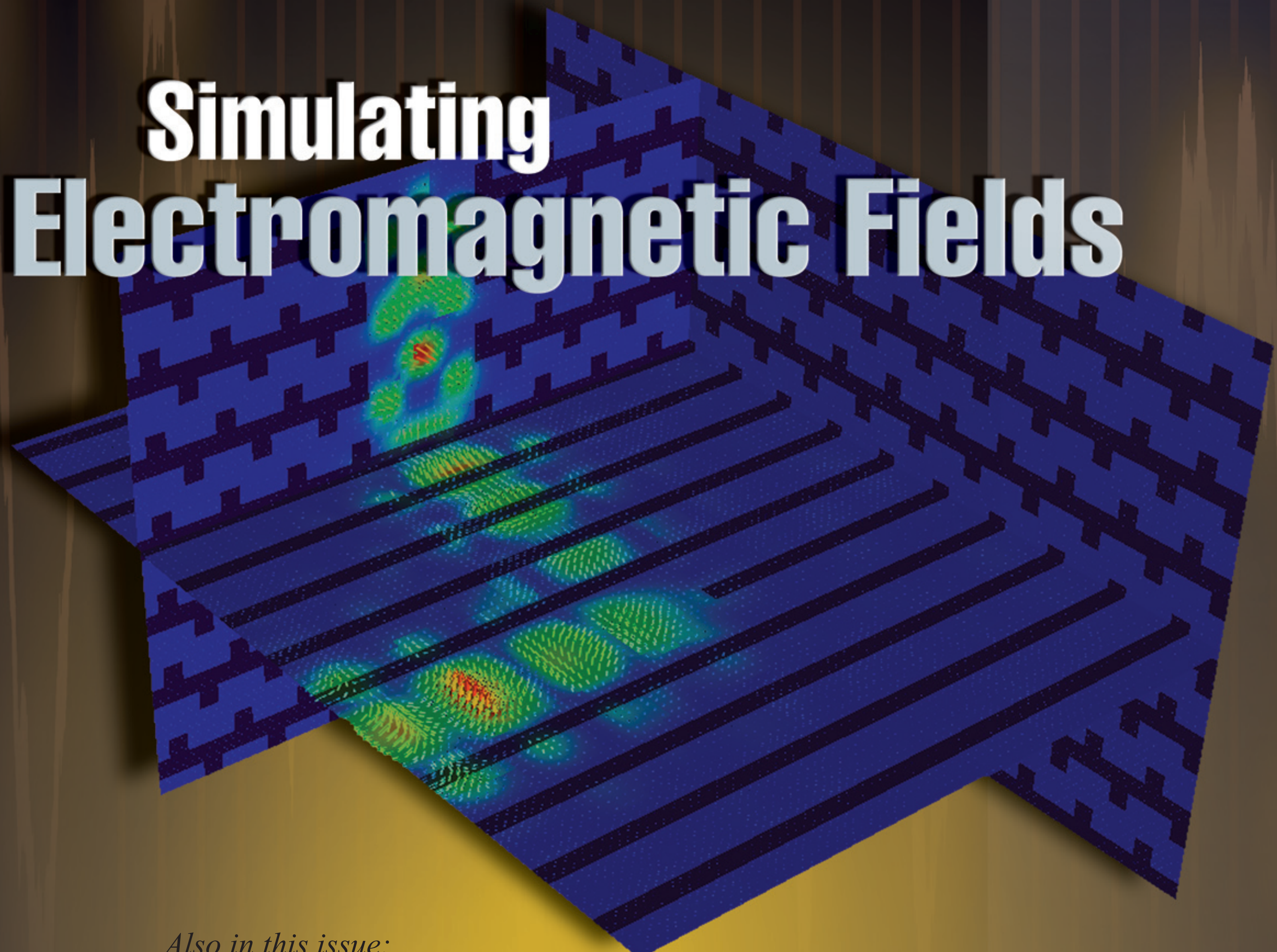
November 2007

Science & Technology REVIEW

National Nuclear Security Administration's Lawrence Livermore National Laboratory

Simulating Electromagnetic Fields

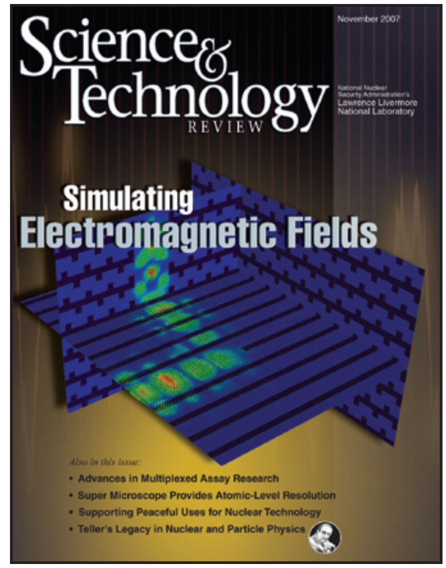


Also in this issue:

- Advances in Multiplexed Assay Research
- Super Microscope Provides Atomic-Level Resolution
- Supporting Peaceful Uses for Nuclear Technology
- Teller's Legacy in Nuclear and Particle Physics

About the Cover

As the article beginning on p. 4 describes, Livermore's EMSolve computer code for simulating electromagnetic fields is proving to be a powerful, accurate, and flexible code for engineering and physics research programs throughout the Laboratory. The code excels at modeling problems with complex geometries containing curved surfaces. EMSolve has been used to accurately simulate electromagnetic fields in structures ranging from a computer chip to a two-story building. The cover shows an EMSolve simulation tracking electromagnetic signals as they travel through a photonic band-gap crystal, making two separate 90-degree bends in three dimensions.



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About the Review

At Lawrence Livermore National Laboratory, we focus science and technology on ensuring 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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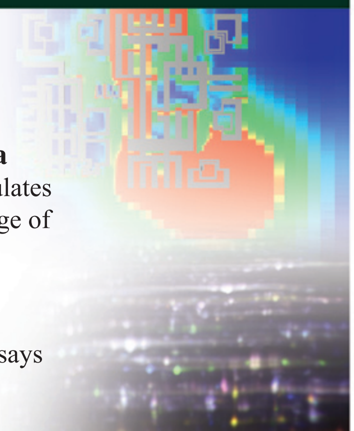

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Effects of irrigation on regional climate

Laboratory scientists Celine Bonfils and David Lobell have found that the rapid expansion of irrigated land in the 20th century has had a cooling effect on California's Central Valley. Although irrigation affects a worldwide land area comparable to urbanization, its regional climatic effects have been much less studied. Scientists have lacked adequate information to incorporate irrigation into regional climate change projections and to help explain historical trends. "Globally, we derive 40 percent of our food from irrigated regions, so we'd like to be able to model future climate changes in these regions," says Bonfils.

Using data from observations of temperature and irrigation trends throughout the state, the authors demonstrated a clear irrigation-induced cooling in agricultural areas and showed that this effect has recently slowed down. In the San Joaquin Valley (the southern portion of the Central Valley), a cooling of 1.8 to 3.2 °C has occurred since irrigation was introduced in 1887. The results of the study, which appeared in the August 14, 2007, edition of the *Proceedings of the National Academy of Sciences*, suggest that this pattern applies to major irrigated regions worldwide.

According to Bonfils and Lobell, the amount of irrigated land in California has stabilized in recent decades, so the suppression of greenhouse warming will gradually lessen in the future. A potential decrease in irrigation may even contribute to a more rapid warming. Changes in irrigation alone are not expected to influence broad-scale temperature patterns, but they may introduce major uncertainties into climate projections in agricultural regions using irrigation.

Contact: Celine Bonfils (925) 423-9923 (bonfils2@llnl.gov).

Successful Phoenix pulsed-power shot in Nevada

On August 4, 2007, at the Laboratory's Big Explosive Experimental Facility at the Nevada Test Site, a team successfully executed helical hydrodynamic test one, or HHT-1. A hydrodynamic test is a nonnuclear scientific experiment that shows how materials react to high-explosives detonation. Hydrodynamic refers to the fluidlike flow of solids under the influence of such an explosion. The shot was the first in a series of tests as part of the Phoenix Project, which will use a pulsed-power system to drive Livermore's isentropic compression experiments.

The Phoenix research is intended to examine the properties of materials at extreme pressures. The focus of HHT-1 was to test a new helical generator system that will be used in future experiments. Program Manager Scott McAllister says, "All of the test data were successfully recorded, and the helical generator performed exactly as predicted."

Livermore participants included McAllister, David Reisman, Fred Ellsworth, David Goerz, and Leon Berzins. In addition, major contributions from other organizations in the Department of Energy complex and the Department of Defense were important components of the test's success.

Contact: Scott McAllister (925) 422-3807 (mcallister1@llnl.gov).

Most energetic laser bay commissioned

In late July, at the National Ignition Facility (NIF), control room operators fired a series of laser shots using a group of eight beams known as bundle 44. The infrared energy output of each beam was approximately 22 kilojoules. This achievement successfully brought to a close the sequential testing of all 96 beams in Laser Bay 2, one of NIF's two laser bays. "With the success of this test, NIF is the world's highest energy laser," says Thomas D'Agostino, head of the National Nuclear Security Administration (NNSA). "The day is coming soon when we will be able to simulate the conditions of extreme temperature and pressure approaching those existing in nuclear explosions."

The next step will be to repeat the process in NIF's other laser bay now that the installation of optics and other components in that laser bay is about 90 percent complete. Overall commissioning is scheduled for June 2009, according to NIF's commissioning manager, Bruno Van Wonterghem. A series of experiments called "Eos" will use the first set of beams from the completed laser bay to validate the performance of NIF's targets.

NIF will convert the infrared energy from its 192 laser beams to 1.8 megajoules of ultraviolet energy. When delivered to millimeter-size targets at the center of NIF's target chamber, this energy will create conditions similar to those in the core of stars and inside exploding nuclear weapons. In addition to supporting NNSA's stockpile stewardship program, NIF will provide opportunities to conduct fusion energy research and to explore regimes of high-energy-density physics in the laboratory.

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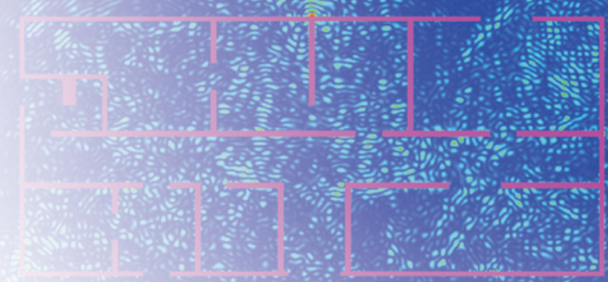


Simulating the Electromagnetic World

MUCH has been written in *Science & Technology Review* and other publications about the remarkable accomplishments of simulation as a full partner with theory and experiment, where they form a threefold foundation for scientific advancement. The steady progression of high-performance computing at Lawrence Livermore has helped ensure our leadership in simulating experiments, often of phenomena for which experimental testing is not an alternative. For example, supercomputer simulations supported by more economical small-scale experiments have replaced underground nuclear testing to help maintain a safe, secure, and reliable U.S. nuclear stockpile.

In the biological sciences, advanced simulations are replacing some aspects of clinical laboratory research to help reveal the mechanisms of pathogenicity. Physical science simulations are allowing us to test ideas in their early stages in place of building expensive hardware prototypes and then iterating experimentally. In chemical research, simulations are revealing how molecules bond to each other and the pathways to new nanomaterials.

Electromagnetic phenomena are ubiquitous throughout the Laboratory's mission, spanning problems from optical regimes to classic microwave and radio-frequency research to the static fields associated with fixed magnets. The accuracy needed for simulations of these problems poses extreme challenges. As described in the article beginning on p. 4, a Livermore code called EMSolve allows us to thoroughly model the electric and magnetic fields of devices ranging from tiny integrated circuits to entire buildings. EMSolve has become increasingly more accurate and efficient over the past decade, thanks to the combined efforts of the Engineering Directorate's Dan White, who is its chief designer; fellow simulation experts; and graduate students.

A premier code, EMSolve has influenced the direction of electromagnetic simulations in government, academia, and industry. It not only simulates complex environments that other codes can't but also offers a platform to couple other kinds of physics that bring intractable problems within reach of our supercomputers. The code is unusually flexible in applying the underlying equations that govern its calculations, allowing the user to perform what-if scenarios across timescales ranging from billionths of a second to tens of seconds.

One reason EMSolve works so effectively is that it was "born parallel." The code was specifically developed to run on the parallel supercomputers located at Livermore and other national laboratories and major research centers. A relatively small number of people are expert at writing complex parallel codes. White and his codevelopers understand the architecture of parallel computers and know how to use the tens of thousands of microprocessors powering these machines. This talent typifies the Laboratory's unique contributions to our nation's technological capability arising from the synergy between collocated high-performance computing specialists, computer scientists, mathematicians, physicists, and computational engineers.

EMSolve developers are currently extending the code to allow it to attack a broader class of problems. They are coupling EMSolve with thermal, structural, and hydrodynamics codes as well as developing the capability to determine electromagnetic properties from a quantum-mechanical perspective. Today, joint projects between computational engineers and computer scientists are focusing on how to adapt the code to the next generation of supercomputers, which will have 10 to 100 times more microprocessors than today's versions.

Our goal is to pose realistic questions concerning complex situations and then simulate the results with the accuracy needed to make meaningful decisions. We will face future challenges for simulating electromagnetic fields, such as those expected in new generations of integrated electronic and optical circuits. Detecting radio signals propagated in caves, tunnels, and "urban canyons" will also be important. In addition, EMSolve will be used to analyze the complex electromagnetic environment of giant lasers such as the National Ignition Facility. We also expect EMSolve to be an extremely powerful tool for quickly interpreting radar signals bounced off high-speed aircraft. Because of the dedicated work of EMSolve developers and their colleagues, we are steadily moving toward making that goal a reality.

■ Steven R. Patterson is associate director for Engineering.

A Code to Model Electromagnetic Phenomena

Livermore's EMSolve code helps scientists understand and predict electromagnetic fields.

AMONG the pantheon of great scientists, few have made contributions as far-reaching as James Clerk Maxwell, the 19th-century Scottish physicist. Maxwell's four equations unified electricity and magnetism for the first time and described light as an electromagnetic wave that varies in space and time. His equations showed how a changing magnetic field produces an electric field, and how a changing electric field generates a magnetic field. In 1931, on the 100th anniversary of Maxwell's birth, Albert Einstein described the change in the conception of reality that resulted from Maxwell's work as "the most profound and the most fruitful that physics has experienced since the time of Newton."

For decades, Livermore engineers and scientists have simulated the propagation and interaction of electromagnetic fields to better understand magnetic fusion energy, lasers, radar, nuclear weapon effects, electronics, and communication systems. Over the years, a number of commercial computer codes have appeared that solve Maxwell's equations for various engineering and physics research applications. None of the codes, however, has proved as powerful, accurate, or flexible as a Livermore code called EMSolve.

The code has been used to accurately simulate electromagnetic fields in structures ranging in size from a computer chip to a two-story building. EMSolve's enormous simulation capabilities require that it run on parallel supercomputers. These machines feature thousands of microprocessors that share computing chores to predict and demonstrate the actions and effects of electromagnetic fields within time frames as short as 1 femtosecond (10^{-15} second).

"EMSolve is used throughout the Laboratory because studying electromagnetic fields is an important aspect of almost every Livermore program," says engineer and computational scientist Dan White, project leader for EMSolve. The code has supported research projects sponsored by the Defense Advanced Research Projects Agency (DARPA), U.S. Air Force, U.S. Navy, and Stanford Linear Accelerator Center.

EMSolve has been cited in more than 30 peer-reviewed journal articles. For example, the March 2007 cover of *IEEE Transactions on Magnetics* features a paper by White and colleagues concerning simulation of magnetic fields in complex geometries. The program has also been licensed to private industry.

White started EMSolve for his Ph.D. dissertation while working in Livermore's Student Employee Graduate Research Fellowship (SEGRF) Program. (See *S&TR,* June 2006, pp. 4–11.) He devised the code to simulate electromagnetic fields using finite-element analysis, a common simulation technique in which a volume is divided into an assemblage of thousands or even millions of simple elements. The changing fields within each element are then calculated. Visually, the collection of elements resembles a wire mesh.

Structured and Unstructured Meshes

The most common method for electromagnetic simulation uses a structured type of mesh to model a geometry of interest. A structured mesh arranges mesh nodes in parallel planes. Such an arrangement works for typical problems but is inadequate for many research applications at Livermore. With EMSolve, researchers can solve Maxwell's equations on an unstructured mesh, which uses elements of simple shapes such as triangles or tetrahedrals in irregular patterns. Because EMSolve is based on unstructured mesh finite-element technology, the code excels at modeling problems with complex geometries containing curved surfaces.

"The code is robust and takes a rigorous approach to solving problems," says White. "It can generate structured meshes for straightforward electromagnetic simulations and unstructured meshes for the enormous simulation challenges Livermore researchers face every day."

Since the code's first release in 1997, it has been continually improved, with funding from Livermore's Laboratory Directed Research and Development Program, the Engineering Directorate, and outside sponsors. Most code advancements, including new algorithms and additional physics, have been done by graduate students. White says, "Ph D. students bring important new ideas about what we can incorporate into the code." Joe Koning, Rob Rieben, and Aaron Fisher, now Livermore employees, based their dissertations on developing new EMSolve capabilities while at the University of California (UC) at Davis. Other contributors include Livermore physicist Niel Madsen, former Livermore postdoctoral researchers Paul Castillo and John Rockway, retired UC Davis professor Garry Rodrigue, and former University of Washington Ph.D. student James Pingenot.

The current development team consists of White and colleagues Mark Stowell and Ben Fasenfest. Stowell is a computer scientist who develops the complex algorithms and data structures required for parallel computations. Fasenfest is an engineer who specializes in EMSolve applications.

EMSolve is one of several codes developed by Livermore engineers. "Livermore's computational engineering community is among the best in the world at solving very large and nonlinear structural and electromagnetic applications," says Robert Sharpe, who leads the Computational Engineering focus area. "Our engineering analysts have expertise in areas such as code development, numerical methods, parallel processing, and material behavior. The development of new codes is driven in part by the increasing expense to execute a comprehensive suite of physical experiments. More and more, we're doing experiments virtually. Because of the codes' proven accuracy, we have confidence in the results."

Sharpe notes that commercial codes are not applicable to the unusual electromagnetic problems encountered in Livermore research. "Our needs go well beyond the scope of codes we can obtain commercially," says Sharpe. Neither can commercial codes be used on the latest massively parallel computers installed at Livermore. "We have the computational resources to explore questions other researchers can't," says Sharpe. Also, he notes, while most commercial codes can make assumptions about physics that are "good enough" for many applications, such assumptions can skew results at the level of detail Livermore researchers require.

EMSolve is used to model events that occur on extremely short timescales. For example, simulations involving a light wave traveling 300 meters in a millionth of a second often require thousands of consecutive time steps, each separated by a few femtoseconds.

Because Maxwell's equations solve for both electric and magnetic fields, EMSolve supplies information on both fields simultaneously. A major challenge is how to visually display the massive amount of data the code supplies. The

EMSolve team works closely with the Livermore computer experts who developed VisIt, a visualization tool that analyzes huge amounts of data generated by supercomputer simulations, to present the code's findings in ways that are readily understood. (See *S&TR,* October 2005, pp. 10–11.) The code also uses software libraries developed at Livermore's Center for Applied Scientific Computing.

One of the EMSolve's most useful features is an error estimator that functions like a self-diagnostic mechanism. The error estimator shows a user those areas in the mesh where the simulation results are not sufficiently resolved. The user can then increase the mesh density to reduce the error. This feature decreases the number of required iterations and makes possible more accurate solutions with less computing power.

Far-Ranging Applications

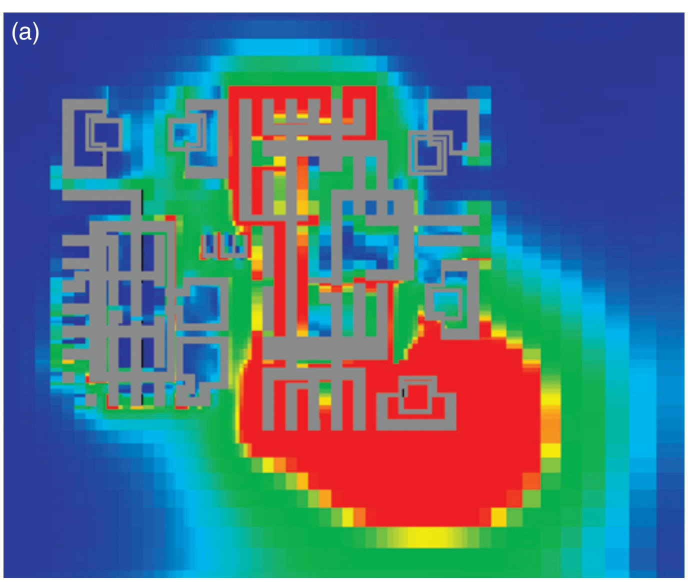
The code has been used to study optical trapping of microparticles, linear particle accelerator components, photonic and electronic devices, aerospace and radar systems, microelectronics devices, radar interrogation of buildings, electromagnetic interference, and cell-phone transmission. EMSolve also supports Livermore's national security missions in stockpile stewardship, homeland security, and the National Ignition Facility (NIF).

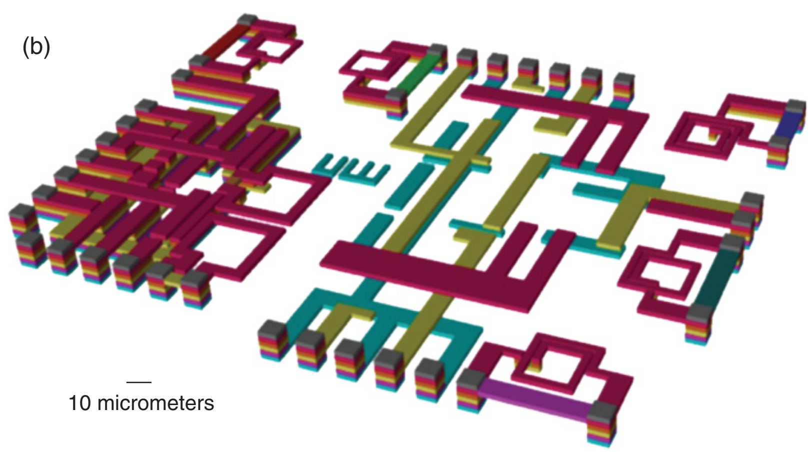
The EMSolve team has performed several studies for DARPA. In collaboration with researchers at the University of Washington, the team simulated electromagnetic waves traveling through an integrated chip containing both digital and analog components. These chips can be found in cell phones and other devices that transmit data. "Digital components generate noise and can interfere with the functions of analog components," says White. "We want to understand electromagnetic interference on the circuits of these chips." The simulations introduced noise consisting of a 5-gigahertz radio-frequency signal and tracked how fast and far the signal propagated through the circuit.

Another DARPA project involved simulating the behavior of radar waves inside a building. Radar uses electromagnetic waves to detect and image objects and to determine their distance from an observer. In principle, a radar system with advanced computer processing of reflected signals could determine a building's internal structure. "We're helping DARPA to better understand the complex radar-scattering mechanisms that occur inside buildings," says White.

The simulation team focused on a generic two-story structure with about 465 square meters (5,000 square feet) of interior floor space with doors, windows, hallways, several rooms, and a stairwell. In one simulation, the structure was made of solid concrete, and in another, it was constructed with cinder block and rebar. The virtual building measured 22.6 meters long by 10 meters wide by 6.75 meters tall. Simulated electromagnetic fields were generated by a radar source outside the structure near the broad side and then the narrow side of the building. The hypothetical radar was a broadband pulsed system with a high frequency of 1 gigahertz and a center frequency of 700 megahertz.

The computational mesh elements varied between 0.75 and 1.4 centimeters on each side. The mesh consisted of more than 10 billion elements, comprising one of the largest electromagnetic simulations ever performed. The simulations, done on

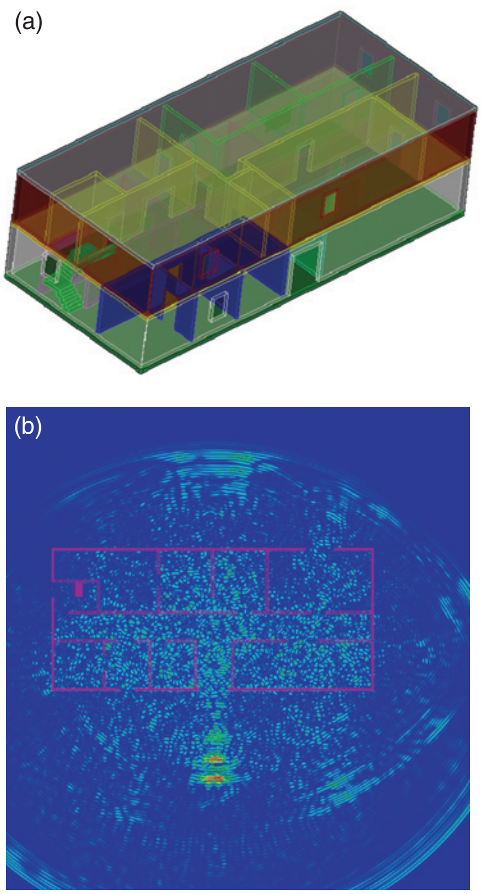




(a) An analysis using the EMSolve code studied noise in integrated circuits containing both digital and analog components. In this simulation, red denotes the highest magnitude and blue the lowest of the electric current in the substrate. (b) A magnified view shows the three-dimensional structure of the chip.

Livermore's Zeus machine, used 1,536 of Zeus's 2,304 processors. The calculations were run long enough for the radar pulse to travel 30 meters when the transmitter was located on the broad side and 50 meters when it was on the narrow side. These distances corresponded roughly to the distances from the transmitters to the farthest corner of the building and back.

The simulations revealed how wall composition affects the propagation of radar waves. Although some of the radar waves were reflected from the outside wall of the building, a significant amount penetrated into the building. Rebar and cinder block walls trapped electromagnetic fields within individual rooms, while concrete walls tended to trap fields within walls and ceilings. The trapped fields in the concrete structure lagged behind the initial pulse because the wave speed within concrete is only 40 percent of the speed of light in air. Another phenomenon, especially evident in continuous concrete, was a wave-guiding effect in which radar waves seemed to be pulled along the building's central corridor toward the far side.



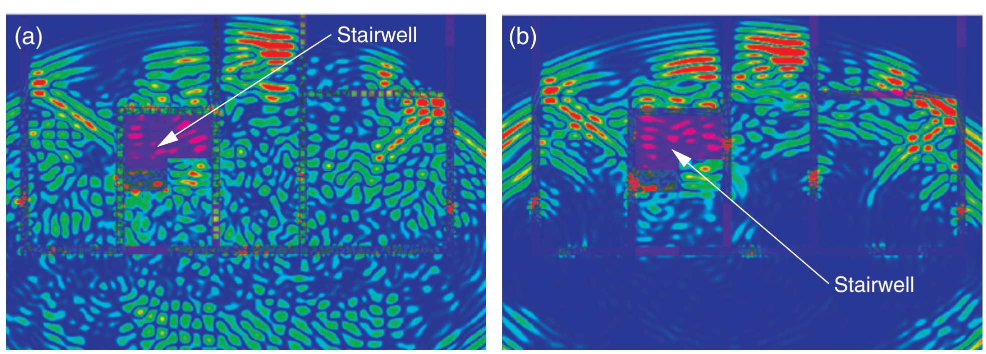
(a) EMSolve simulated the interaction of radar waves inside a hypothetical two-story building. (b) A snapshot captured 140 nanoseconds after the launch of the radar wave shows the electric-field plane through the center of the first floor. The small red block is the stairwell, which tends to trap electromagnetic energy.

Tracking Light in a Crystal

The Livermore team has also studied the three-dimensional (3D) electromagnetic field intensities of photonic band-gap (PBG) crystals, also called photonic crystals. A revolutionary concept for guiding light, PBG crystals consist of alternating layers of various insulating materials. The devices can stop the propagation of light, allow propagation only in certain directions, localize light in certain areas, or prevent the transmission of light within a certain frequency range.

While a graduate student, Rieben used EMSolve to provide the first-ever 3D simulation of light in a PBG crystal. He modeled PBG structures operating at 11 gigahertz and measuring 1.1 by 1.1 by 1.2 centimeters. The crystal was arranged in a 90- by 13- by 7-layer configuration of aluminum oxide cylinders. The simulations tracked the propagation of signals making two separate 90-degree bends in three dimensions, which were made possible by three defects introduced in the crystals. The finite-element structured mesh consisted of 419,328 hexahedral elements. Within each element, the electric field was represented by a cubic polynomial. In contrast, other simulations assume only linear variations. The simulations ran for 6,500 time steps, with each step separated by 300 femtoseconds.

The EMSolve team also simulated the operation of an induction cell, which is used to accelerate a beam of electrons in a linear accelerator. The simulation, done for the Stanford Linear Accelerator Center (SLAC), was conducted as part of the design effort for the International Linear Collider (formerly called the Next Linear Collider). A global collaboration of particle physics laboratories, including Livermore, is involved in designing the machine, which will collide electrons with positrons to produce exotic subatomic particles. (See *S&TR*, September 2004, pp. 22–24). SLAC



These close-up views show EMSolve simulations of a building made of (a) rebar and cinderblock and (b) solid concrete. The rebar and cinderblock walls trap fields within individual rooms, whereas the concrete walls tend to trap fields within walls and ceilings. In the solid concrete building, an inner-wall wave-guiding effect is evident. In both cases, electric fields accumulate in the stairwells.

computational scientists have recently built on EMSolve software to create a version tailored for their physics research.

Modeling Electromagnetic Pulses

EMSolve is used increasingly in Livermore programs. One of the most challenging applications for EMSolve is advancing the understanding of electromagnetic pulses (EMPs), which result from laser–target interactions in high-power laser facilities. An EMP is an intense burst of electromagnetic energy caused by an abrupt, rapid acceleration of electrons. The burst lasts 10 to 1,000 times longer than the original laser pulse.

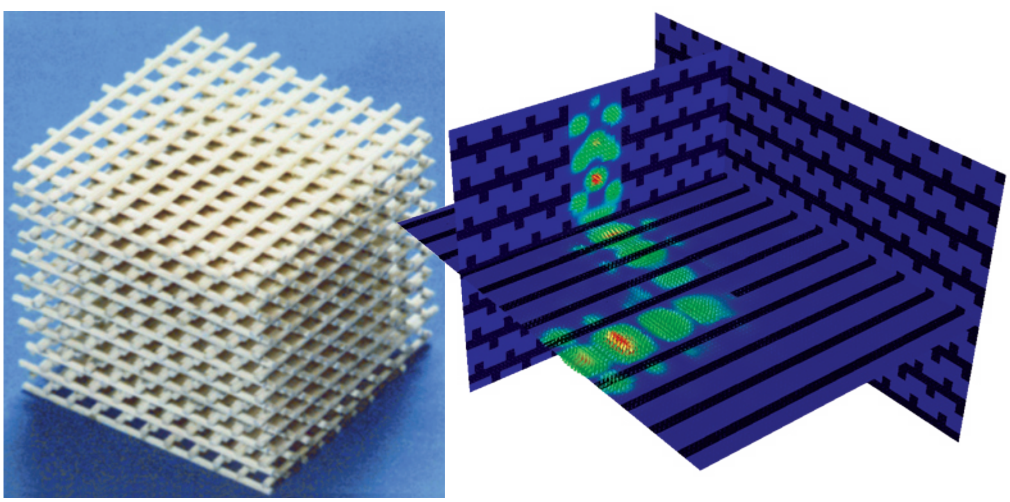
Researchers have reported many cases of EMP-induced diagnostic damage and data loss at short-pulse, high-energy laser facilities even when instruments have been isolated and shielded. Because of this damage, scientists want to improve their understanding of EMPs for current laser facilities and for the next generation of short-pulse, high-power lasers, including NIF, France's Laser Megajoule (LMJ), and a new short-pulse capability at the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics. Effective mitigation techniques require detailed data on the properties of EMP and the mechanisms by which it is produced.

The main source of strong EMPs at laser facilities is believed to be the small fraction of electrons—produced by laser–plasma interactions—that escape the target. As the electrons exit, they leave behind a positively charged target, thereby creating a strong electrostatic field that causes electron currents from throughout the chamber to flow and neutralize the positive charge. The electrons hit the target chamber wall, creating an EMP, which induces currents to flow back and forth. Physicist Dave Eder, group leader for facility modeling at NIF, compares the target chamber to a violin string that rings after being plucked.

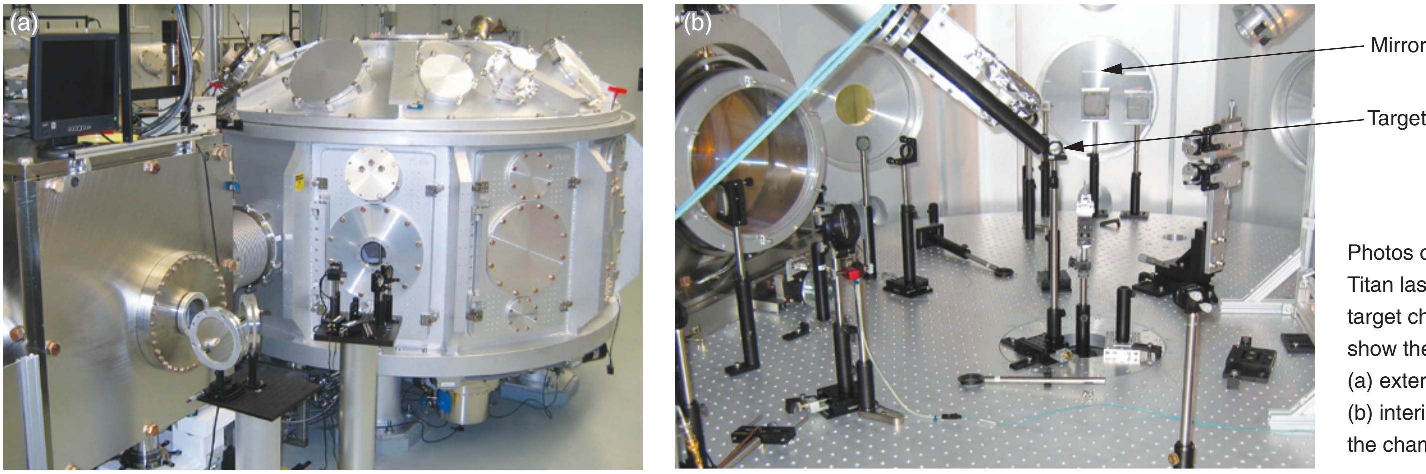
Scientists are obtaining the first quantitative understanding of EMP processes from a laser by using the Titan laser at Livermore's Jupiter Laser Facility. Researchers measure the number of escaping electrons, the time and spatial distribution of the electrons, the EMP, and the resulting transient currents. The recorded properties of the electron stream are compared to 3D EMSolve simulations of the same experiments. In this way, they are validating the code's accuracy and effectiveness as a tool to predict the strength, duration, and electromagnetic frequency of EMPs generated on Titan and other laser facilities. The effort is funded by the Laboratory Directed Research and Development Program and is an Engineering Directorate technology-base project.

"We're developing a predictive simulation capability that can be applied to existing and future laser facilities to mitigate EMPs and greatly reduce the occurrence of diagnostic upset or damage and data loss," says Eder. Scientists hope to use the simulations to develop ways to reduce EMP for a wide range of target–laser conditions. Mitigation options include reducing the number of electrons escaping, installing shields that the electrons strike before they impact the target chamber walls, and developing new grounding and shielding configurations for instruments that are sensitive to EMP.

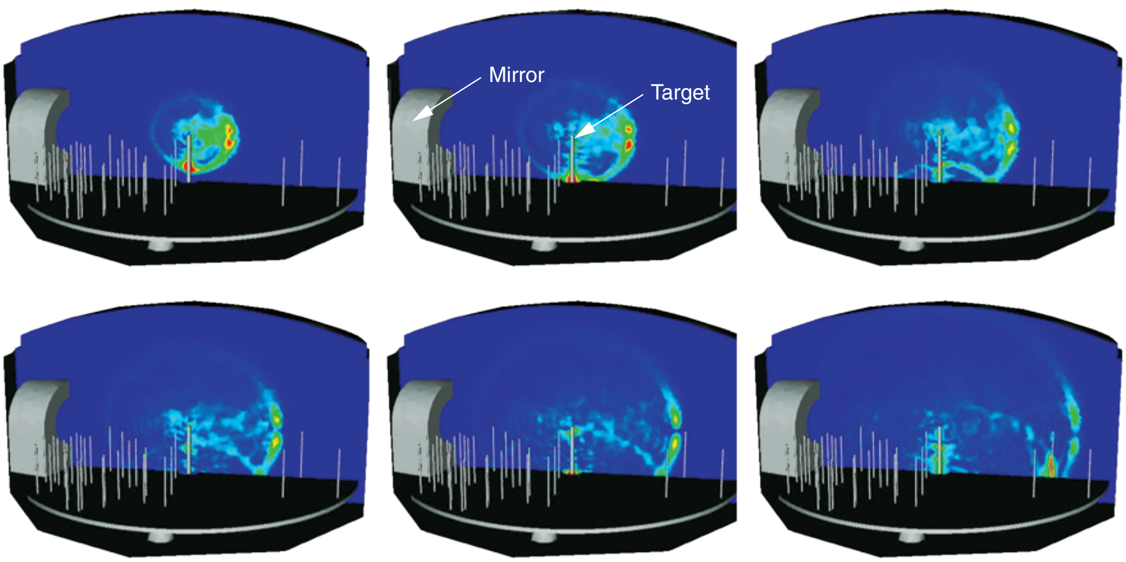
The EMSolve simulations shown on p. 9 begin with a detailed 3D model of the Titan target chamber, which is crowded with optical stands. The simulations depict electromagnetic fields flowing from the moving electron pulse as it speeds to the chamber wall, inducing currents to flow throughout the chamber. In these depictions, which represent a "slice" through the 3D data, red indicates the strongest magnetic fields while blue shows a zero magnetic field. A portion of the electron stream can be seen striking the top of a metal post supporting an experimental target. The suddenly positively charged stand is then neutralized by electrons coming up from the table that supports the experimental target.



The first three-dimensional EMSolve simulation of light in a photonic band-gap crystal tracked the propogation of signals as they made two separate 90-degree bends.



Photos of the Titan laser target chamber show the (a) exterior and (b) interior of the chamber.

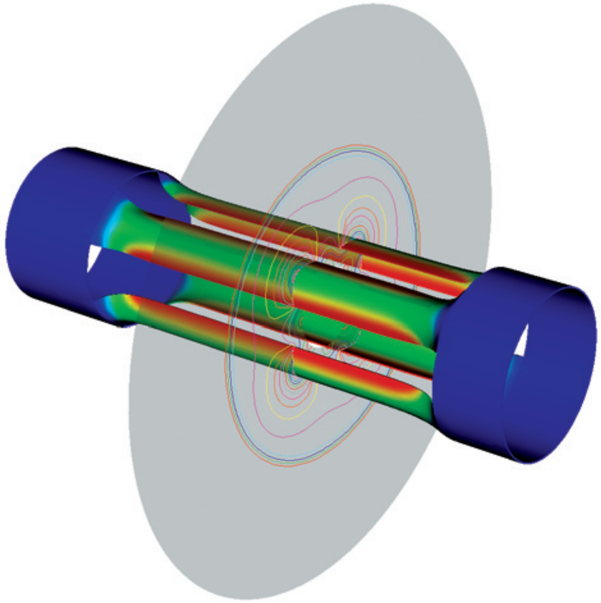


This EMSolve simulation shows the electromagnetic pulse generated by high-energy electrons streaming from the Titan laser target in time intervals separated by several picoseconds. The pulse travels from left to right, eventually hitting the target chamber wall (not shown). The stalks represent stands for diagnostic instruments and mirrors. The large curved object at left represents a mirror that directs the laser beam onto the target.

Eder is hopeful that the simulation capability can be applied equally successfully to planning experiments on other laser facilities, including NIF and LMJ. The NIF target chamber has stainless-steel louvers about 10 centimeters in length designed to reduce the amount of ablated material generated in fusion experiments. Fine structures in the target chamber, such as louvers and stands, affect high frequencies. As a result, Eder hopes to use EMSolve to model the effects of NIF louvers on EMPs. LMJ, currently under construction, will use louvers made of aluminum.

Building More Comprehensive Codes

White notes that some solid mechanics codes have grown into "multiphysics" codes, with the addition of fluid dynamics, heat transfer, and chemistry. Multiphysics codes are needed for stockpile stewardship to ensure the safety, performance, and reliability of the nation's nuclear weapons. However, most multiphysics codes do not yet solve for Maxwell's equations. Such a capability would make possible electro-thermal-mechanical (ETM) simulations, which have long been sought by engineers and scientists. An ETM simulation includes electromagnetics, heat transfer, and nonlinear mechanics (deformation of materials and friction).



This coupled electro-thermal-mechanical simulation shows a current pulse generating magnetic pressure through a 7.5-centimeter-diameter tube. The magnetic field is so intense that it crushes the tube. The solid colors represent the velocity at which it is being crushed, with red being the highest. The contour plot shows the magnitude of the magnetic field.

Because EMSolve is based on a modular software architecture, the core finite-element technology can be readily incorporated into other codes to produce ETM simulations. For example, the team has added several EMSolve modules into ALE3D, which models the response of materials to heat and explosives and other processes. The code can also model potential glass damage mechanisms in NIF, which is the most energetic laser system in the world as well as the largest optical instrument ever built. The giant laser has 7,500 large optics and more than 30,000 small optics, all of which can slowly accumulate damage from repeated firings. Physicists believe that EMSolve, coupled with ALE3D, one of Livermore's hydrodynamics codes, can help them better understand the mechanisms of glass damage and point the way to mitigation strategies.

The team has also added EMSolve modules to Diablo, a new Livermore 3D solid mechanics code developed for long-duration stockpile-stewardship-related simulations. In addition, EMSolve finite-element modules have been incorporated into HYDRA, a radiation–hydrodynamics code developed by Livermore's Inertial Confinement Fusion Program to simulate laser–plasma interactions.

Other ETM applications include electromagnetic launchers, inductive heating and mixing of metals, and microelectromechanical systems—tiny devices that integrate mechanical elements, sensors, and electronics on a silicon substrate. Sharpe notes that ETM codes will be required to accurately simulate Office of Naval Research railgun experiments. A railgun works by sending electric current along parallel rails, creating an electromagnetic force so powerful it can fire a projectile at tremendous speed. Future U.S. Navy ships may use stored electromagnetic energy to power railgun-launched offensive and defensive weapons. Livermore researchers are also interested in railguns as a possible technology for achieving velocities and pressures beyond those of Livermore's two-stage gas guns.

White predicts that EMSolve will continue to grow in adaptability, accuracy, and capability. The code is sure to play an important role in Livermore scientists' and engineers' exploration of the electromagnetic fields critical to advancing countless research programs.

—Arnie Heller

Key Words: ALE3D code, electromagnetic pulse (EMP), electromagnetism, electro-thermal-mechanical (ETM) simulations, EMSolve code, finite-element analysis, Maxwell's equations, National Ignition Facility (NIF), photonic band-gap (PBG) crystals, radar, railgun, Titan.

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Characterizing Virulent Pathogens

Multiplexed assays and proteomics research are helping the nation counter potential biothreats.

SECURING the nation against potential terrorist attacks is an increasingly complex challenge. Today's global environment requires that homeland security officials be prepared for a range of threats. One concern is that terrorists may use biological organisms to attack the U.S. To address this potential threat, the Department of Homeland Security's (DHS's) Director for Science and Technology allocates more than 40 percent of its budget to chemical and biological countermeasures research.

When Lawrence Livermore began working on the problem of biological threats in the 1990s, few solutions existed for the early detection and characterization of biological agents. Researchers in Livermore's Global Security Principal Directorate attacked the problem by integrating expertise in biology, chemistry, engineering, and computation to develop a succession of increasingly capable, rapid, and rugged biodetection instruments. Anticipating the importance of detection technologies and threat signatures in countering biological attacks, Global Security initiated several forward-thinking projects with Livermore's Laboratory Directed Research and Development

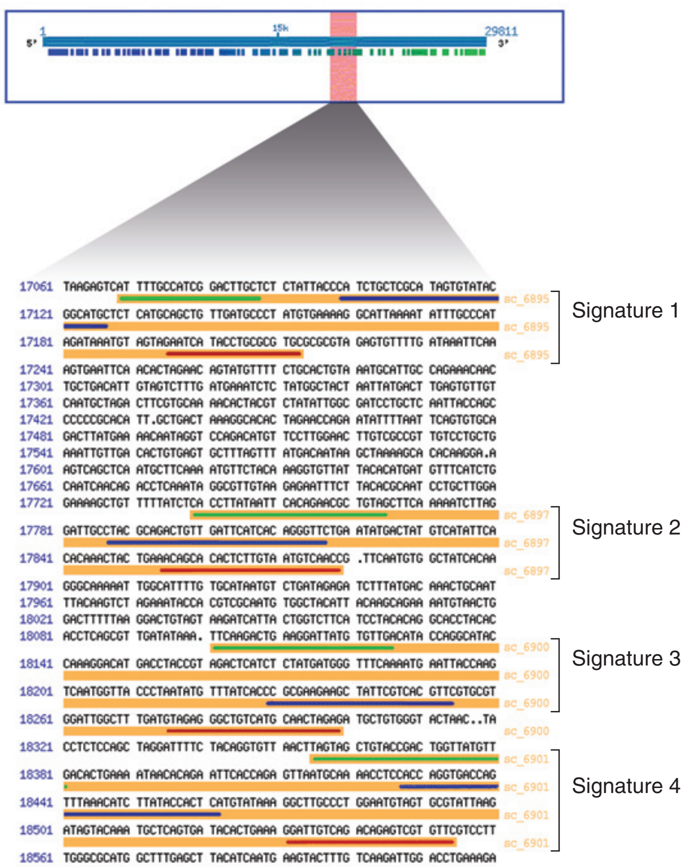
Program. They also formed partnerships with the Centers for Disease Control and Prevention (CDC), other national laboratories, and universities to develop assays for pathogens that might be used in a biological attack and those that could cause a disease epidemic.

Natural or Intentional Outbreak

Determining whether a pathogenic (disease-causing) organism has appeared through natural mechanisms or has been introduced in an act of biological terrorism is challenging. Many microorganisms occur naturally in the environment and cannot be genetically distinguished from those that might be used in an intentional release. Because of the potential impact to the country if a bioterrorist attack were to occur, scientists must be able to quickly characterize the organism in question.

Livemore researchers are addressing some of the knowledge gaps that exist in characterizing pathogens, their disease transport, and host–pathogen interaction mechanisms. "Given the capabilities of modern biotechnology," says computer scientist Tom Slezak, who leads the Laboratory's bioinformatics group, "we don't know if a disease outbreak is due to an intentional release or a natural outbreak until we can check the genome closely."

The 2002–2003 outbreak of severe acute respiratory syndrome (SARS) is a case in point. The outbreak began in China and quickly spread to Singapore, Vietnam, and Canada. Although the casualties numbered fewer than 1,000 people, the rapid spread of the disease and the lack of preparedness for an outbreak caused widespread concern. It took the international public health community about 90 days from the time unusual disease symptoms were first noticed in China until the SARS virus was finally isolated, sequenced, and identified as a new type of coronavirus. Subsequent studies identified numerous wildlife hosts, confirming that SARS was an emerging natural pathogen.



Livermore researchers used the computational design system KPATH to produce four DNA signatures of severe acute respiratory syndrome. Each signature has a forward primer (green underline), a reverse primer (red underline), and an internal probe (blue underline). An entire signature amplicon (a small, replicating DNA fragment) includes all three components.

Computers Speed Signature Analysis

Researchers develop laboratory assays to help detect organisms. The most promising assays are experimentally validated to meet rigid criteria. Researchers start with a map of the microbe's genome and determine a set of candidate signatures—patterns of DNA sequences of nucleotides unique to the organism's genome. Once validated, these signatures enable scientists to rapidly and confidently diagnose the presence of the pathogen.

Livermore's bioinformatics group, which includes biologists, computer scientists, mathematicians, and statisticians, is the largest in the world focusing on pathogen signatures, and it was first to use computers for identifying candidate signatures at a whole-genome scale. (See *S&TR*, April 2004, pp. 4–9.) The group's computational DNA-signature generation and analysis system, called KPATH, uses efficient algorithms to compare the genome of a target pathogen to a library of microbial genomes, searching for areas unique to the target organism or to the family of related pathogens. Designed after the September 11, 2001, terrorist attacks and implemented in 2002, the automated system can deliver microbial signature candidates spanning 200- to 300-plus base pairs of DNA in minutes to hours. SARS was the first natural-outbreak pathogen the group used to test KPATH's capability. When CDC asked the Livermore team to develop candidate signatures for SARS in 2003, Slezak's group did so in just three hours.

During a disease outbreak involving potentially tens of thousands of sick people, time is of the essence. Medical personnel need to know what tests to perform—for example, which bodily fluids to sample to look for the presence of a particular virus. "Clinicians must pick one of five fluid types to test," says Slezak. "Choosing the wrong bodily fluid to test could have devastating consequences in terms of the number of people who might get sick or die. Any delays can accelerate the spread of disease."

In 2006, a Livermore-developed signature for SARS was used in a landmark study to detect the virus in the bodily fluids of long-tailed macaque monkeys. For this study, researchers from the U.S. Army Medical Research Institute of Infectious Diseases infected the animals with the SARS-CoV *Urbani* strain. A key finding was that researchers did not find the virus where expected. "Conventional wisdom said the virus would appear in the feces," says Slezak. "However, in all but one monkey, the virus was found in the urine." These results will help researchers develop effective SARS vaccines and therapies. "If SARS were to reappear," says Slezak, "clinicians now know where to look for the virus in the body and when."

Nationwide Warning System

Early detection and response to the release of a potentially lethal microorganism are crucial for saving lives. In 2003, DHS launched the BioWatch program, a nationwide early-warning system that detects trace amounts of specific microorganisms in the air. The program is a collaboration of federal and state agencies, including CDC, the Environmental Protection Agency, Los Alamos and Lawrence Livermore national laboratories, the Federal Bureau of Investigation, and state and city environmental monitoring agencies.

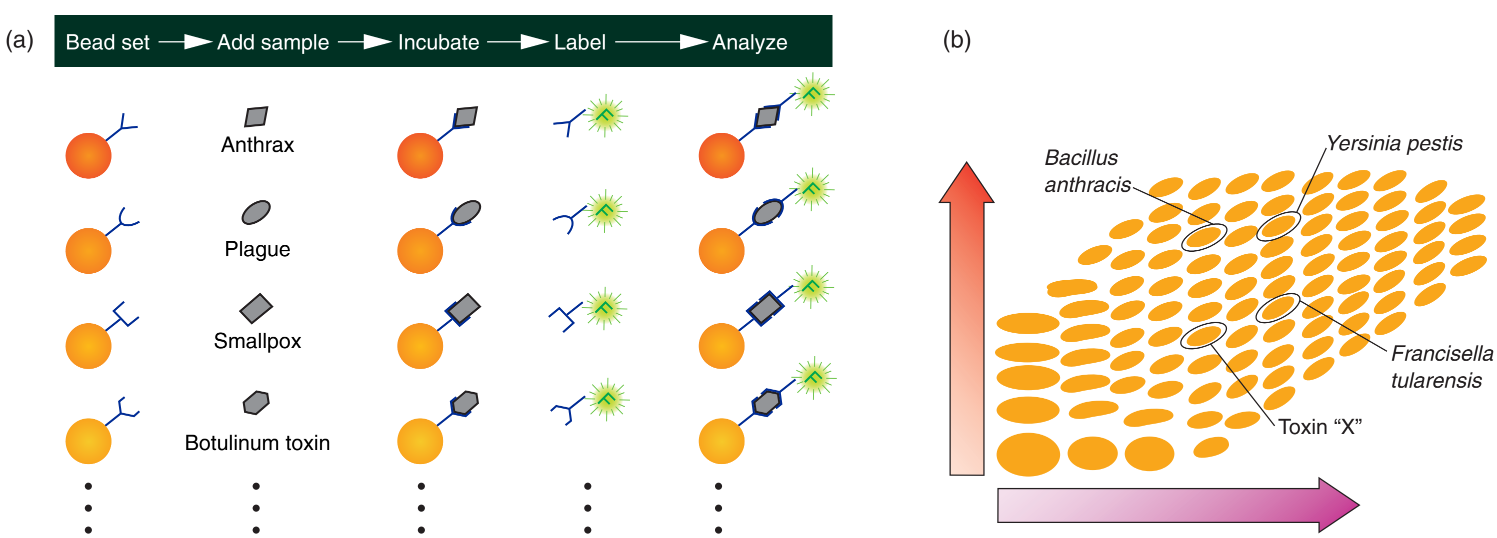
BioWatch detectors, in place in about 30 cities in the U.S., use the architecture originally developed for Livermore's and Los Alamos's Biological Aerosol Sentry and Information System (BASIS) as well as up-to-date versions of the DNA signatures used in BASIS. (See *S&TR*, October 2003, pp. 6–7.) Local agencies monitor BioWatch instruments, and CDC coordinates sample analysis through the nation's Laboratory Response Network. Scientists at participating laboratories analyze the samples using polymerase chain reaction (PCR)—a technique that replicates and amplifies a fragment of DNA to produce copies of a sequence so it can be detected.

Fast Multiplexed Assays

Typical PCR is a singleplex process—that is, it detects one signature on an organism's genome. If the result is positive for a target organism, the technician tests the sample with other signatures related to the organism to confirm the initial finding. To speed the analysis process, a Livermore team funded by DHS and CDC developed a multiplexed nucleic-acid assay that can detect multiple biological threat agents at one time. The team, led by molecular virologist Pejman Naraghi-Arani, includes James Thissen, Alda Celena Carrillo, Jason Olivas, Sally Smith, Linda Danganan, and Lance Tammero.

In developing the assay, Naraghi-Arani asked Slezak's group to screen the available genomic sequence information of selected pathogens and identify regions of interest on the genomes. Candidate signatures were compared with other microorganisms, including related strains and genetic near-neighbors of the target pathogens. The computational screening included DNA from more than 2,300 aerosol samples collected with BioWatch detectors as well as samples from soils, bacteria, insects, animals, and humans to test for cross-reactivity.

Naraghi-Arani's team then developed the multiplexed assay using a bead-based liquid array technology that extracts nucleic acids from the sample and amplifies the DNA. Polystyrene microbeads are tagged with a sequence of



(a) Multiplexed assays simultaneously detect multiple bacterial spores and cells, viruses, and toxins. (b) Using a Luminex instrument, scientists can resolve up to 100 different classes of biological organisms by their fluorescence intensity.

nucleotides that complement the signatures of interest. If a target organism is present, it will combine with a microbead. The beads are embedded with precise ratios of red and infrared fluorescent dyes. When excited by a laser, the two dyes emit light at different wavelengths. The ratio of each dye reflected emits light at a unique frequency that identifies the organism. An additional dye is used to indicate if the bead detected the unique signature DNA of the pathogen of interest.

The multiplexed assay requires only picogram quantities of DNA and contains all verification signatures in one reaction. "The sensitivity is as good as the best singleplex assay," says Naraghi-Arani, "and the cost savings is about 90 percent." The team subjected the multiplexed assay to a series of verification tests. "Even in a mixture containing large amounts of a variety of DNA masking the target DNA, the assay panel still identified the presence of the target organisms," says Naraghi-Arani. "These results demonstrate that with a rigorous bioinformatics process, a multiplexed assay can be simpler to run than a singleplex assay."

Next-Generation BioWatch

DHS and CDC have evaluated the multiplexed assay to determine if it could be incorporated into BioWatch sample screening. In collaboration with the agencies, Thomas Bunt, associate program leader for Livermore's biological monitoring and response group, conducted a six-month pilot study to compare the multiplexed assay performance to that of the existing BioWatch format. Naraghi-Arani's team participated in the pilot. Says Bunt, "The multiplexed assay contained more than 25 pathogen signatures. Labor and reagent costs were dramatically reduced because we were able to combine multiple BioWatch verification assays into a single reaction."

The researchers analyzed more than 12,000 filter extracts. Results demonstrated that the multiplexed assay yielded faster verification results while maintaining sensitivity of pathogen detection. DHS is incorporating the multiplexed assays into the BioWatch system. "Livermore has been involved in every step of the development process, from bioinformatics to assay validation, protocol development, and data management," says Bunt. "We also operate two BioWatch laboratories so we are end users as well."

Testing for Animal Diseases

DHS is also funding work at Livermore and elsewhere on multiplexed assays to detect agricultural diseases. A number of very serious animal diseases are endemic in other parts of the world but have not appeared in the U.S. for several decades. (See *S&TR*, May 2006, pp. 11–17.) Agriculture is a major sector of the U.S. economy, accounting for more than 13 percent of the gross domestic product and employing more than 15 percent of the U.S. population. Homeland security officials are concerned that terrorists might attempt an attack on the nation's agricultural industry.

Molecular virologist Ray Lenhoff, veterinary epidemiologist Pam Hullinger, and chemist Ben Hindson are collaborating with the Department of Agriculture's National Veterinary Services Laboratory and the Foreign Animal Disease Diagnostic Laboratory at Plum Island, New York, the agency responsible for testing and investigating foreign animal diseases. Plum Island conducts about 300 investigations each year, but during a major outbreak, demand could rise to 100 investigations per week.

The clinical signs of foreign animal disease often closely mimic many diseases that regularly occur in animals. A particular concern is foot-and-mouth disease, an extremely contagious viral disease of cattle, pigs, sheep, goats, deer, and other ruminants. "Traditional tests use a single detection assay to look for one virus at a time," says Lenhoff. "A negative test result could mean either that the assay failed or that the disease wasn't present." The team's first version of the multiplex assay screens for both DNA and RNA viruses and looks for 17 target signatures, including seven major strains of foot-and-mouth disease.

An outbreak of a foreign animal disease, such as foot-and-mouth disease in the U.S., could be devastating to the nation's economy.

The researchers are working on two additional assays: one for diseases affecting cattle and one for those affecting swine. Once they complete the initial development and characterization studies, they will send the assays to Plum Island for additional testing. The team has also developed a high-throughput, semiautomated system that can process more than 1,000 samples in 10 hours using a single line of equipment and two technicians.

In 2006, Hindson led an exercise involving 14 laboratories that belong to the National Animal Health Laboratory Network to evaluate the performance of the multiplexed assays in the hands of end users. Hindson's team "spiked" the test samples with known domestic viruses that mimic foot-and-mouth disease. The laboratories then analyzed the samples and reported their findings to Livermore. The exercise allowed researchers to test the assays with multiple users and obtain a large data sample to measure the performance of the signatures included in the multiplexed panels.

Identifying Virulent Proteins

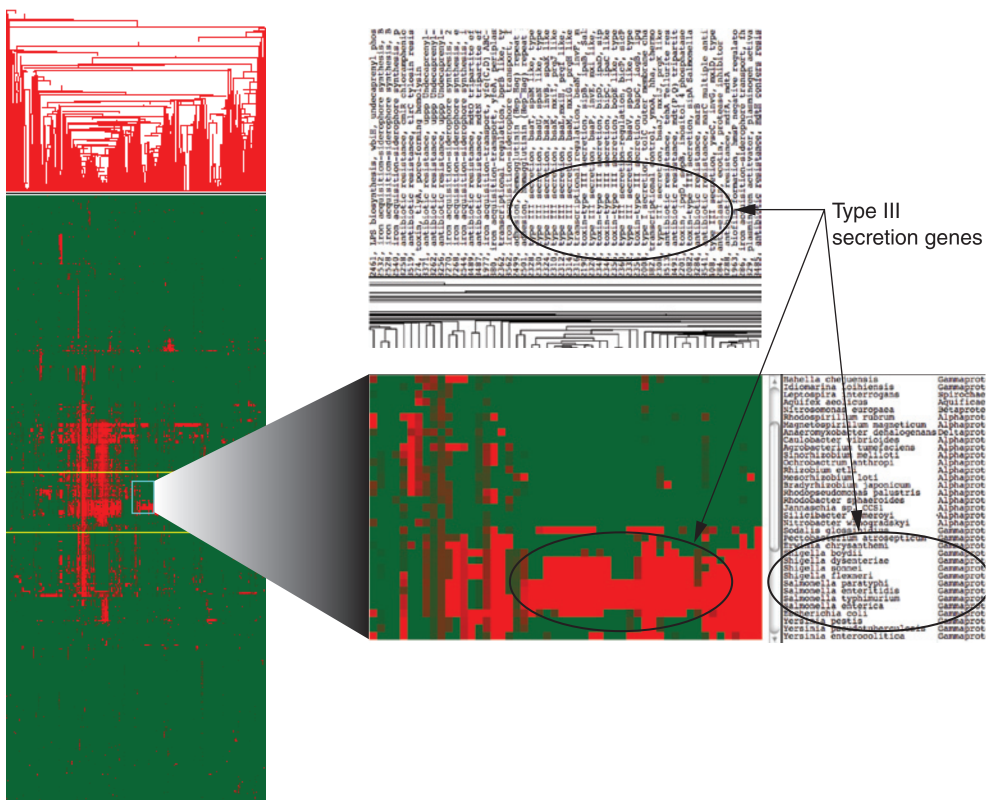
Although an assay can confirm the presence of a microbial species, it is limited in the information it can provide about the species' strain and virulence. For example, of the SARS signatures Slezak's group developed in 2003, it is not clear which, if any, identify genes related to virulence factors or which types of hosts the virus could infect. To develop countermeasures against a particular disease, scientists must understand the pathogen's replication mechanism, including how it confers virulence. Slezak's group is using computational analyses to determine patterns characteristic of an organism's potential virulence mechanisms, including antibiotic resistance. They are applying the data to develop recognition assays using NimbleGen® microarrays, which detect up to 390,000 specific genetic features that serve as signatures for particular functional mechanisms. The microarrays provide a "parts list" of functional elements to more fully characterize a BioWatch positive hit or other sample.

Livermore researchers are also conducting proteomic experiments to study virulence mechanisms. Proteomics characterizes all proteins within a cell, including protein expression levels. Some pathogen proteins, known as virulence factors, are responsible for conferring a pathogen's virulence. The key to characterizing a pathogen's virulence potential lies in knowing which proteins and how much of them are expressed.

A Livermore team led by protein chemist Sandra McCutchen-Maloney identified virulence-inducing mechanisms in the *Yersinia pestis* bacterium, the pathogen that causes plague. The *Y. pestis* work draws on earlier Laboratory studies. (See *S&TR*, March 2002, pp. 4–9.) The team, which includes Brett Chromy, Todd Corzett, and Ann Holtz, is collaborating with Walter Reed Army Medical Center, Texas A&M University, University of California at Davis, University of Minnesota, and Pacific Northwest National Laboratory. To augment the gene expression research, McCutchen-Maloney's team provides proteomic data on pathogens and host response to pathogen exposure. The researchers will use these data to improve the assays so that they characterize threat pathogens and can identify exposure in humans and animals before symptoms become apparent.

Naturally occurring plague is transmitted from infected fleas or rodents to humans. Three forms of the disease exist: bubonic, septicemic, and pneumonic. Bubonic and septicemic forms can most often be treated with antibiotics; the disease of pneumonic plague is suppressed at the temperature of a flea (26 °C). However, at 37 °C, the body temperature for humans, virulence factors are expressed. By activating virulence mechanisms in *Y. pestis* through laboratory-induced growth conditions and then measuring cell contents, researchers can link proteomic data with genomic data and better understand pathogen virulence levels.

Dozens of proteins are responsible for virulence in *Y. pestis*. McCutchen-Maloney's team is studying 22 *Y. pestis* strains representing diversity of origin, virulence level, and countermeasure



Computed data compare known virulence and antibiotic-resistance mechanisms (columns) for all sequenced genomes (rows). Red indicates a mechanism is present, while green indicates it is not. Type III secretion is a mechanism that occurs in many pathogens, including *Shigella*, *Salmonella*, *Yersinia*, and *Escherichia coli*.

resistance to determine individual protein expression levels. Adding fluorescent dyes to multiplexed gels allows the researchers to measure differences in the abundance of expressed proteins among the various strains. Then using mass spectrometry, they can identify the proteins of interest—data that will guide the assay development work.

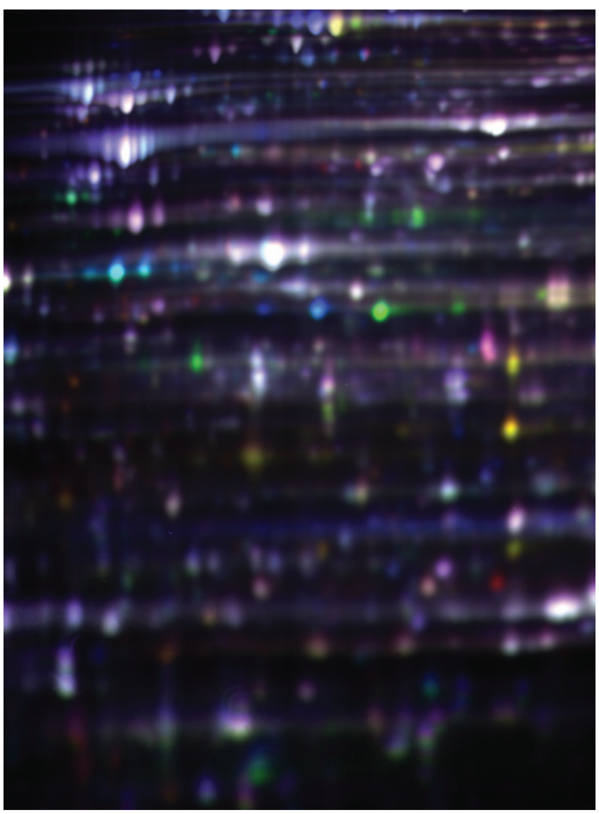
Host–Pathogen Interactions

The team is also attacking the problem from the other end—observing how a host's body interacts with the pathogen. Host–pathogen interactions contain biomarkers such as protein by-products that reveal virulence characteristics. McCutchen-Maloney says, "A lot of people can start showing up sick, as in the SARS cases in 2003. When health officials don't know what they are dealing with, it would be helpful to test patients for biomarkers that could identify the pathogen."

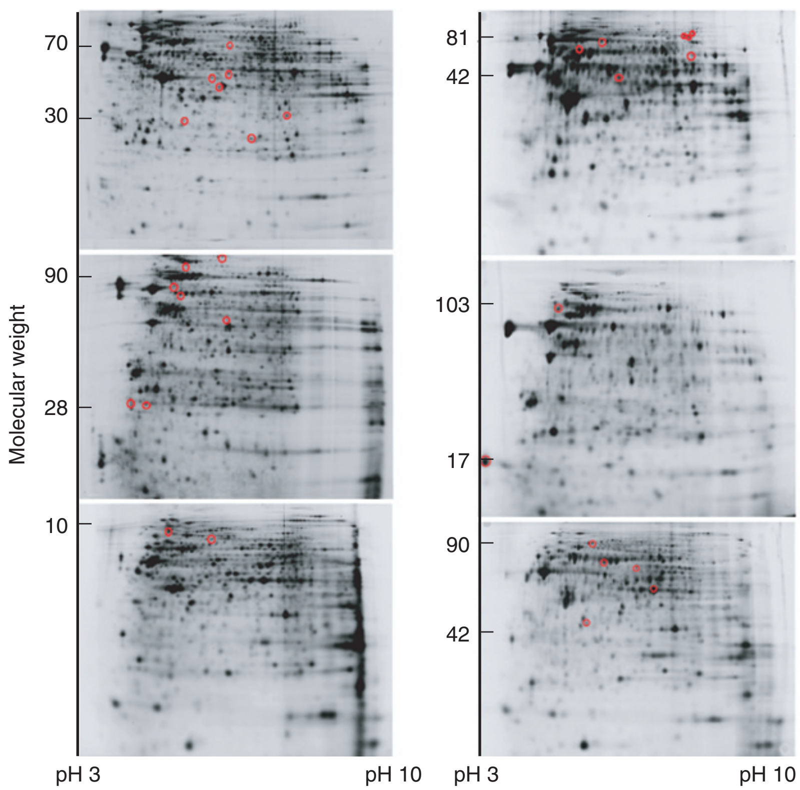
In one experiment, the Livermore team exposed human monocytes to *Y. pestis* and *Y. pseudotuberculosis*. The group identified 16 differentially expressed host proteins in the *Y. pestis* exposure and 13 host proteins in the *Y. pseudotuberculosis* exposure. Only two of the proteins were shared between the two exposures, indicating different immune response mechanisms.

The team also examined virulence mechanisms in two closely related strains of *Y. pestis*, one of which caused pneumonic plague in an animal model. Although the two strains are virtually identical at the gene level, they exhibited more than a 1,000-fold difference in pathogenicity, or virulence level. The research demonstrates that detection alone does not reveal virulence potential. "Near-neighbors can be that important," says McCutchen-Maloney. "It can be the difference between quick death and an upset stomach." The work will help researchers look for better ways to detect and understand virulence within the multiple strains of a species.

The team is working to build a pathogen reference library of information on known, unusual, and emergent pathogens. "The more organisms we can catalog in the



A two-dimensional gel map of 22 strains of *Yersinia pestis* shows more than 2,800 differentially expressed proteins (spots). The colored protein spots represent a *Y. pestis* strain that expressed a large amount of a particular protein.



Gel images of human macrophage cells exposed to *Yersina pestis* (left) and *Y. pseudotuberculosis* (right) display distinct profiles. Proteins from three different protein components are measured according to their molecular weight and pH level. Scientists then perform mass spectrometry on selected areas (red circles) to measure the amount of expressed proteins.

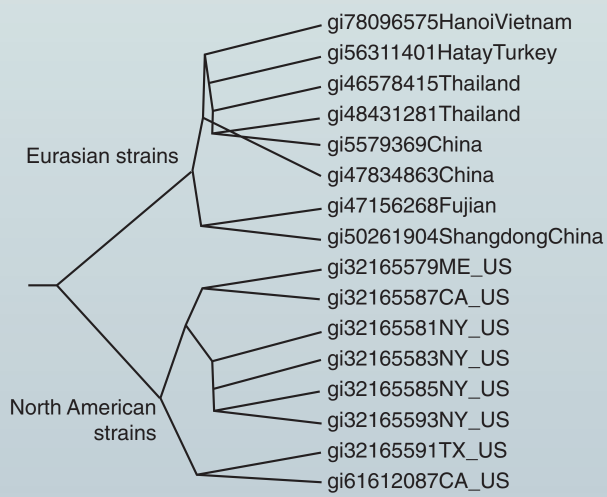
Nature's Ever-Changing Organism

Influenza, or the flu, sickens millions of people and is responsible for up to 500,000 deaths worldwide each year. New influenza viruses are produced by mutation or by reassortment—a process in which two similar viruses infect the same cell and their genetic material mixes. New flu vaccines are formulated every year based on the strains observed in the previous year and on expert opinion about which strains are expected to dominate worldwide in the next flu season.

In 2004, the Centers for Disease Control and Prevention called on Livermore scientists to develop candidate signatures for human and avian influenza viruses. Health officials are concerned about the possibility of a flu epidemic from any host since the influenza virus mutates so rapidly. Beth Vitalis, lead biologist for Livermore's pathogen bioinformatics group, explains, "Numerous strains of influenza circulate through the population every year, and a concern is that one of these strains could acquire an extreme virulence potential similar to the 1918–1919 influenza strain. A potentially more serious threat is that a lethal avian strain will mutate such that it can become readily human transmissible." The 1918–1919 pandemic killed approximately 50 million people worldwide. With today's travel patterns, an unchecked similar pandemic could be even more devastating.

As in the 1918–1919 flu pandemic, the body's immune system often accelerates the host's death. For example, when the body is attacked by a pathogen, one of its defense mechanisms may be to produce a higher level of inflammatory cytokines—proteins that are activated by immune cells and cause inflammation. The resulting inflammation can cause overwhelming damage to body tissues and organs.

Avian influenza infections of humans are relatively rare and have yet to occur in North America. Nevertheless, health officials want to prepare for the possibility that a strain of avian flu could become transmissible from human to human. "The influenza virus evolves rapidly," says Vitalis, "so diagnostics and vaccines must be continually evaluated and updated to be effective against circulating strains."



A computational clustering technique is used to group H5 avian influenza strains based on geographic lineages. All avian strains of influenza infecting humans have been of Eurasian lineage. To date, domestic avian influenza is not transmissible to humans.

library, the better we will be able to say with confidence, 'this looks like *Bacillus anthracis*, but it's not *anthracis*,'" says McCutchen-Maloney.

One of McCutchen-Maloney's next goals is to study viruses, which are more diverse than bacteria and can mutate or change much more rapidly. (See the box above.) As with bacteria, the mechanisms that drive viruses must be understood if researchers are to develop detection methods and countermeasures against them. However, viral mechanisms are more complicated than bacterial processes. Bacteria essentially carry all the parts they need to infect their hosts. In contrast, viruses must recruit or hijack some parts from a host's cells to do their damage.

By developing assays screened by a rigorous bioinformatics process and identifying pathogen replication mechanisms and host-response biomarkers, Livermore researchers are helping DHS and other health and security agencies strengthen the nation's biodefense preparedness programs. Events such as the 2003 SARS outbreak and the potential for an avian influenza outbreak or epidemic provide on-the-job training that prepares Laboratory scientists for rapid response. "We don't want to be unprepared, whether a disease outbreak is intentional or unintentional," says Slezak. "Our research is aimed at helping public health and homeland security officials make informed decisions about responding to and limiting the effects from any type of outbreak."

—Gabriele Rennie

Key Words: biological agents, BioWatch, foot-and-mouth disease, foreign animal disease, influenza, KPATH, multiplexed assays, pathogen, severe acute respiratory syndrome (SARS), virulence.

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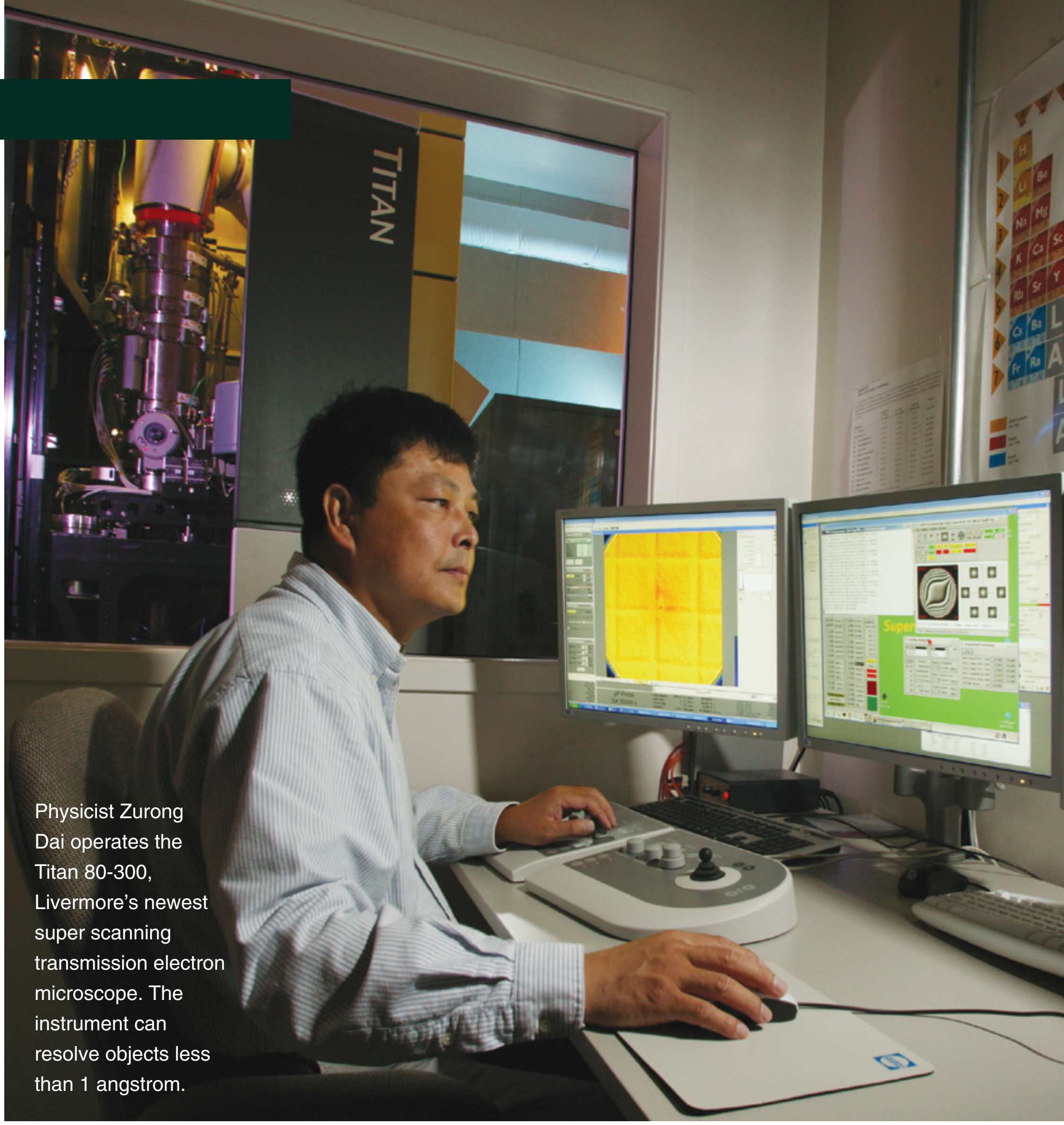
Imaging at the Atomic Level



Physicist Zurong Dai operates the Titan 80-300, Livermore's newest super scanning transmission electron microscope. The instrument can resolve objects less than 1 angstrom.

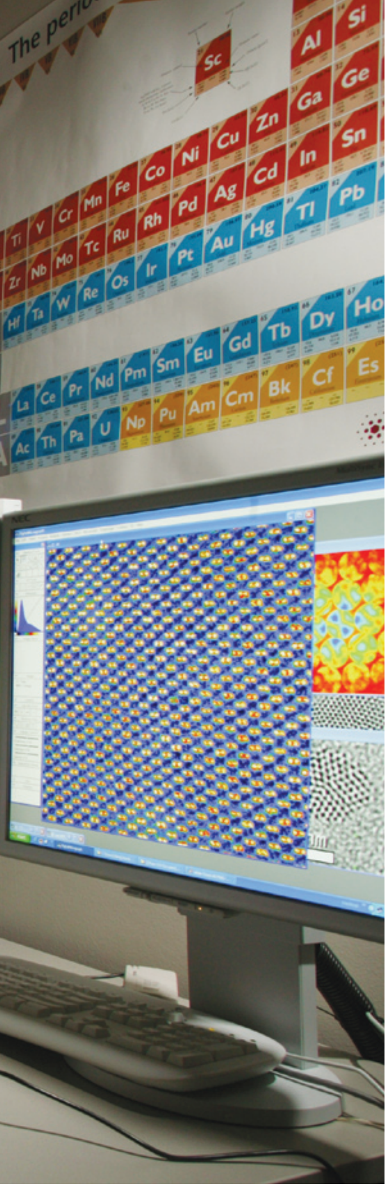
FOLLOWING the successful recovery of the National Aeronautics and Space Administration's (NASA's) Stardust sample-return capsule in January 2006, scientists began extracting and analyzing samples from Comet Wild 2 that were embedded in the spacecraft's cometary particle collector. Particles were trapped both in the collector's silica aerogel cells and in craters that formed in the aluminum foil wrapped around the collector grid walls. In December 2006, Livermore scientists were among the researchers who announced results of some of the first cometary particle analyses. (See *S&TR,* April 2007, pp. 4–11.) Those analyses were greatly aided by the Laboratory's super scanning transmission electron microscope known as SuperSTEM—the highest resolution microscope in the world.

"Stardust particles are aggregates of carbonaceous matter, glass, and crystals with a grain size of 2 to 5 nanometers," says physicist John Bradley, director of Livermore's branch of the University of California's Institute of Geophysics and Planetary Physics. "Understanding such complex assemblages requires mapping them with the highest possible spatial resolution because a portion of the most significant information is detectable only on the atomic scale."

SuperSTEM technology uses monochromators and image correctors for analyzing a particle's composition on the atomic scale, resulting in stunning pictures magnified more than l million times. Using SuperSTEM and other analytical instruments, many of them located at Livermore, scientists have found Comet Wild 2 is full of complex minerals and other material that originated in the inner solar system. Yet, the comet was formed a long distance from the Sun, far beyond the orbit of Neptune.

SuperSTEM is an advanced form of a transmission electron microscope, which evolved from the first electron microscope developed in Germany in 1931. A transmission electron microscope uses a focused beam of energetic electrons to penetrate an extremely thin-sliced specimen. The instrument allows researchers to analyze the shape and size of particles making up a specimen, its constituent elements and compounds, and the arrangement of the atoms in the specimen's crystalline lattice.

SuperSTEM focuses an electron beam on a narrow area of the sample and then scans it in a raster pattern. The rastering of the electron beam makes possible analysis techniques such as electron



energy-loss spectroscopy (EELS), which provides information on the electronic properties of materials. EELS can derive the identity and chemical and electronic states of atoms by measuring the amount of energy lost in interactions with electrons from SuperSTEM's beam. This information is obtained simultaneously as an image builds up, thereby forming a direct correlation between the image and electronic data.

Record Resolution

Bradley focused on emerging SuperSTEM technology in 1999 with the goal of achieving a resolution of less than 1 angstrom (0.1 nanometer) to address challenges in astromaterials science. "We had never achieved subangstrom resolution, but I knew we could effectively use this technology to examine fine-grained extraterrestrial materials from Stardust and other space missions," says Bradley. (Atoms range in diameter between 1 and 3 angstroms; the space between atoms in a crystalline lattice is about 4 angstroms.)

Bradley met with microscope experts from the FEI Company in Eindhoven, Netherlands, to discuss the essential elements of a SuperSTEM. The goal was to image structures with atomic resolution and simultaneously provide information on the chemical composition, bonding, and electronic structure of the material under analysis. SuperSTEM's monochromator would reduce energy spread in the electron probe from about 1 to 0.1 electronvolt—a capability comparable to that provided by synchrotron facilities. In addition, spherical aberration correctors would remove image blurring in the lens of the microscope to improve image resolution by nearly tenfold.

The use of both aberration correctors and monochromators, not previously combined in transmission electron microscopes, would mean tighter, brighter beams yielding a stronger signal, higher imaging contrast, greater analytical sensitivity, and unprecedented spatial and spectral resolution. The specifications also included digital imaging, an ultrahigh-stability power supply, and systems to suppress mechanical vibration and electronic noise.

The first machine produced by FEI, called Tecnai, was funded jointly by NASA's Sample Return Laboratory Instrument and Data Analysis Program and Lawrence Livermore. Tecnai was installed at Livermore in 2004 in a laboratory designed specifically to dampen vibrations, suppress ambient magnetic fields, and reduce variations in temperature. "The instrument is so sensitive that I have to hold my breath when taking a picture to keep the image from blurring," says Livermore physicist Zurong Dai.

Tecnai, which can achieve about 1.4-angstrom resolution, incorporates some but not all of the SuperSTEM features Bradley requested. Its most important feature is a monochromator that operates at 200 kiloelectronvolts. The monochromator, located at the beam source, reduces energy spread in the beam for high-resolution EELS to reveal bonding, valence state, and electronic properties. Tecnai's energy resolution (0.1 electronvolt) provides more than 100 times improved spatial resolution.

Livermore scientists and colleagues from other research institutions have used Tecnai to study the mineralogical and chemical composition of Stardust samples. Materials scientists and biologists have also found the machine's extreme powers of magnification to be invaluable.

Miaofang Chi, a University of California at Davis student and a participant in Livermore's Student Employee Graduate Research Fellowship Program, used EELS on Tecnai to identify osbornite (titanium nitride), a mineral formed at high temperatures that was found imbedded in Stardust silicates. "The machine is easy to operate and user friendly," she says. "Everything is computerized. For example, the microscope alignment can be stored and easily reloaded for another experiment."

Chi has applied her expertise gained from the Stardust project to study man-made compounds called vanadium perovskites. These compounds have strong electron correlations with physical properties that can be tailored by substituting different elements. Some of them are candidates for multiferroic materials, which exhibit both magnetic and ferroelectric properties.

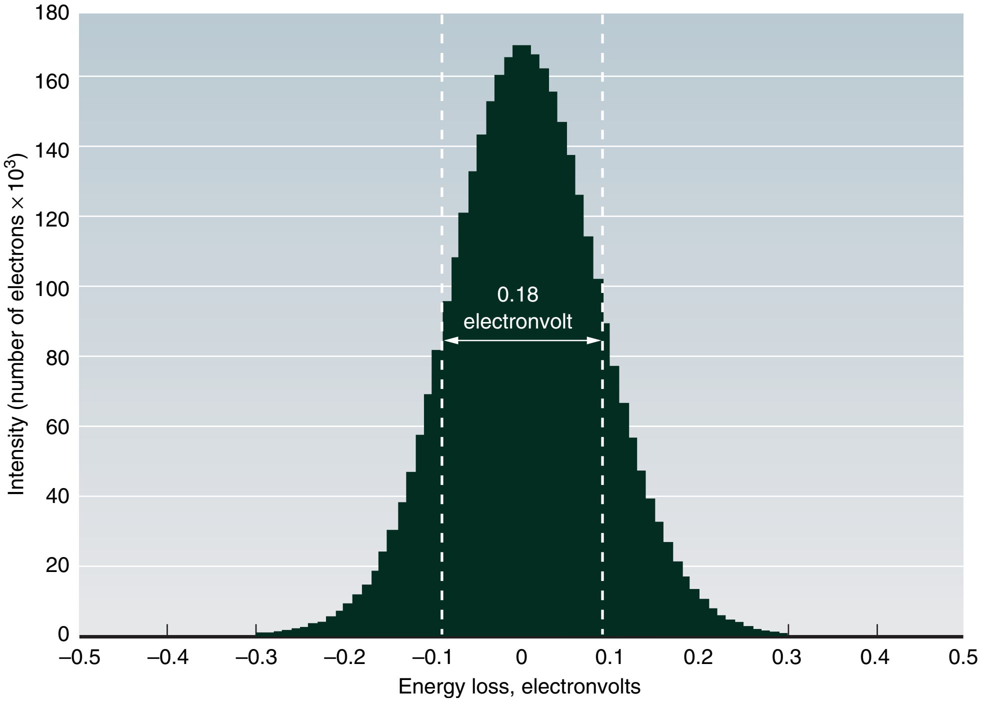
Vanadium perovskites are useful for semiconductor devices, switches, and data storage. Working with chemist Nigel Browning of the Chemistry, Materials, Earth, and Life Sciences Directorate, Chi is examining the electronic and atomic structures of perovskite thin films and nanomaterials. In addition to improving understanding of electron correlated materials, this work could lead to entirely new materials.

Titan More Advanced

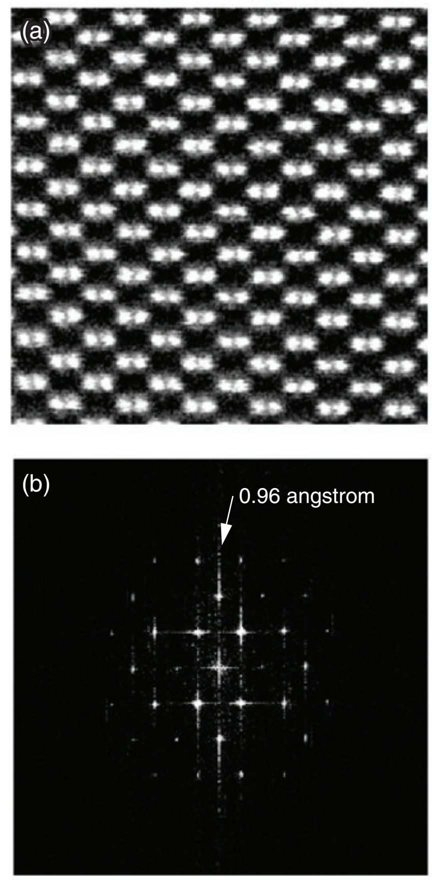
Tecnai is being replaced with a more advanced SuperSTEM called Titan 80-300. This machine features the same monochromator as Tecnai but has two additional spherical aberration correctors to resolve features as small as 0.8 angstrom. Spherical aberrations have long interfered with the ability to clearly image material interfaces with atomic detail.

Titan operators will be able to choose voltages accelerating between 80 and 300 kiloelectronvolts. A higher voltage improves spatial resolution and permits thicker samples to be examined. However, some specimens can be sensitive to damage by high-energy electrons. In such instances, operators will be able to choose a lower setting.

Titan will be used in Livermore's continuing Stardust particle analysis effort and in an increasing number of materials science–related research projects, especially those involving novel nanomaterials. Bradley explains that in nanomaterials, the atomic structure of layer interfaces and the thickness of extremely thin



Titan's monochromator reduces energy spread in the beam used for high-resolution electron energy-loss spectroscopy, which yields information on the electronic properties of materials. This graph shows that Titan achieves an average 0.18-electronvolt energy resolution when operating at 300 kiloelectronvolts. In contrast, other 300-kiloelectronvolt scanning transmission electron microscopes typically obtain about 0.75-electronvolt resolution under ideal conditions.



(a) Titan's resolving power of less than 1 angstrom is shown here with silicon "dumbbells." (b) A corresponding diffraction pattern of the same sample indicates that a subangstrom spatial resolution was achieved.

layers, many measuring less than 1 nanometer, determine their properties. Therefore, images with ultrahigh atomic resolution are needed to understand a material's properties and dimensions and to improve its performance. Chi, for example, plans to use Titan to study the effects of oxygen vacancies within atomic lattices on nanomaterials used in electronic switches and fuel cells.

Bradley notes that SuperSTEM is one of several advanced analytical instruments at Livermore. Other machines include the nanometer-scale secondary-ion mass spectrometer known as NanoSIMS, a dual-beam focused ion beam, an ultramicrotome (for cutting cell sections), and a clean room.

By combining microanalytic instruments such as these, Livermore researchers are at the forefront of characterization materials at the nanoscale. Bradley says, "We are developing an integrated microanalysis capability to enable a new level of investigations into the mineralogical, chemical, and isotopic properties of nanomaterials. The initial development is being carried out on natural nanomaterials captured during the Stardust mission. The Stardust studies are developing capabilities directly applicable to Laboratory missions in stockpile stewardship and homeland security that require characterization on the nanoscale and beyond."

For example, researchers plan to use Titan to determine the microstructure of natural uranium minerals as references for nuclear forensics investigations. Other applications include studying grain boundaries in semiconductors and determining the composition of room-temperature gamma-ray detectors.

The National Center for Electron Microscopy at Lawrence Berkeley National Laboratory has also purchased a Titan 80-300. "Over the next few years, I expect that many institutions will be acquiring a similar machine," says Bradley. As word spreads about SuperSTEM's capabilities, Livermore researchers in disciplines ranging from biological science to semiconductors are planning to use it as a powerful tool for imaging and analysis. Their results should allow them to better understand existing materials and to develop new materials with novel characteristics.

—Arnie Heller

Key Words: electron microscope, electron energy-loss spectroscopy (EELS), monochromator, nanomaterials, Stardust spacecraft, super scanning transmission electron microscope (SuperSTEM).

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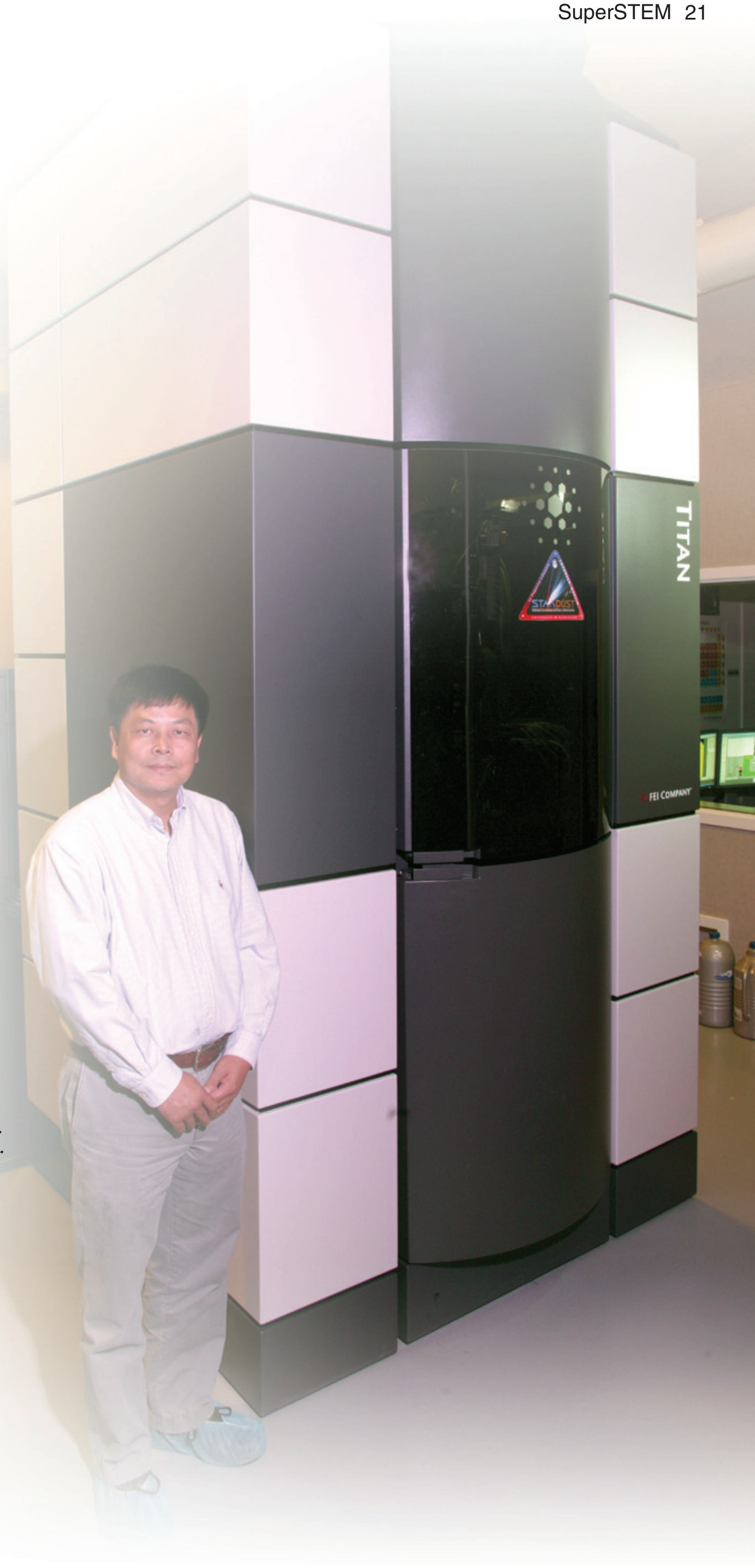

Scientists without Borders

Lawrence Livermore is one of five U.S. national laboratories participating in the International Nuclear Safeguards and Engagement Program. The U.S. has signed arrangements with 10 countries (blue dots). An arrangement with Malaysia (green dot) is being negotiated.

THE International Nuclear Safeguards and Engagement Program (INSEP) operated by the Department of Energy National Nuclear Security Administration (DOE/NNSA) supports international outreach akin to Doctors without Borders, the international organization that provides emergency medical treatments to people caught in disaster situations. Instead of offering medical aid, INSEP provides expertise on the peaceful uses of nuclear science and technology and nuclear infrastructure preparedness. Begun in the early 1980s as the Sister Laboratory Program, INSEP established cooperative institutional relationships between U.S. national laboratories and their counterparts in other nations. Today, the program seeks to assist cooperating nations in meeting the technical requirements associated with civilian nuclear power development in a manner that promotes international nonproliferation norms.

"The idea had its genesis in the Department of State and DOE as a way to engage with nonnuclear countries that had signed the Nuclear Non-Proliferation Treaty," says Mo Bissani, who manages the sister laboratory activities in the Global Security Principal Directorate's Nonproliferation Program. "Through bilateral cooperative arrangements, these activities establish direct lines of communication between nuclear specialists in the U.S. and those in the participating countries."

A Program for Peace

The Treaty on the Non-Proliferation of Nuclear Weapons is part of a decades-long international effort to control the proliferation of nuclear weapons while making the peaceful use of nuclear technology widely available. Under the terms of this treaty, the five acknowledged nuclear weapon states—the U.S., U.S.S.R., United Kingdom, France, and China—agreed not to transfer nuclear weapons, other nuclear explosive devices, or related technology to the signatory states with no nuclear weapons. The five nations also pledged to work toward eventual elimination of their own nuclear stockpiles. The signatory nonnuclear states, in turn, agreed not to acquire or produce nuclear weapons or nuclear explosive devices. In exchange, these states would have access to peaceful nuclear technologies for such applications as energy generation, medical use, and research.

The International Atomic Energy Agency (IAEA) oversees the primary multilateral methods for helping the nonnuclear countries use these technologies through its Technical Cooperation Programme. One way the U.S. provides technical cooperation is through INSEP. "Nuclear energy is bound to play an increasing role in the future as oil reserves are depleted—even in countries that export oil," says Bissani. "Countries must have the information and technical expertise they need to make this a safe, secure, and successful endeavor."

INSEP addresses the growing interest in nuclear energy in several ways. Assistance in nuclear safeguards helps participating countries meet international standards for nuclear material accounting and control. Nuclear infrastructure preparedness assistance provides them with the technical capabilities to develop nuclear power safely and securely while meeting international norms and requirements. Specific topics for cooperation include radiation protection, reactor operations, and radioactive waste disposition.

Through INSEP, scientists from Lawrence Livermore and other national laboratories work with their international counterparts, exchanging information on subjects ranging from radiation protection and health physics to radioactive waste management, research reactor optimization, radioisotope production, neutron activation, and emergency response protocols. “At Livermore, we have decades of experience that we can share with our counterparts across the world,” says Bissani, “and we are happy to pass this expertise on to others.”

Mexico was the first beneficiary of the nuclear engagement program. In 1982, its National Institute of Nuclear Research was paired with Los Alamos National Laboratory. Today, the list of participating countries includes Algeria, Argentina, Egypt, Libya, Morocco, Peru, Romania, Thailand, and Vietnam. Five national laboratories participate: Lawrence Livermore, Los Alamos, Sandia, Oak Ridge, and Argonne. Universities such as the University of Texas at Austin, University of California at Davis, Texas A&M University, Massachusetts Institute of Technology, and University of Missouri also contribute.

Livermore leads collaborations with the North African region, which includes Algeria, Egypt, Libya, and Morocco. “The program started with exclusive laboratory-to-laboratory links,” says Bissani. “Since then, NNSA has restructured it so that people can be pulled from any participating laboratory or university. That way, the best experts are assigned to each collaboration.”

INSEP offers unclassified technical assistance at different levels. Once a bilateral arrangement is signed, U.S. researchers meet with a facility’s scientists and engineers to develop action sheets that outline the scope of a specific project, its schedule and tasks, and the roles and responsibilities for all participants. “When the action sheets are signed, we send experts from Livermore and other organizations on a brief expert mission,” says Bissani. “These people stay in the host country for a week or so, where they provide hands-on training, attend seminars, and give presentations on the subject.”

In 2002, for example, Livermore researchers traveled to Morocco for an expert mission with researchers at the Moroccan National Center for Nuclear Energy Sciences and Techniques. The Moroccan equivalent to a U.S. national laboratory, the center operates the newly constructed research reactor at the Nuclear

At left, two scientists from Morocco receive training on nuclear reactor safety from a colleague at the University of Texas at Austin. Above, Livermore scientist Paris Althouse (background) demonstrates a sampling technique used for a baseline characterization project in Morocco.

Members of the U.S. delegation working with Libya's Tajura Nuclear Research Center are (from left) Mary Ann Parker, Population Services International; Chris Eves, U.S. Embassy in Libya; Greg Jones, Livermore; Maggie Manning, Department of Energy (DOE); Dewey Sprague and Mo Bissani, Livermore; and Ken Apt, DOE.

Research Center in Maamora. Built to international nuclear safety standards, the research reactor will be used for such civilian purposes as basic science and research, industrial applications, and medical isotope production. It will also lay the groundwork for nuclear-generated electrical power, should Morocco choose to develop this energy source.

On the 2002 trip, the Livermore team analyzed environmental samples to characterize the background, or baseline, of nonradiological constituents in various media at the Maamora facility. Samples included surface soil and water, groundwater from underground wells, short-lived vegetation such as grass, and long-lived vegetation such as oak trees. At the time of sampling, most of the buildings and laboratories had been built, but no construction activities had begun in the area zoned for the research reactor.

Action sheets may also specify a hands-on activity that can only be supplied in the U.S., such as training personnel on reactor operations. For these projects, the program authorizes scientists from the foreign facility to visit the U.S. for up to two months, depending on funding availability. Livermore also leverages its resources by using IAEA fellowships to meet some of the training requirements.

"We complement the IAEA program," says Bissani, "we don't compete with it." For instance, IAEA fellowships supported three researchers traveling to Livermore from Morocco. One scientist stayed more than four months to study Lawrence Livermore's approach to nuclear waste characterization, sampling, treatment, and disposal. A second Moroccan researcher focused on nuclear chemistry, and a third learned about techniques for managing nuclear waste.

Another approach to international cooperation is to provide regional training through workshops and seminars. "We often send our experts into a country to conduct a workshop and invite scientists in nearby countries to participate," says Bissani.

"When our team led a workshop at the Egyptian Atomic Energy Authority in Cairo on neutron and prompt gamma activation analyses, we also invited our colleagues from Algeria, Libya, and Morocco." Conducting workshops in a participating country instead of in the U.S. often makes travel and other logistics easier for the attendees.

The NNSA program can also facilitate material exchanges of goods and equipment between a U.S. laboratory and a participating facility. For example, researchers can arrange to transfer samples, materials, and components to their counterpart laboratories or help them acquire reference materials and difficult-to-obtain items, such as radiation monitoring and waste treatment equipment.

Partnership with Libya

In 2005, the U.S. and Libya signed an agreement for cooperation focusing on the Tajura Nuclear Research Center. Action sheets define interactions between the parties in the areas of reactor operation, radiation protection and health physics, neutron activation analysis, environmental safety and health, quality assurance, and radioactive waste management.

Livermore health physicists Greg Jones and Dewey Sprague have traveled to Libya several times in the past two years on behalf of the agreement. The Tajura reactor originally used highly enriched uranium fuel. Through DOE's Global Threat Reduction Initiative, it has been converted to low-enrichment uranium fuel, which is preferred for meeting nonproliferation goals.

"They restarted the reactor with the new fuel in April 2007," says Jones. "The whole process is like putting a new engine in a car. You go slowly and test the system before you take it up to speed. We offer our technical expertise and train personnel, for example, showing them how to safely handle fuel elements during refueling. Some of their instruments and monitoring systems are 27 years old—the age of the original reactor—and they want to upgrade this equipment as well."

Livermore is also assisting Libya in such areas as basic radiation monitoring, contamination control, and surveying. The Tajura facility recently upgraded from a film dosimetry system to a thermoluminescent system, and Jones and Sprague helped their colleagues calibrate the more modern dosimetry reader. "The two countries have similar regulatory systems in place," says Jones, "but the regulations and legal limits differ. We tailor our training materials to their systems and listen to what they say they need. It's exciting to make the connections. The program's success depends on building trust among the participants."

Sprague, who leads the radiation protection activities with Libya, adds that participants must be open to different cultures and philosophies. "Things move differently in Libya than in the U.S., which is true of many Mediterranean countries," he says. "Anyone taking on this sort of work must be considerate of the differences between our cultures."

Participating in the program requires stamina as well as diplomacy. "We spend weeks preparing for a one-week mission," says Sprague. "Libya is 10 time zones ahead of California, and traveling there requires two days. The U.S. delegation must hit the ground running, often launching into a full day of meetings and presentations. We're prepared to work 10 to 14 hours a day, doing everything we can to ensure a positive outcome."

Cooperation Opens Doors

Developing good relationships is the key to INSEP's success, and each relationship is unique. "First, we build trust at the highest level," says Bissani. "Then we get the technical experts of both sides involved. We know we've succeeded when a problem crops up and our counterparts call to ask for our assistance and guidance. The Livermore people who participate do so with passion and derive great satisfaction from their work."

In June 2007, the U.S. signed an arrangement with Algeria to cooperate at the laboratory-to-laboratory level on peaceful uses of nuclear energy. "Algerian scientists and engineers are excited about this opportunity," says Bissani. "It was front-page news in the Algerian media. The arrangement will provide an important mechanism to establish meaningful cooperation aimed at real technical issues. In the near future, we will send a technical team to Algeria to do what we do best: provide training and consultations, help solve technical problems, and collaborate on technical activities related to the peaceful uses of nuclear applications."

In January 2008, INSEP plans a regional conference at Livermore for colleagues from the national nuclear laboratories in North Africa and the Middle East. "Our goal is to support nascent interest in nuclear power development consistent with nonproliferation and national security objectives in North Africa," says Bissani. "We also want to strengthen the relationship between NNSA and participating countries—each of which is considering the introduction of nuclear power—while laying a foundation for increased cooperation, bilaterally and regionally, in the future."

—Ann Parker

Key Words: Algeria, Argentina, Egypt, international nonproliferation cooperation, International Nuclear Safeguards and Engagement Program (INSEP), Libya, Morocco, Peru, Romania, Thailand, Treaty on the Non-Proliferation of Nuclear Weapons, Vietnam.

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Probing Deep into the Nucleus

Teller's Contributions to Nuclear and Particle Physics

January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the eighth in a series of 10 honoring his life and contributions to science.

As researcher, theoretician, colleague, educator, and mentor, Edward Teller influenced every field of physics. His contributions to the fast-growing fields of nuclear physics and particle physics were part of the Golden Age of Physics, in which discovery after discovery produced an increasingly clearer picture of the nucleus and the fundamental interactions of the subatomic particles contained within the nucleus.

The Teller–Gamow theory on beta decay appeared in 1936 and was immensely influential in the growing field of particle physics.

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Selection Rules for the β-Disintegration

G. Gamow and E. Teller, *George Washington University, Washington D. C.*

(Received March 28, 1936)

§1. The selection rules for β-transformations are stated on the basis of the neutrino theory outlined by Fermi. If it is assumed that the spins of the heavy particles have a direct effect on the disintegration these rules are modified. §2. It is shown that whereas the original selection rules of Fermi lead to difficulties if one tries to assign spins to the members of the thorium family the modified selection rules are in agreement with the available experimental evidence.

§1.

According to the theory of β-disintegration given by Fermi[1] no change of the total nuclear spin should occur in the most probable transformations, i.e., in transformations located on the first Sargent curve.[2] The transformations corresponding to the second Sargent curve approximately 100 times less probable should correspond to changes ±1 or 0 of the angular momentum of the nucleus. One may expect the existence of still lower curves for higher changes in the nuclear spin. This selection principle is based on the assumption that the spin of the heavy particles does not enter in the part of the Hamiltonian which is responsible for the β-disintegration. The same assumption was made in the modified theory of Konopinski and Uhlenbeck[3] who introduced the derivative of the neutrino wave function in the Hamiltonian in order to get a better fit with the experimental curves of the energy distribution in β-spectra. We should like to note here that this selection rule will be changed if the spins of the heavy particles are introduced into the Hamiltonian, a possibility proposed in many discussions about this subject.

We shall first give the derivation of Fermi's selection rule in a somewhat generalized form. The probability of β-disintegration is proportional to the square of the matrix element.

$$M_1 = \sum_l \int (\Omega_l^{N,P}\psi_i)\psi_f^* \delta q_l \{0(\psi_\nu^*\psi_e^*)\}. \quad (1)$$

Here ψ_i and ψ_f are the proper functions of the heavy particles, protons and neutrons, for the initial and final state, respectively. These functions depend on the positions of the heavy particles, on their spins, and on a third variable[4] which corresponds to the charge of the heavy particles and which is capable of two values, in a manner similar to the spin variable, the value 1 corresponding to a proton and the value 0 to a neutron. The operator $\Omega_l^{N,P}$ acts on this last variable converting the lth particle in ψ_i into a proton if it was a neutron and giving $\Omega_l^{N,P}\psi_i = 0$ if the lth particles is already a proton. The integration in (1) includes summation over the spin and charge coordinates of the heavy par

[1] Fermi, Zeits. f. Physik **88**, 161 (1934).
[2] Sargent, Proc. Roy. Soc. **A139**, 659 (1933).
[3] Konopinski and Uhlenbeck, Phys. Rev. **48**, 7 (1935).
[4] Introduced by Heisenberg, Zeits. f. Physik **77**, 1 (1932).

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Teller's contributions often were made in collaboration with some of the greatest luminaries of 20th-century physics such as Enrico Fermi, George Gamow, and Hans Bethe. Even in his earliest papers on nuclear physics, Teller's style is readily apparent: a complete command of mathematics, an intuitive understanding of physics, and elegant arguments.

As a student of Werner Heisenberg in the late 1920s and early 1930s, Teller's early work in theoretical physics focused on applying the new theory of quantum mechanics to understanding phenomena in molecular and condensed-matter physics. However, the rapidly developing field of nuclear physics soon caught his attention. Fermi, James Chadwick, Hideki Yukawa, and others made the first important steps in understanding that the atomic nucleus is composed of protons and neutrons held together by a strong nuclear force, now considered as one of the four fundamental interactions of nature. Further clues to the fundamental interactions came from studying the decays of unstable nuclei. These nuclei may undergo alpha decay, in which they emit a helium nucleus, or beta decay (controlled by the weak force of nature), in which nuclei eject an electron (or positron) and a neutrino.

Teller fled Nazi Germany in 1934, going first to the Niels Bohr Institute in Copenhagen and then to University College in London. In 1935, Gamow invited him to join the faculty at George Washington University. Soon, the two were collaborating on a

This photo, taken in 1982, shows Edward Teller with Chen Ning Yang, who was Teller's student in the late 1940s. (Courtesy of Brookhaven National Laboratory.)

paper that eventually proved to be a crucial leap in understanding fundamental physics.

In 1934, Teller's lifelong friend Fermi proposed a significant beta-decay theory, in which Fermi stipulated that the spin of nucleons (protons and neutrons) tended to remain constant. In a 1936 paper published in *Physical Review*, Teller and Gamow focused on the experimental evidence presented by the complicated beta-decay scheme of thorium. They wrote that several observed nuclear spin assignments and beta- and gamma-decay rates contradicted Fermi's theory. They proposed modifications that allowed a nucleon to flip its spin during transition when emitting an electron and antineutrino, which became known as the Gamow–Teller transition.

The Teller–Gamow paper unexpectedly and quickly led to a better understanding of the generation of nuclear energy in the Sun. Bethe had just proposed the carbon–nitrogen–oxygen cycle as a mechanism for catalyzing the transformation of hydrogen into helium, which works for heavier, hotter stars than the Sun. Bethe, along with Gamow and Charles Critchfield, realized that another mechanism must be required for the Sun. Together, they proposed the proton–proton chain reaction, which relies on the Gamow–Teller spin-flip transformation of two protons into deuterium, releasing a positron and a neutrino as one proton changes into a neutron.

Both the original Fermi and Gamow–Teller theories of beta decay obeyed the symmetry of parity (or mirror symmetry). In the 1950s, Chen Ning Yang, a student of Teller's, and Tsung-Dao Lee explored the conservation of parity in beta decays. They discovered that, unlike gravitation and electromagnetism, parity was not conserved in some weak decays described by a novel mixture of the Gamow–Teller and Fermi theories. Yang and Lee were awarded the Nobel Prize in Physics in 1957 for this work. Later, the unification of weak and electromagnetic interactions grew out of these and other insights. Thus, the Gamow–Teller transitions, originally proposed to explain nuclear phenomena, proved to be a key step toward the standard model of fundamental interactions.

Teller also worked on other aspects of nuclear physics. In 1937, he wrote a set of papers with Julian Schwinger, who shared the Nobel Prize in Physics with Sin-Itiro Tomonaga and Richard Feynman in 1965. These papers focused on the coherent behavior of neutrons scattering off hydrogen molecules—similar to x rays scattering off crystals. The scattering of slow neutrons provided a new tool for understanding the behavior of molecular and condensed-matter systems and explained the basic binding of neutrons and protons into deuterons. During this era, Teller also worked with John Wheeler analyzing nuclei rotations.

A decade later, Teller and Maurice Goldhaber—another refugee from Germany—proposed that the giant dipole nuclear resonance observed in high-energy, gamma-ray reactions with nuclei was the result of a collective vibration of the neutrons and protons. Realizing that the resonance was analogous to the oscillating behavior of sodium and chlorine ions within a crystal of salt in the presence of light, Goldhaber sought out Teller because he had understood and proposed important general laws governing the interaction of light and salts. Together, they went on to invent their giant dipole resonance model.

Edward Teller and Enrico Fermi converse on the University of Chicago campus in 1951. (Courtesy of American Institute of Physics Emilio Segré Visual Archives.)

During the late 1940s and early 1950s, many nuclear physicists shifted their focus to probing the properties of newly discovered fundamental particles. In the 1930s, Yukawa hypothesized a new particle called pi meson (or pion) as the intermediary of the strong nuclear force that binds protons and neutrons. In 1947, scientists debated whether the newly discovered mu meson (or muon) was the long-sought pion. Teller, together with Fermi and Victor Weisskopf, showed that the muon could not be the pion. Several months after their paper appeared, other researchers discovered the real pion.

After the founding of Lawrence Livermore in 1952, Teller focused on developing the hydrogen bomb and related areas of science at the new laboratory. In the 1960s, he worked with Livermore physicists, including Mort Weiss and Stewart Bloom, on the interactions of K mesons with matter. Teller also worked with George Chapline, Montgomery Johnson, and Weiss on one of the earliest papers regarding the collisions of heavy ions.

For more than four decades, Teller made key contributions to nuclear and particle physics, including a major step toward the unification of fundamental interactions.

—Arnie Heller

Key Words: Edward Teller, nuclear physics, particle physics, standard model.

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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

Thin Layer Chromatography Residue Applicator Sampler
Peter J. Nunes, Fredrick R. Kelly, Jeffrey S. Haas, Brian D. Andresen
U.S. Patent 7,247,273 B2
July 24, 2007
A thin-layer chromatograph residue applicator sampler provides for rapid analysis of samples containing high explosives, chemical warfare agents, and other items of interest under field conditions. The residue applicator sampler includes a sampling sponge that is resistant to most chemicals and is fastened via a plastic handle inside a hermetically sealed tube containing a known amount of solvent. During sampling, the wetted sponge is removed from the sealed tube and used as a swiping device across an environmental sample. The sponge is then replaced in the tube, where the sample dissolves in the solvent. A small pipette tip is also contained in the sealed tube. The sponge is removed and placed into the pipette tip, where a squeezing out of the dissolved sample from the sponge into the pipette tip results in a droplet captured in a vial for later analysis. Alternatively, the droplet is applied directly to a thin-layer chromatography plate for immediate analysis.

Conversion of Raw Carbonaceous Fuels
John F. Cooper
U.S. Patent 7,252,901 B2
August 7, 2007
Three configurations of an electrochemical cell are used to generate electric power from the reaction of oxygen or air with porous plates or particulates of carbon. Waste heat from the electrochemical cells flows upward through a storage chamber or port containing raw carbonaceous fuel. These configurations allow combining the separate processes of devolatilization, pyrolysis, and electrochemical conversion of carbon to electric power into a single-unit process, fed with raw fuel and exhausting high-British thermal unit gases, electric power, and substantially pure carbon dioxide during operation.

List Mode Multichannel Analyzer
Daniel E. Archer, S. John Luke, Joseph Mauger, Vincent J. Riot, David A. Knapp
U.S. Patent 7,253,387 B2
August 7, 2007
A digital list-mode multichannel analyzer (MCA) is built around a field programmable gate array for onboard data analysis and modification of system detection and operating parameters. This MCA can collect and process data in short time periods (less than 1 millisecond) when used in histogram or list mode.

Autofluorescence Detection and Imaging of Bladder Cancer Realized through a Cystoscope
Stavros G. Demos, Ralph W. deVere White
U.S. Patent 7,257,437 B2
August 14, 2007
Near-infrared imaging using elastic light scattering, tissue autofluorescence, and interior examination techniques and equipment are explored for medical applications. This approach uses cross-polarized elastic light scattering or tissue autofluorescence in the near infrared coupled with image processing and interimage operations to differentiate human tissue components.

Nonlinear Optical Crystal Optimized for Ytterbium Laser Host Wavelengths
Christopher A. Ebbers, Kathleen I. Schaffers
U.S. Patent 7,260,124 B1
August 21, 2007
A material for harmonic generation has been made by changing the crystal $LaCa_4(BO_3)_3$, also known as LaCOB, to the form $Re1_xRe2_yRe3_zCa_4(BO_3)_3O$. In this form, Re1 and Re2 (rare-Earth ions 1 and 2) are selected from the group consisting of scandium, yttrium, lanthanum, cerium, praseodymium, neodymium, samarium, europium, gadolinium, terbium, dysprosium, holmium, erbium, thulium, ytterbium, and lutetium. Re3 is lanthanum, and $x + y + z = 1$.

Real-Time Detection Method and System for Identifying Individual Aerosol Particles
Eric E. Gard, Keith R. Coffee, Matthias Frank, Herbert J. Tobias, David P. Fergenson, Norm Madden, Vincent J. Riot, Paul T. Steele, Bruce W. Woods
U.S. Patent 7,260,483 B2
August 21, 2007
An improved method and system have been developed for identifying individual aerosol particles in real time. Sample aerosol particles are collimated, tracked, and screened to determine which ones qualify for mass spectrometric analysis based on selection criteria. Screening techniques include determining particle size, shape, symmetry, and fluorescence. Only qualifying particles that pass all screening criteria are subject to desorption ionization and single-particle mass spectrometry to produce corresponding test spectra. The test spectra are used to determine the identities of each of the qualifying aerosol particles by comparing the test spectra against predetermined spectra for known particle types. In this manner, activation cycling in a particle-ablation laser of a single-particle mass spectrometer is reduced.

Awards

The **Federal Laboratory Consortium for Technology Transfer** (FLC) honored three teams of Livermore scientists for technology transfer efforts in a Far West Regional competition. The award for **Outstanding Technology Development** was presented to **George Caporaso**, **Steve Sampayan**, and **Genaro Mempin** for the Dielectric Wall Accelerator for Proton Therapy. Two Laboratory teams were honored with **Outstanding Commercialization Success** awards: **Jesse Wolfe**, **Randall Elder**, and **Ted Saito** for the Durable Silver Reflector for High-Efficiency Solar Cells; and **Mark Rowland**, **Catherine Elizondo**, **Dan Dietrich**, and **Raymond Pierce** for their work on the Fission Meter, a portable neutron-source identifier.

A nationwide organization of federal laboratories, FLC provides a forum to develop strategies and opportunities for linking the laboratory mission technologies and expertise with the marketplace. The Far West is one of six regions in the FLC network, and its eight states encompass more than 100 federal laboratories and facilities.

A Code to Model Electromagnetic Phenomena

A Livermore code called EMSolve is being used to accurately simulate electromagnetic fields. EMSolve's enormous simulation capabilities require that it be run on parallel supercomputers. EMSolve is used throughout the Laboratory because studying electromagnetic fields is an important aspect of almost every Livermore program. The code has supported research projects sponsored by the Defense Advanced Research Projects Agency, U.S. Air Force, U.S. Navy, and Stanford Linear Accelerator Center. Based on unstructured-mesh finite-element technology, the code excels at modeling problems with complex geometries containing curved surfaces. One EMSolve simulation showed the interaction of radar waves inside a hypothetical two-story building. A challenging application for the EMSolve code is advancing the understanding of electromagnetic pulses. Because EMSolve is based on modular software architecture, the core technology can be readily incorporated into other codes to produce electro-thermal-mechanical simulations.

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Characterizing Virulent Pathogens

Livermore researchers are developing candidate signatures for pathogens that might be used in a bioterrorist attack and for bioorganisms that can cause a disease epidemic. To speed pathogen detection, scientists have developed multiplexed assays that simultaneously detect for multiple bacteria, viruses, and toxins. The assays will be incorporated into BioWatch, a nationwide early warning system that detects trace amounts of specific microorganisms in the air. Researchers are also developing multiplexed assays to detect foreign animal diseases such as foot-and-mouth disease. In addition to pathogen detection technologies, Livermore scientists are studying how a host's body interacts with a pathogen. Host–pathogen interactions contain biomarkers that health officials may be able to use to identify the pathogen in patients before symptoms appear.

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Coming Next Month

Safeguarding Nuclear Materials

For 15 years, Livermore has been working to protect nuclear materials in the Russian Federation.

Also in December

- *Communication technologies using ultrawideband radar are improving national security.*
- *Calculating the permeability of partially melted metals in a mineral matrix unlocks secrets about the formation of Earth's core.*

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