the normal operation of the bearing system to provide a passive bearing system that has virtually no losses under equilibrium conditions, that is, when the supported system is not subject to any accelerations except those of gravity.
Craig R. Wuest	**Microgap Flat Panel Display** U.S. Patent 5,847,509 December 8, 1998	A microgap flat panel display that includes a thin gas-filled display tube that uses switched X–Y "pixel" strips to trigger electron avalanches and activate a phosphor at a given location on a display screen. The panel uses the principle of electron multiplication in a gas subjected to a high-voltage electric field to provide sufficient electron current to activate standard luminescent phosphors located on an anode. The X–Y conductive strips, which are a few micrometers wide, may be deposited on opposite sides of a thin insulating substrate or on one side of the adjacent substrates and function as a cathode. They are separated from the anode by a gap filled with a suitable gas. Electrical bias is selectively switched onto X and Y strips to activate a "pixel" in the region where these strips overlap. A small amount of a long-lived radioisotope is used to initiate an electron avalanche in the overlap region when bias is applied. The avalanche travels through the gas-filled gap and activates a luminescent phosphor of a selected color. The bias is adjusted to give a proportional electron multiplication to control brightness for a given pixel.
Lawrence M. Wagner Michael J. Strum	**Load Regulating Expansion Fixture** U.S. Patent 5,848,746 December 15, 1998	A free-standing, self-contained device for bonding ultrathin metallic (such as 0.001-inch beryllium) foils. The device will regulate to a predetermined load for solid-state bonding when heated to a bonding temperature. The device includes a load-regulating feature, whereby the expansion stresses generated for bonding are regulated and self-adjusting. The load regulator comprises a pair of friction isolators with a plurality of annealed copper members located between them. The device, with the load regulator, will adjust to and maintain a stress level needed to successfully and economically complete a leak-tight bond without damaging thin foils or other delicate components.

Abstracts

Structural Biology Looks at the Ties That Bind

Over the last five years, Lawrence Livermore has established a program in structural biology to further its work on DNA damage and repair processes. This new program supports a number of other newer projects as well, including the development of antidotes, detection systems, and countermeasures for minimizing the threat of exposure to biological warfare agents. Laboratories have been established for x-ray crystallography and nuclear magnetic resonance spectroscopy, the only methods for obtaining high-resolution, three-dimensional data about individual molecules. This experimental structural biology work is supplemented by computational efforts in molecular modeling and protein prediction.

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Duplicating the Plasmas of Distant Stars

Livermore researchers are creating in the laboratory the same kinds of extremely hot plasmas found in distant stars. The experimental program, conducted at Sandia National Laboratories' pulsed-power facilities, focuses on cepheids (big pulsating stars), supernovae (the brightest objects in the universe), and stars that generate x rays through a process called accretion. A key aspect of the experiments is testing advanced Livermore atomic models—OPAL for the cepheid and supernova experiments and LXSS for the x-ray tests. The data from these experiments will help scientists better understand the birth and evolution of stars, galaxies, and the universe itself. The new experimental techniques, strengthened codes, and diagnostics developed for the tests are also helping the Department of Energy's Stockpile Stewardship Program keep the nation's aging nuclear weapons safe, secure, and reliable in the absence of nuclear testing.

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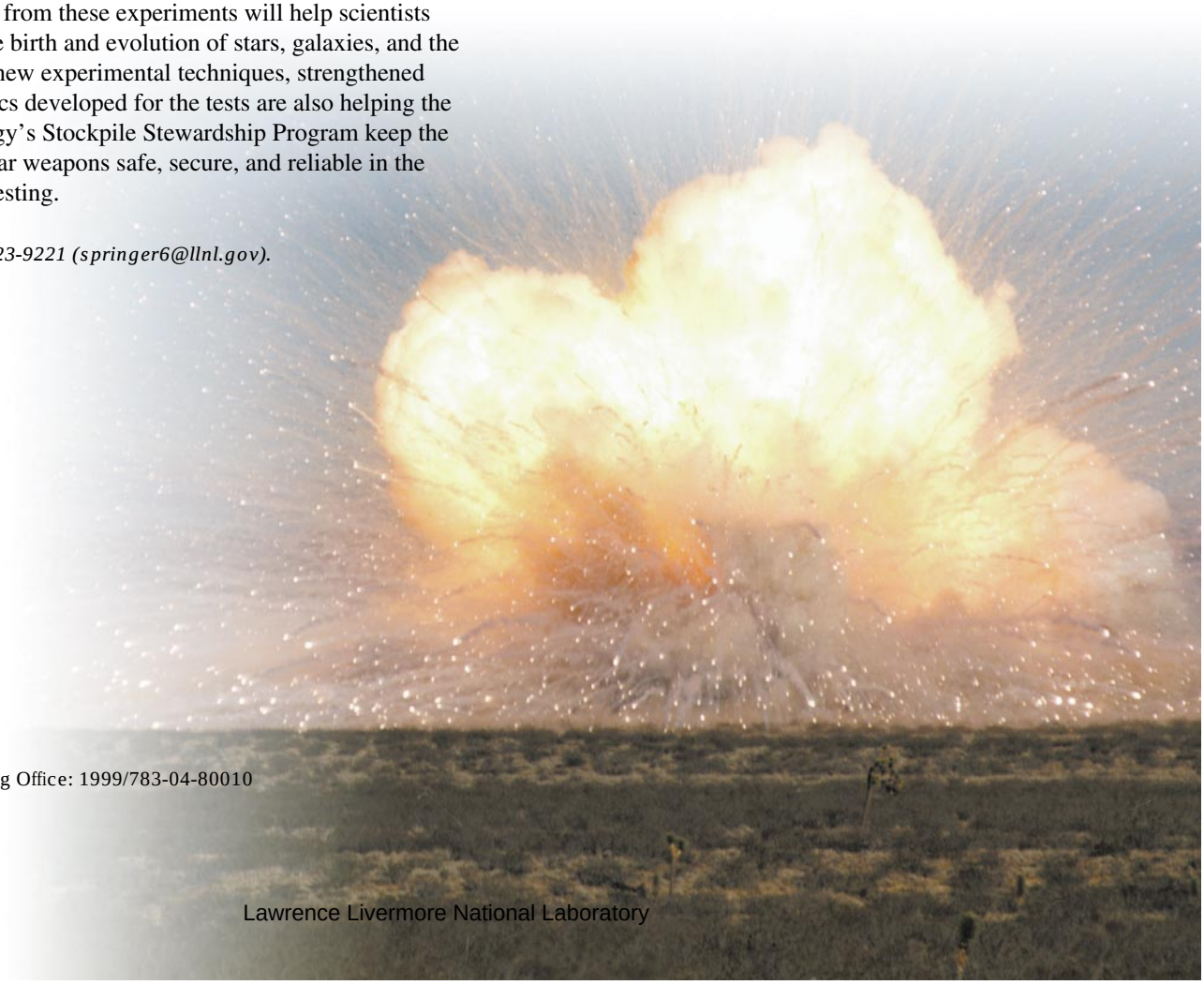
Coming Next Month

Leveraging Science and Technology in the National Interest

A report on recent Lawrence Livermore projects in support of the Department of Defense.

Also in May

- *Putting acoustic signals to novel uses.*
- *Data communication at the speed of light*



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