Lawrence Livermore National Laboratory

Science & Technology Review

October/November 2012

Livermore Captures Six R&D 100 Awards

2012 R&D 100 50th ANNIVERSARY

Also in this issue:

A Precisely Engineered Hydrotest

Simulating Nerve Agent Decontamination

About the Cover

Laboratory researchers won six R&D 100 awards in *R&D Magazine*'s annual competition for the top 100 industrial innovations worldwide. The award-winning technologies are described beginning on p. 4. They include a power divertor for nuclear fusion reactors, a method to produce protective coatings that prevent surface degradation in extreme environments, a beam-shaping device to improve laser beam performance and operational reliability, plastic scintillators for neutron and gamma-ray discrimination, a protective coating to extend the life of steel components that experience high-impact forces, and a portable optical velocimetry system for shock-physics experiments. Since 1978, Livermore researchers have received 143 R&D 100 awards. The R&D 100 logo is reprinted in this issue courtesy of *R&D Magazine*.

Cover design: George A. Kitrinos

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure 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 eight 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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Sequoia Ranks Number 1 in Top500

The Laboratory's Sequoia ranked as the world's most powerful supercomputer on the Top500 list released in June 2012. Sequoia, a 96-rack IBM BlueGene/Q system developed in partnership with the National Nuclear Security Administration (NNSA), demonstrated a sustained performance of 16.32-quadrillion floating-point operations per second (petaflops) on the industry standard LINPACK benchmark. Sequoia will enable simulations that explore phenomena at a level of detail never before possible. The computer is dedicated to NNSA's Advanced Simulation and Computing (ASC) Program for stewardship of the nation's nuclear weapons stockpile, a joint effort of Lawrence Livermore, Los Alamos, and Sandia national laboratories.

"Computing platforms such as Sequoia help the United States keep its nuclear stockpile safe, secure, and effective without the need for underground testing," says NNSA Administrator Thomas D'Agostino. "While Sequoia may be the fastest, the underlying computing capabilities it provides give us increased confidence in the nation's nuclear deterrent as the weapons stockpile changes under treaty agreements, a critical part of President Obama's nuclear security agenda. Sequoia also represents continued American leadership in high-performance computing, key to the technology innovation that drives high-quality jobs and economic prosperity."

"Sequoia will provide a more complete understanding of weapons performance, notably hydrodynamics and properties of materials at extreme pressures and temperatures," says Bob Meisner, NNSA director of the ASC Program. "In particular, the system will enable suites of highly resolved uncertainty quantification calculations to support the effort to extend the life of aging weapons systems; what we call a life-extension program."

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A Faster, Lower-Cost Desalination Technique

A team of Laboratory researchers led by Michael Stadermann has developed a capacitive desalination technique that could ultimately lower the cost and time of desalinating seawater. In capacitive desalination (CD), a voltage is applied between two porous electrodes to adsorb ions onto the electrode surface and thus remove them from the feed stream. Traditionally, due to the small pore sizes of the electrodes, the feed stream flows between the electrodes and through a dielectric porous separator. The new technique, called flow-through electrode CD, uses porous carbon materials with a hierarchical pore structure, which allows the saltwater to easily flow through the electrodes themselves.

The Livermore approach offers several advantages relative to traditional flow-between systems, including faster and more energy efficient desalination with more salt removed for each charge of the capacitor. Finally, flow-through can be used with a thinner separator because the separator is no longer a flow channel, thereby reducing the overall and electrical resistance of the device, which further decreases costs.

"By leveraging innovative porous carbon materials recently developed at Livermore, our method removes the diffusion limitations afflicting traditional CD cells. The desalination process now only takes as long as it takes to charge the electrodes, on the order of minutes or less," says Matthew Suss, a Lawrence scholar and first author of a paper that appeared online June 26, 2012, in *Energy & Environmental Science*. "The new method currently removes salt five to ten times faster than previous CD systems and can be further optimized for increased speed. It also reduces the concentration of the feed up to three times as much per charge." Other Livermore researchers on this project include Theodore Baumann, William Bourcier, and Christopher Spadaccini.

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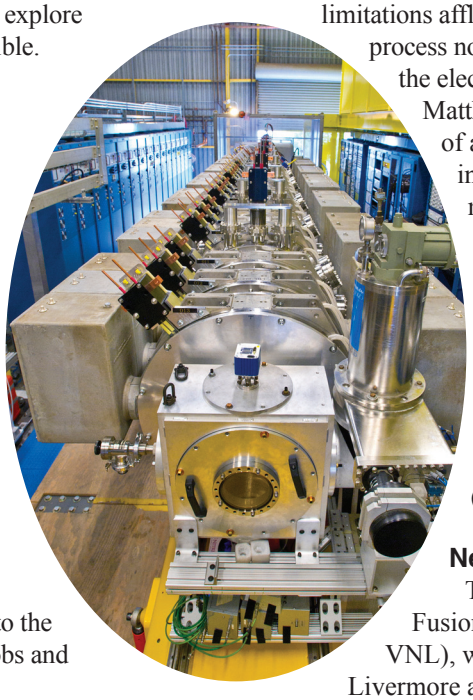

New Accelerator Ready to Go

The Department of Energy's Heavy-Ion Fusion Science Virtual National Laboratory (HIFS-VNL), whose member institutions include Lawrence Livermore and Lawrence Berkeley national laboratories and the Princeton Plasma Physics Laboratory, has recently completed a new accelerator designed to study an alternate approach to inertial fusion energy. Housed at Lawrence Berkeley, NDCX-II (shown center; photo courtesy of Roy Kaltschmidt, Lawrence Berkeley National Laboratory) is a compact machine designed to produce a high-quality, dense beam that can rapidly deliver a powerful punch to a solid target.

Research with NDCX-II will introduce advances in the acceleration, compression, and focusing of intense ion beams that can inform and guide the design of major components for heavy-ion fusion energy production. Livermore developed most of the physics design for NDCX-II under a subcontract to Lawrence Berkeley. The Laboratory also provided the accelerating cells, which were previously used for its Advanced Test Accelerator, and the Blumleins, which are 250,000-volt, pulsed-power sources that provide the rapid final acceleration.

"NDCX-II represents the first conversion of electron induction accelerator components into a pulse-compressing ion accelerator," says Livermore's Alex Friedman, the project's beam acceleration task area leader. "With NDCX-II, we will be able to study fusion-relevant intense-beam physics, properties of ion-heated matter, and elements of target physics for ion-beam-driven inertial fusion energy."

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Commentary by William W. Craig

Innovation Rooted in Exploratory Research

LAWRENCE Livermore is honored to have won six R&D 100 awards in 2012. Each year, *R&D Magazine* presents these "Oscars of Invention" to the top 100 technological advances that contribute to meeting an important national or societal need. This year's R&D 100 Award winners bring the Laboratory's total to 143 since Livermore began participating in 1978.

This issue of *S&TR* features the prize-winning efforts (see the movie at www.llnl.gov/news/newsreleases/2012/Jun/attach/rd100.mov). They are a tribute to Livermore's multidisciplinary approach to tackling difficult challenges from idea conception and the underpinning scientific discovery to engineering development of prototype systems. Visible and tangible results, such as those honored with R&D 100 awards, often take more than a decade to come to fruition in a problem-solving breakthrough. Early steps include exploratory research and typically a "proof-of-principle" feasibility demonstration to attract sponsor support and transform the idea into a product that meets an important mission need.

In this regard, the Laboratory Directed Research and Development (LDRD) Program, authorized by Congress in 1991, is critically important. It is the primary means by which the Laboratory pursues innovative, long-term, high-risk, and potentially high-payoff research in support of its missions. Such groundbreaking work is necessary to meet emerging national needs but usually deemed "too risky" for direct support by sponsors. It is noteworthy that about two-thirds of our R&D 100 Award-winning technologies over the past decade have had their roots in LDRD projects, including three of this year's awards.

The award-winning development of plastic scintillators for neutron and gamma-ray detection (see p. 10) is an illustrative example. In 2007, the Laboratory launched a three-year exploratory research project aimed at improving capabilities to effectively detect and identify fissile materials. Better detectors are needed to counter nuclear smuggling and proliferation. With LDRD support, systematic surveys were completed of 150 materials, leading to a better understanding of the physics of scintillation and the development of efficient, low-cost materials. This highly successful effort was followed up with programs at the Laboratory funded by the National Nuclear Security Administration's (NNSA's) Office of Nonproliferation Research and Development and the Department of Homeland Security's Domestic Nuclear Detection Office. The R&D 100 Award is a testimony to the importance of the breakthroughs that were made and the substantial progress that is being made toward enhancing our nation's security.

Similarly, both the "snowflake" power divertor for nuclear fusion reactors (see p. 4) and multiplexed photonic Doppler velocimetry (MPDV, see p. 14) have deep roots in LDRD projects at Livermore. The snowflake power divertor, an ingenious method for dissipating exhaust power from hot plasmas in tokamaks, has been tested at institutions that are partner recipients of the award. MPDV technology, first demonstrated in LDRD work at Livermore, has since been used at Los Alamos National Laboratory and the Nevada National Security Site to collect key data in hydrodynamic experiments in support of national security work. NNSA's National Security Technologies, LLC, is our partner in the award.

LDRD is not only key to mission success; it is also vital to the long-term health of our institution. This point was emphasized in the 2012 report of a National Academy of Sciences study examining science and technology at Lawrence Livermore, Los Alamos, and Sandia national laboratories. Because LDRD supports exciting innovative projects, the program helps attract and retain top talent in new and emerging fields of science and technology with important national-security applications. At Livermore, the LDRD Program supports most of the Laboratory's postdoctoral researchers, many of whom later become full-time employees. LDRD is also behind nearly 50 percent of our patents, more than 25 percent of Livermore copyrights, and about 20 percent of our peer-reviewed publications.

Livermore serves the nation by exploring science and technology that can make a big difference with application to important current and emerging national needs. Our six R&D 100 awards this year are one of many indicators of continuing success in meeting those needs.

Hearty congratulations go to all the contributing Laboratory scientists and engineers and their collaborators from the many partnering research institutions mentioned in the stories.

■ William W. Craig is director of the Laboratory Directed Research and Development Office.

A Major Step for Fusion Energy

AN R&D 100 Award-winning technology will help the world move away from a fossil-fuel-based electricity supply. Sustaining natural resources, reducing carbon emissions, and stabilizing greenhouse gas levels are essential in the face of global warming.

One of the most attractive solutions for humankind's future energy needs is controlled thermonuclear fusion. Controlled fusion with magnetically confined plasmas in a doughnut-shaped tokamak is actively being pursued by countries worldwide to bring this energy source to fruition.

However, one problem that has yet to be resolved is the safe dissipation of the power exhaust from the hot plasma in a commercial tokamak reactor: hundreds of megawatts of power are released in the form of charged particles that must be accommodated in the reactor chamber. The general approach to solving this problem was identified decades ago and consists of creating a magnetically guided exhaust channel that diverts the plasma from the walls of the chamber and directs it to thermally and mechanically hardened and actively cooled absorbers. This component of a tokamak reactor is called the "divertor."

The design of a standard divertor is sufficient for the lower power densities of existing experimental tokamak research facilities. However, despite significant effort, a steady-state, practical method has not been found to spread the heat over a large enough surface to reduce the power density to a manageable level for a future commercial reactor. The characteristic power load would be about 100 megawatts per square meter—more than is generated on the surface of the Sun. No materials could survive the exposure to such heat fluxes.

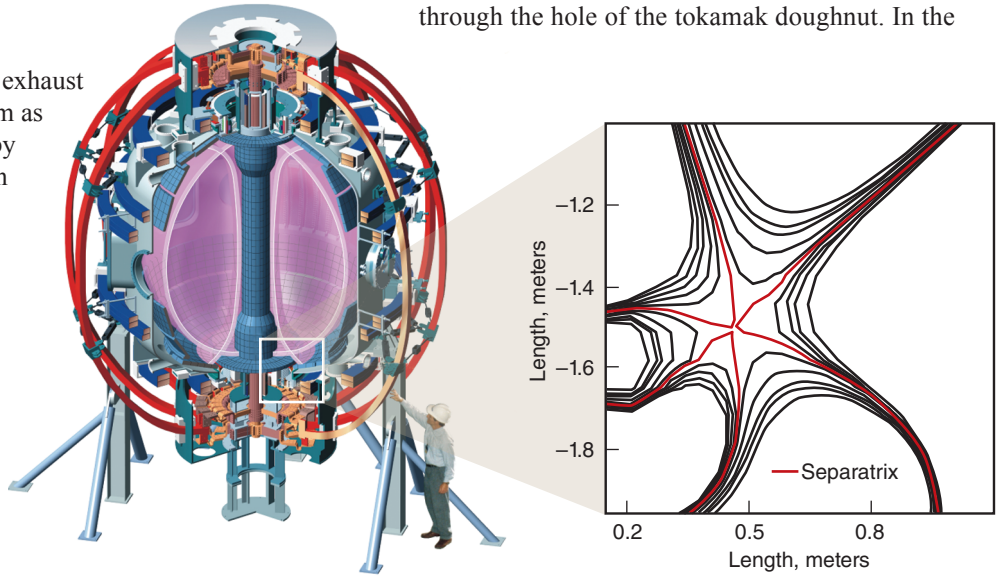
> ***. . . the heat flux to the material [divertor plates] was reduced by an order of magnitude . . . the core plasma behavior was not influenced by the snowflake divertor at the edge [a critical result because in fusion plasmas the edge can strongly affect behavior in the core], and . . . harmful impurity concentration in the core was reduced by the snowflake.***
>
> **—S. Prager, Director**
> Princeton Plasma Physics Laboratory

A Simple Solution

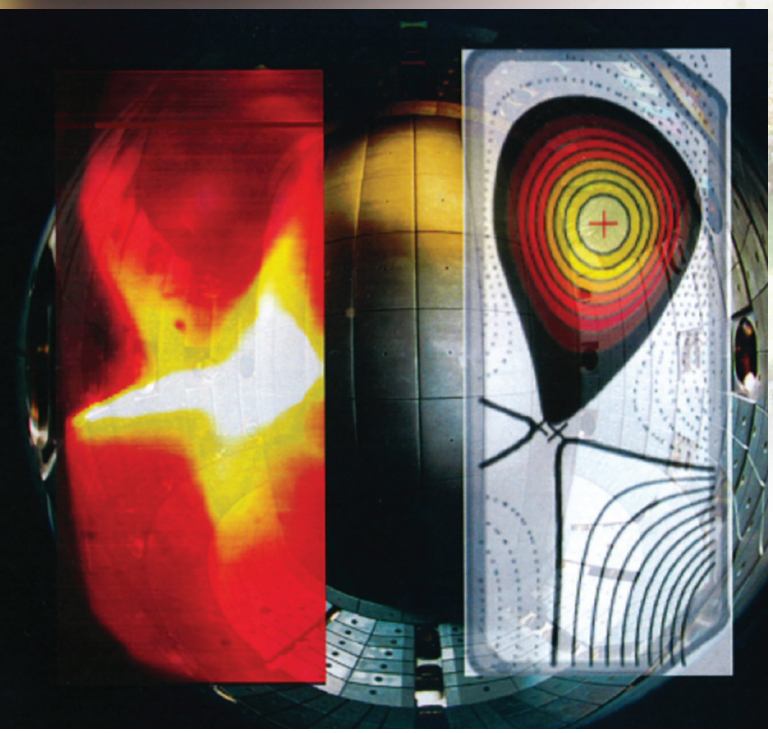
Various efforts are under way to handle the exhaust blast. But none addresses this daunting problem as well as the solution discovered by a team led by Livermore physicist Dmitri Ryutov. In addition to scientists from Livermore, Ryutov's team includes researchers at Princeton Plasma Physics Laboratory (PPPL), the École Polytechnique Fédérale de Lausanne Center for Research in Plasma Physics (CRPP) in Switzerland, and Oak Ridge National Laboratory.

"Our 'snowflake' power divertor uses a newly discovered configuration of the divertor magnetic field," says Ryutov. This configuration spreads out the magnetic field in a shape reminiscent of a snowflake. The magnetic field lines spread the exhaust over a larger area, effectively reducing the heat flux by a factor of 10 to a manageable 10 megawatts per square meter.

The distribution and magnitude of the heat fluxes in the divertor are determined by the shape of the poloidal magnetic field—the component of the magnetic field that loops through the hole of the tokamak doughnut. In the



A "snowflake" power divertor is installed at the bottom of the tokamak at the National Spherical Torus Experiment at Princeton Plasma Physics Laboratory (PPPL). (inset) A snowflake magnetic configuration shows the characteristic hexagonal shape of the separatrix, which is the singular magnetic field line that determines the overall field geometry.



A vertical cross section of the divertor region of the experimental tokamak at the École Polytechnique Fédérale de Lausanne Center for Research in Plasma Physics (CRPP) in Switzerland shows (left) the snowflake-shaped spreading of the exhaust plasma and (right) its magnetic field lines on the background of the confining vessel.

Livermore development team for the snowflake power divertor: (from left) Thomas Rognlien, Maxim Umansky, Dmitri Ryutov, and Ronald Cohen; (inset) Livermore team member Vsevolod Soukhanovskii. (Not shown: Stefano Coda, Basil Duval, Jean-Marc Moret, and Francesco Piras of CRPP; Egemen Kolemen and Jonathan Menard of PPPL; and Joon-Wook Ahn of Oak Ridge National Laboratory.)

new configuration, a large zone of a very weak poloidal magnetic field is created in the divertor. This zone induces a large flaring of the plasma flow and dramatically decreases the heat fluxes in the divertor.

"The redistribution is technologically simple but remained unnoticed prior to our discovery and subsequent publications," says Ryutov. The figure on p. 4 illustrates the snowflake power divertor at work on the National Spherical Torus Experiment at PPPL. This effort was led by Livermore's Vsevolod Soukhanovskii, who is on a long-term assignment at PPPL.

The snowflake divertor also has been tested on an experimental tokamak at CRPP. (See the figure above.) The tokamaks at PPPL and CRPP have quite different plasma shapes, but in both of them, the confinement of the hot core plasma remained good when the snowflake configuration was achieved. In both facilities, the control systems allowed experimentalists to maintain the plasma configuration close to the snowflake shape for extended periods. Says Ryutov, "We are pleased that the snowflake configuration has proven to be so flexible."

Wide Acceptance

The beauty of the snowflake power divertor is that it does not require any expensive or complex changes to the overall configuration of a tokamak. Nor does it call for significant changes in the already well-developed scenarios for operation of a commercial tokamak.

This exciting technology has been well received. Several new experimental tokamak facilities plan to install the snowflake power divertor. One facility is an upgraded version of the existing experimental facility at PPPL, whose higher magnetic current and power will serve as a testing ground for fusion reactors still in the planning phase. Other tokamaks that will incorporate the snowflake power divertor are being designed in Italy and China.

—Katie Walter

Key Words: fusion energy, R&D 100 Award, snowflake power divertor, tokamak.

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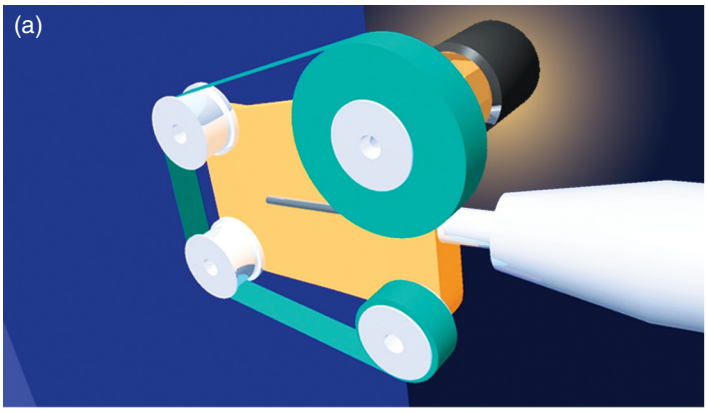
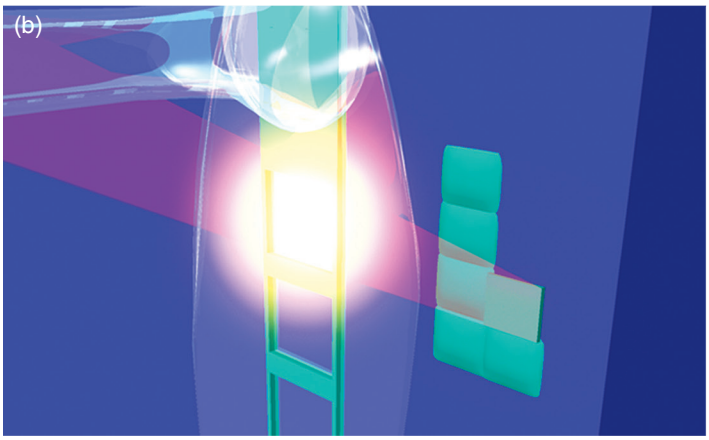
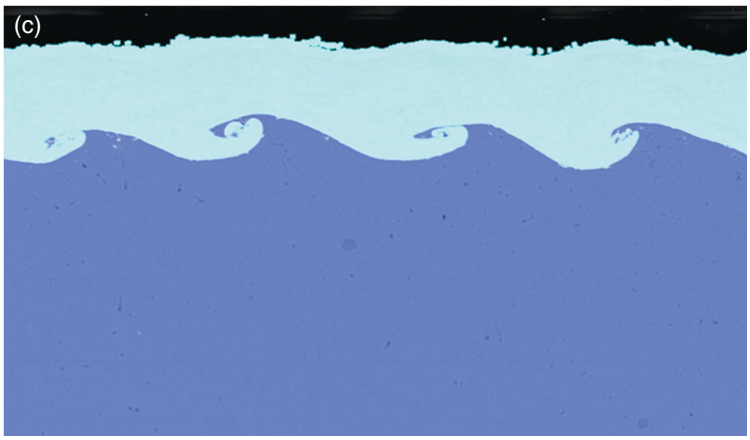
High-Performance Metal Coatings Produce Exceptional Bond Strength

HIGH-VELOCITY laser-accelerated deposition (HVLAD) uses advanced lasers to produce protective coatings with ultrahigh-strength, explosively bonded interfaces. These coatings prevent corrosion, wear, and other modes of degradation in extreme environments. HVLAD leverages high-power pulsed laser technology developed for laser inertial-confinement fusion research as well as key components of laser peening technology. Laser peening, which was also developed by the Laboratory and won an R&D 100 Award in 1998, has been in commercial production for nearly a decade, extending the fatigue life of aerospace equipment. (See *S&TR,* October 1998, pp. 12–13.) The HVLAD process can be applied using the hardware in current use for laser peening, with the addition of a water-delivery fixture and a coating-film cartridge. Livermore chemical engineer and corrosion scientist Joe Farmer and physicist Alexander (Sasha) Rubenchik, along with Lloyd Hackel of Curtiss-Wright Surface Technologies–Metal Improvement Company, won an R&D 100 Award for their development of the technology.

The high-power pulsed lasers produce coatings using materials that are difficult to deposit by other means, at room temperature and pressure, and with exceptional bond strength. Unlike some competing processes, HVLAD can be conducted in open production areas including factory floors, shipyards, and aircraft hangers. HVLAD enables the deposition of a variety of heat-resistant materials that can withstand temperatures above 538ºC—for example, tantalum, titanium, and tungsten—onto high-temperature steels and other inexpensive materials. Such materials are often used in power plants and shipyards and in the aerospace, chemical, gas, and oil industries.







(a) For high-velocity laser-accelerated deposition (HVLAD), a special head is adapted to a laser-peening device and associated robotics. (b) Patches of high-performance corrosion-resistant film are accelerated and bonded to a substrate in a controlled process. (c) A scanning electron microscope image shows a heat-resistant tantalum coating on a copper substrate. The tantalum was accelerated at the copper interface, and the shear forces at the interface caused the mixing of the two materials, resulting in an exceptionally strong interfacial bond. This coating was produced at room temperature and pressure, with no special process equipment other than the laser. (Renderings by Clayton Dahlen.)

Livermore development team for HVLAD: Alexander Rubenchik (left) and Joe Farmer.

How It Works

The HVLAD process uses the world's most powerful and highest-repetition-rate production lasers for localized explosive bonding. A high-intensity laser pulse is focused onto an advancing filmlike target material, which is covered by a thin layer of water that serves as a tamper. The laser pulse generates a high-temperature plasma and with it very high pressure that shears out a patch of the filmlike material, accelerating it to hypersonic velocities. The accelerated patch hits the substrate at an oblique angle, where the high-impact velocity induces plastic shear flow at the film–substrate interface, resulting in the mixing of target and substrate materials at the interface. Exceptionally strong interfacial bonds are created that approach the ultimate tensile strength of the substrate.

Farmer says, "We can place coating film on complex surfaces with millimeter resolution, adjusting the incidence angle on every pulse to attain highly uniform coverage, as we do for laser peening. The transition to HVLAD is a straightforward adaption of this established capability."

Coatings produced with conventional and physical vapor deposition processes, according to Farmer, are completed at a slow rate due to mass transport limitations. Low mass flux, or flow, and roughness amplification place limitations on coating thicknesses as well. Conventional thermal and cold-spray coatings have bond strengths on the order of only 680 atmospheres (10,000 pounds per square inch), while the HVLAD-bonded materials have ultimate tensile strengths of about 6,800 to 34,000 atmospheres (100,000 to 500,000 pounds per square inch). Furthermore, conventional coating processes rely on difficult-to-handle powder feeds through a hypersonic nozzle.

Another advantage of the HVLAD system is that it is very cost effective. "The HVLAD beam-delivering robot can be configured nearly exactly as that now used in the laser peening process for treating F-22 fighter jets, Navy arrestment hook shanks, and gas and steam turbine blades," says Farmer. "Thus, almost no additional capital investment is required to implement this technology."

Industrial Applications

Application of the HVLAD technology can be beneficial in a variety of industries. For example, HVLAD coatings could make possible the use of high-temperature materials in fossil-fuel, solar thermal, and nuclear power plants, leading to an increase in efficiency. Increasing the operating temperature of an energy conversion system from 325°C to 900°C could lead to a 20-percent gain in efficiency. Another application could involve coating a thin layer of titanium on conventional ship hulls made of steel as a cost-effective means of corrosion prevention.

Oxide-dispersion-strengthened (ODS) steels have very good high-temperature strength, are radiation resistant, and are leading candidate materials for next-generation nuclear power plants. However, these materials lack corrosion resistance in exotic high-temperature coolants. The HVLAD process could be used to deposit high-temperature corrosion-resistant coatings of expensive alloys such as tantalum–tungsten on the less corrosion-resistant ODS steel.

HVLAD coatings help prevent corrosion and pitting and leave materials resistant to stress corrosion cracking and failure from fatigue. These protective coatings and cladding with high-integrity interfacial bonds are capable of extending the operating life of valuable equipment in the aerospace, marine, and energy arenas.

—Cindy Cassady

Key Words: corrosion-resistant coating, high-strength bonded interface, high-velocity laser-accelerated deposition (HVLAD), laser peening, R&D 100 Award.

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Improving Laser Beam Performance and Operational Reliability

THE National Ignition Facility (NIF) houses the world's most energetic laser built to study the fusion processes that occur inside stars, supernovae, and exploding nuclear weapons. It was designed to create the conditions required to ignite controlled fusion reactions that could someday serve as an energy source.

To enhance the performance and operability of this and other laser facilities as well as meet the requirements of future laser-driven fusion power plants, a team led by Livermore's John Heebner in collaboration with Meadowlark Optics in Colorado developed the LEOPARD (laser energy optimization by precision adjustments to the radiant distribution) system. The system is now operational on NIF, and the team has won an R&D 100 Award for the new technology.

LEOPARD precisely adjusts a laser beam's radiant distribution or intensity profile, enabling the correction of residual imperfections in a beam. The system also protects fragile regions containing flaws on downstream optics by locally shadowing the beam where it overlaps the flaws. This technique allows the maximum amount of energy to be extracted from the laser amplifiers while preserving a high degree of reliability among the optical components.

Hybrid Design Provides Unique Capability

At the heart of LEOPARD is a hybrid design consisting of two liquid-crystal-based spatial light modulators. The first modulator is of the type found in conventional liquid crystal display (LCD) projectors; that is, it is pixelated and can be electrically controlled or addressed with a digital image. The second modulator is unconventional in that it is nonpixelated, analog, and optically addressed by the images projected from the first. Both contain twisted nematic liquid crystal molecules used in most LCD TVs, monitors, and projectors.

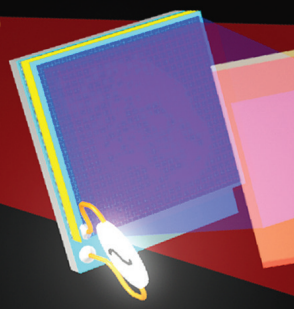
To preserve the existing NIF laser beam quality while adding the capability to create smooth beam shapes, the team customized the second modulator in the hybrid design. This modulator, called an optically addressable light valve (OALV), contains a liquid crystal cell, but unlike a conventional, pixelated liquid crystal cell matrix, it consists of only a single, giant pixel.

The orientation of the liquid crystal molecules is controlled with a voltage applied across transparent electrode layers surrounding the liquid crystal layer. The LEOPARD design also incorporates a photoconductor layer adjacent to and in series with the liquid crystal layer. As a result, the local voltage across a patch of the liquid crystal layer can be controlled by the local brightness of light illuminating the photoconductor. This control can happen only if the photon energy of the illuminating light is higher than the bandgap energy of the photoconductor such that it can be absorbed, turning the insulator into a conductor. The process short-circuits the photoconductor layer, allowing the voltage to be applied locally to the liquid crystal layer and opening a local transmission window for the laser beam. This mechanism enables a weak, incoherent image pattern consisting of bright and dark features to control the pattern of transmission for a much higher energy coherent laser beam.

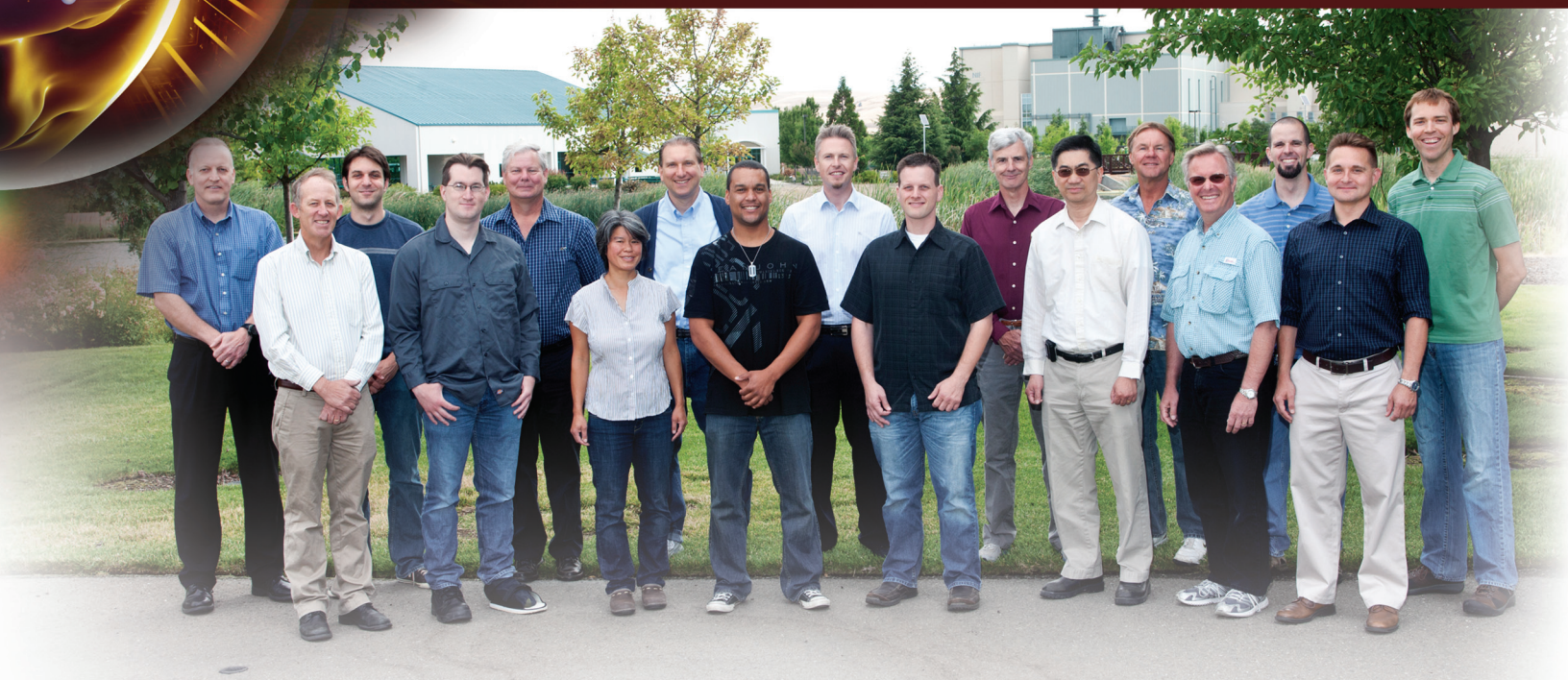
Because OALV is unpixelated and analog, it is well suited for creating ultrasmooth laser beams with arbitrary shapes. For the NIF application, it also had to satisfy a set of stringent requirements typically not possible with conventional, pixelated liquid crystal modulators. These requirements included achieving a more than 90-percent transmission, imparting minimal wavefront distortions, and avoiding the creation of temporal interference patterns (also known as amplitude modulation), all in a plug-and-play module.

LEOPARD's Spots

The LEOPARD capability added to NIF's 192-beam laser system enables operators to introduce obscurations, or "blockers,"

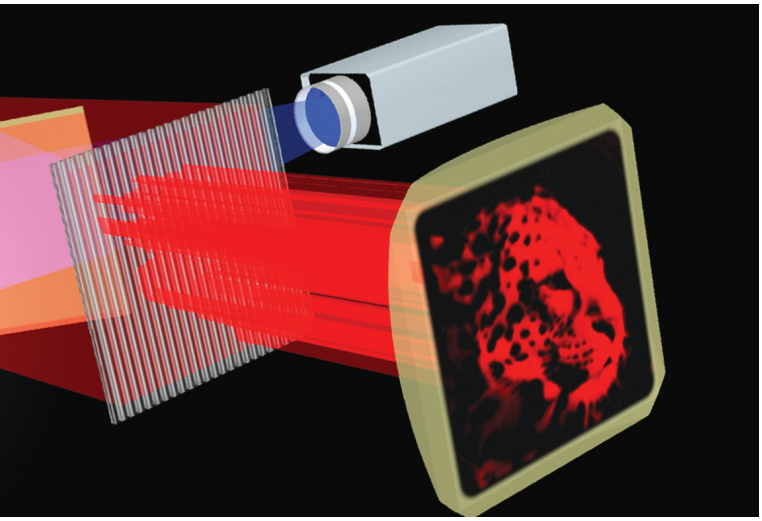


LEOPARD (laser energy optimization by precision adjustments to the radiant distribution) allows a detailed intensity profile to be encoded in a high-power laser beam with no pixelation artifacts. An incoherent light source (purple) illuminates a photoconducting layer with a pixelated image. The layer is adjacent to and controls the transmission of a single large liquid crystal in a process that smooths any jagged edges. As the coherent laser light (red) passes through, it picks up the smooth intensity profile (in this case, the face of a leopard). (Rendering by Clayton Dahlen.)



Livermore development team for LEOPARD: (from left) Michael Borden, Phil Miller, Marcus Monticelli, Matt Rever, Mark Franks, Nan Wong, Michael Taranowski, Eric Imhoff, Gordon Brunton, Jeff Jarboe, Steve Hunter, Eddy Tse, Kim Christensen, Jeff Wilburn, Edward Von Marley, John Heebner, and Kevin Williams. (Not shown: Jean-Michel Di Nicola, Sham Dixit, Lynn Seppala, Mike Scanlan, Tracy Budge, Larry Smith, and Abdul Awwal.)

upstream, which shadow flaws downstream in the final optics. In preparation for each high-energy firing sequence, the laser beam is first imaged at low power and overlaid with inspection images of the final optics. An automated control system then decides whether the beam fluence needs to be reduced in areas containing flaws that could grow with repeated laser shots. Temporarily shadowing a flaw buys time, enabling the continued operation of NIF until the optic can be removed, refurbished, and reinstalled.



"The LEOPARD system was designed to dramatically improve the performance and operational reliability of laser systems," says Heebner. "The system saves NIF an estimated $5 million annually in direct refurbishing costs and eliminates operational delays that might be incurred by the refurbishing cycle. Many other high-energy lasers worldwide could be optimized for increased extractable energy and achieve greater operational lifetimes using LEOPARD."

NIF is designed to produce the first demonstration of controlled inertial-confinement fusion where the energy released is greater than the laser energy input. For NIF's 192 beams (48 quads) to be operated at optimum performance and with high reliability, a system of 48 precisely programmable beam shapes is essential. The LEOPARD system meets this need and sets a new defining standard for precise control of the most energetic laser system ever constructed.

—Cindy Cassady

Key Words: fusion energy, laser energy optimization by precision adjustments to the radiant distribution (LEOPARD), liquid crystal modulator, optically addressable light valve (OALV), R&D 100 Award, shadow blocker.

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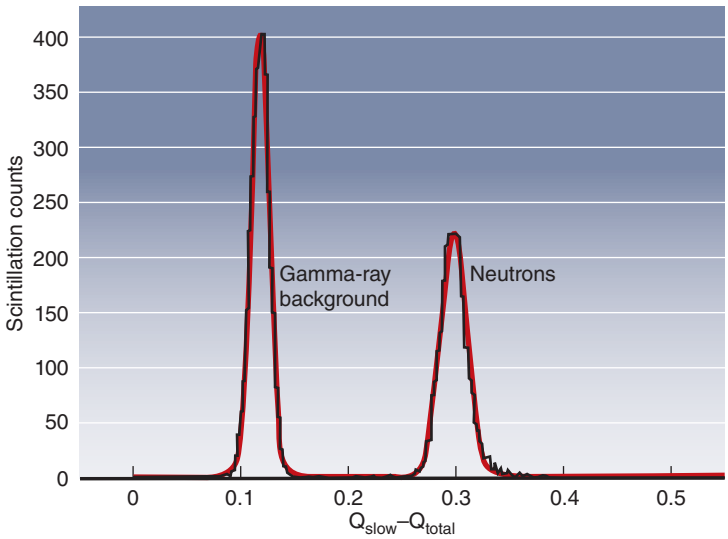
A Solid Solution for Neutron and Gamma-Ray Differentiation

ACCURATELY detecting illicit radioactive material moving through customs, border crossings, and pedestrian and transportation inspection portals is a critical national security objective for the U.S. Although highly sensitive and reliable detection systems are available today, existing systems consist of certain materials that are difficult to deploy in large volumes. What's needed is a new material that is easily fabricated and deployed. An effective detector in portal-inspection applications must also differentiate potentially dangerous radioactive sources from nonthreatening sources, such as cosmic rays, fertilizers, ceramics, decorative uranium glassware, welding rods, medical radioisotopes administered to cancer patients, and even bananas.

Lawrence Livermore scientists joined forces with collaborators from Eljen Technology in Texas to develop an enhanced plastic scintillator material that is a solid solution to efficient neutron and gamma-ray differentiation. The breakthrough material consists of a very high concentration of scintillating dye suspended in a polyvinyltoluene polymer matrix. This unique dye–polymer combination is extremely soluble. While plastic scintillators have been around since the 1950s, using such a high concentration of dye had not been considered to be a viable pathway. The team has received an R&D 100 Award for their work.



The new plastic scintillator is the first of its kind to discriminate between the desired neutrons and the gamma-ray background. In this experimental test with a Californium-252 fission source, the measured scintillation pulses from the neutrons are clearly distinguishable from the background signal. (Q_{slow}–Q_{total} is the ratio of delayed light to total light.)

Scintillating Materials Detect Radiation

Simply put, a scintillator is a substance that lights up when excited by ionizing radiation. This property makes scintillators useful in gamma-ray detection devices. For years, plastic scintillators have been used in gamma-ray detectors at transportation portals and at international crossing points. They have also been used in high-energy-physics experiments conducted at CERN in Switzerland and at Fermilab in the U.S. While conventional plastic scintillators can detect both gamma rays and neutrons, they have not been capable of distinguishing one from the other.

Organic crystals currently serve as one of the best types of neutron detectors, but the crystals can be difficult to grow and obtain in large volumes. Liquid scintillators present several hazards that hinder their use. Negative aspects of organic liquid neutron-detector materials include their toxicity, flammability, freezing points, and the difficulties in handling large amounts of these materials in field conditions.

Conversely, plastic scintillators pose none of the hazards or difficulties associated with those scintillator options. Given the low cost of plastic scintillator material, the material could be economically fabricated onto far larger surface areas than is possible with other neutron-detector materials, improving the nation's ability to identify radiation from illicit sources at transportation portals. Despite these benefits, plastic scintillators have always been considered to be far inferior to crystals or liquids. "It has been established opinion since the 1950s that organic crystals and liquid scintillators can work for detecting neutrons, but that plastics are not suitable for neutron detection," says materials scientist Natalia Zaitseva, who led the Livermore team.

Overcoming the Skeptics

After studying the available options and long-standing concerns, researchers at the Laboratory decided that the ease at which plastic scintillators can be shaped and fabricated makes them an extremely

Livermore physicist Natalia Zaitseva leads a research team that has developed the first plastic material capable of efficiently distinguishing neutrons from gamma rays.

useful material for gamma-discrimination applications. Further studies indicated that dye concentration in the plastic had to be at least 10 times greater than the amount previously used to achieve efficient discrimination of neutrons from gamma rays using plastic scintillators.

The thought that plastic scintillators could be created to efficiently discriminate neutrons from gamma rays came about, in part, from growing crystals with mixtures of the scintillating chemicals diphenylacetylene (DPAC) and stilbene. "We mixed DPAC with stilbene at 5 percent, 10 percent, and 15 percent, with no results," recalls Livermore materials scientist Steve Payne. "Suddenly at 18 percent, we could distinguish neutrons from gamma rays. Once we hit 40 percent, we had the full function." The result was the development of enhanced plastic scintillators that efficiently discriminate between neutrons and gamma rays.

Scintillators coupled to an electronic light sensor enable pulse-shape discrimination (PSD). PSD is a technique for detecting neutrons in the presence of background gamma radiation where particles are identified by the decay characteristics of the electronic pulse. These characteristics can then be analyzed and provide meaningful information about the particles that struck the scintillator. Tests have shown that the performance of the first plastic scintillators with PSD capability is comparable to that of the best commercially available liquid scintillators. (See the figure on p. 10.) Also, it may become possible to obtain scintillator plastics that are as good as the best scintillator crystals now in use.

"When we started this work, we had little understanding of how PSD was affected by the chemical composition of the scintillating materials. We have found some of the major principles of molecular interaction that determine the presence or absence of PSD properties in organic scintillators," Zaitseva says.

Reversing more than five decades of prevailing opinion by skeptics who said it could not be done, this diverse team of Laboratory researchers has demonstrated that their enhanced plastic scintillator material can efficiently differentiate neutrons from the gamma rays emanating from radioactive substances. Moreover, Eljen Technology, Livermore's industrial partner, has rapidly commercialized the new formulation and will have a product on the market within a few months.

—Geri Freitas

Key Words: diphenylacetylene (DPAC), gamma ray, neutron, organic crystal, plastic scintillator, polyvinyltoluene, pulse-shape discrimination (PSD), R&D 100 Award, radiation, stilbene.

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Livermore development team for plastic scintillators: (standing from left) Paul Martinez, Andrew Glenn, Sebastien Hamel, Steve Payne, and Keith Lewis; (sitting from left) Nerine Cherepy, Natalia Zaitseva, Iwona Pawelczak, Michelle Faust, and Leslie Carman. (Not shown: Ben Rupert; Charles Hurlbut, Loretta Hernandez, and Matt Jackson of Eljen Technology.)

Making Boring Cutting Edge

Glassy alloy powder is delivered onto a metal substrate and fused with it using lasers to form a NanoSHIELD (super-hard inexpensive laser-deposited) coating. (Courtesy of Oak Ridge National Laboratory.)

THROUGHOUT history, tunnels have been used for aqueduct, storm-drain, and sewer systems and for pedestrian, motor-vehicle, and rail-train passageways. In urban environments today, tunnels are often used instead of bridges for transportation because unlike bridges, tunnels hide traffic and allow land to be retained for other uses.

The development of the tunnel-boring machine (TBM) in the mid-1900s revolutionized tunnel building. A modern TBM is an enormous piece of equipment with 20 or more disc cutters mounted in a rotating circular plate 6 meters in diameter or larger. The machine advances into the tunnel in increments of 1.5 meters called "pushes." During these pushes, the crown area of the disc cutters pulverizes the rock face. Wear on the disc cutters is so severe that they must be replaced frequently, typically every few days depending on the type of host rock, which is costly in terms of both time and money.

Attempts have been made to extend the life of disc cutters by applying hardened coatings. However, during each rotation, the disc cutters experience a combination of tensile and compressive stresses that has thwarted these attempts—that is, until these barriers were shattered with the development of the NanoSHIELD (super-hard inexpensive laser-deposited) coating. NanoSHIELD is a nanostructured protective coating that can extend the life of disc cutters by at least 20 percent, potentially saving millions of dollars over the course of a project.

The coating is created by lasers that fuse a specially formulated iron-based amorphous alloy powder onto a steel substrate, forming a metallurgical bond. While the NanoSHIELD coating was first designed to prolong the life of cutting discs used for tunnel boring, it can also be used in other applications such as rock-mixing paddles, machining tools, and geothermal drilling tools.

A team of scientists and engineers from Lawrence Livermore and Oak Ridge national laboratories and collaborators at Strategic Analysis, Inc.; Ozdemir Engineering, Inc.; Colorado School of Mines; and Carpenter Technology Corporation have won an R&D 100 Award for the technology. The team's efforts benefited from previous work performed under the Structurally Amorphous Materials (SAM) Program, which was cosponsored by the Defense Advanced Research Projects Agency and the Department of Energy.

Exploiting Key Technologies

In crystalline alloys, atoms form an orderly three-dimensional lattice, which allows the alloy to stretch or bend. However, under high enough stress, crystalline alloys are prone to metal deformation. In contrast, structurally amorphous materials, such as iron-based amorphous alloys, have the disordered atomic structure of glass, making them harder, stronger, and more resistant to wear. The SAM Program developed innovative iron-based amorphous alloys with the correct balance of hardness, ductility, and wear resistance for tunnel-boring applications. Powder forms of SAM alloys are now commercially produced in bulk quantities via gas atomization and are used in the NanoSHIELD coating.

NanoSHIELD development also has benefited from advancements in additive manufacturing. (See *S&TR*, March 2012, pp. 14–20.) Instead of machining away material to shape a

part, additive manufacturing can build components in layers from materials such as SAM powder.

A Choice of Fabrication Methods

To apply the NanoSHIELD coating onto a disc cutter, the team uses a method that involves depositing SAM powder by aspiration onto the cutter with a polymer-based binder. The binder retains the powder in place until laser fusing. The powder is applied in striped or freckled patterns, which allows for distortion or deformation of the steel substrate without disturbing the coating, similar to the use of expansion joints in concrete to accommodate thermal strains. The laser fuses the powder to the substrate, forming a strong metallurgical bond. Then the excess binder and powder are extricated by a variety of means, including scrubbing with a wire brush. This method is preferred for coating disc cutters because of their size.

Another method involves fusing the NanoSHIELD coating to a steel substrate using a direct metal deposition free-form laser and robotic system. Binders are not applied; rather, the powder is delivered to an area by argon gas where it is fused by the laser and solidified in place. The sophisticated software controlling the laser and robot allows the system to coat more complex geometries. For example, paddles used in aggregate mixers have been successfully coated with this method.

The team's experiments in laser fusing of NanoSHIELD coatings have led to unique nanocrystalline, glassy, and nanocrystalline–glassy composites with incredible metallurgical properties. For example, a sufficient coating thickness for improving the wear resistance of a cutting disc is only 0.1 to 0.7 millimeters. The coating can have from 1.3 to more than 7 times the hardness of the steel substrate without affecting the intrinsic toughness and elasticity of the substrate.

Performing Field and Laboratory Experiments

According to the Colorado School of Mines, in over 25 years of testing and research and development on coated disc cutters, NanoSHIELD-coated discs are the first to not spall or fracture after one linear cut of granite on a linear cutting machine used for simulating full-scale rock-cutting conditions in the laboratory. The granite is cast in concrete within a heavy steel box to provide the necessary confinement during testing. After each cut, the granite is moved sideways by a preset spacing to duplicate the action of multiple cutters on a TBM. "In laboratory tests at Colorado, the coating showed no signs of spalling even after more than 100 cuts on granite," says Livermore scientist Frank Wong, who led the disc-cutter collaboration.

Livermore NanoSHIELD codeveloper Frank Wong.

Following these positive laboratory tests, full-scale field tests were performed at the Combined Sewer Overflow Tunnel Project in Atlanta, Georgia. Four of the 52 disc cutters on a 9.7-meter-diameter TBM were replaced with NanoSHIELD-coated discs, adjacent to uncoated cutters. The coated cutters survived 13 pushes without cracking or spalling. Most remarkable, the coated cutters maintained their sharpness at least 20 percent longer than the uncoated cutters, resulting in less down time for disc replacement, higher penetration rates, and lower energy consumption.

—Geri Freitas

Key Words: direct metal deposition, disc cutter, glassy metal, iron-based amorphous alloy, nanocrystalline, NanoSHIELD (super-hard inexpensive laser-deposited) coating, R&D 100 Award, tunnel-boring machine (TBM).

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Ten Times More Data for Shock-Physics Experiments

FOR years, scientists conducting shock-physics experiments were limited to measuring sudden velocity increases at only a few discrete points on a target's surface. For example, as recently as a year ago, the high costs and complexity of setup forced researchers at the National Nuclear Security Administration (NNSA) laboratories to collect velocity data at only a dozen or so points on a moving surface as part of stockpile stewardship experiments. These scientists then used extrapolation, assumptions, and models to determine what was occurring in regions of the experimental target not observed directly.

Today, scientists are routinely recording 96 channels of optical velocity data at a fraction of the former cost to acquire data from just a few channels. This new technology, for which its developers earned an R&D 100 Award, is called multiplexed photonic Doppler velocimetry (MPDV).

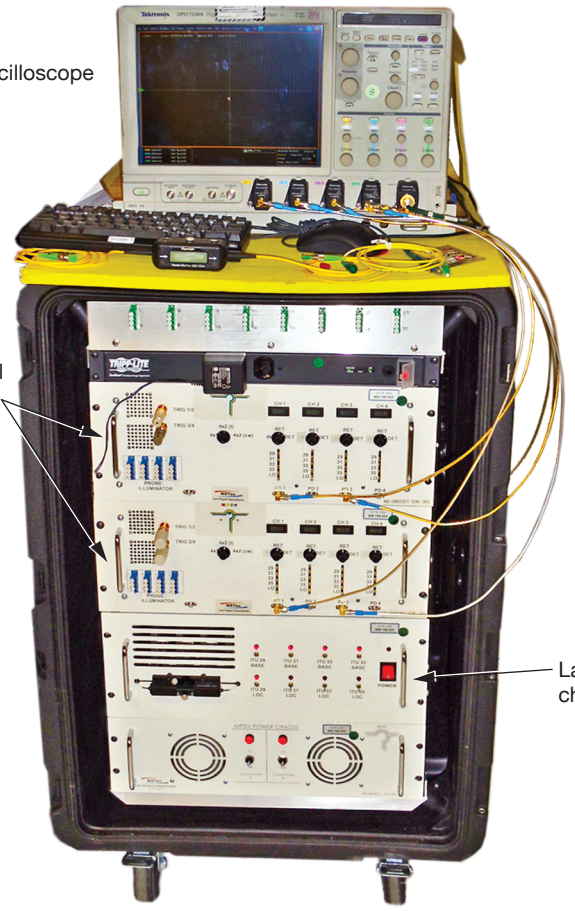
The MPDV system was designed and developed by a team from NNSA's National Security Technologies (NSTec), LLC, the managing and operating contractor for the Nevada National Security Site and its related facilities, including operations in Los Alamos and Nevada. Senior scientist Ed Daykin led the development team together with Livermore physicist Ted Strand. The project began under NSTec's Site Directed Research and Development Program, and final development was conducted under the Shock Wave Related Diagnostic Development Project, which addresses the diagnostic needs of the NNSA nuclear design laboratories (Lawrence Livermore, Los Alamos, and Sandia national laboratories) in the area of shock physics.

Beat Frequency a Matter of Subtraction

MPDV is an optical velocimeter, a group of noncontact diagnostics that measure the velocities of explosively driven metal surfaces in single-shot shock-physics experiments. These surfaces may be driven to kilometer-per-second velocities in less than a billionth of a second. MPDV is a significant improvement over photonic Doppler velocimetry (PDV), which was pioneered by Strand. He searched in the early 2000s for an optical-based technique that was easier to deploy and more cost-effective than two other instruments: the Fabry–Perot velocimeter, developed at Livermore, and the commercially available VISAR (velocity interferometer system for any reflector).

PDV is based on determining the "beat frequency," the difference in frequency between two waves, in this case, the difference in frequencies between a reference laser and the Doppler-shifted light reflected from a moving surface. Over the years, PDV became a standard diagnostic tool available to Livermore researchers. (See *S&TR,* July/August 2004, pp. 23–25.)

Strand explains that although highly reliable, PDV cannot economically provide the many dozens of simultaneous



A compact multiplexed photonic Doppler velocimetry (MPDV) system includes a 20-gigahertz digital oscilloscope for recording data, 32 optical channels for simultaneously measuring 32 discrete surface velocities, and a chassis for powering the lasers that are used to determine the beat frequency—a combination of the Doppler-shifted light from one laser and the reference light from another laser.

measurements needed to improve physical understanding and experimental accuracy in some stockpile stewardship experiments. In particular, Los Alamos and Lawrence Livermore scientists performing hydrodynamics experiments requested a more portable and cost-effective diagnostic system that could record more than 100 points of optical velocimetry data. Hydrodynamics experiments monitor the movement of a curved imploding surface inside a domelike configuration. In these experiments, the detonation of high explosives sends a shock wave through the test material, causing a liquidlike flow. Liquid behavior is described by hydrodynamic equations, so the experiments are often called hydrotests. (See the related article beginning on p. 16.)

Livermore MPDV codeveloper Ted Strand.

More Information at Reduced Cost

In response to the experimenters' requests, the MPDV development team increased the data-recording capacity of PDV by nearly an order of magnitude and reduced the cost per data channel fivefold. Built entirely from commercially available components, MPDV incorporates frequency- and time-division multiplexing to provide increased channel count, simultaneously measuring up to 32 discrete surface velocities onto a single digitizer. Frequency-division multiplexing sends signals in several distinct frequency ranges at a given time. Time-division multiplexing involves sequencing groups of data from individual input streams, one after the other, in such a way that they can be associated with the appropriate receiver. The equipment is designed to be set up and operated by one person per 32-channel system. While traditional PDV cannot discern between forward- and backward-traveling surface motion, MPDV measures the direction of travel.

MPDV uses a fiber-optic interferometer that measures the beat frequency resulting from a combination of the Doppler-shifted light from one laser and the reference light from another laser—an approach referred to as the heterodyne method. The Doppler-shifted light from four different probes is combined with four different reference light frequencies and applied to a photodetector. This process is accomplished within a fiber-coupled system that leverages commercially available telecommunications hardware. The beat frequency is recorded onto a high-bandwidth (20-gigahertz) digitizing oscilloscope and is then analyzed to determine velocity versus time at any of the surface locations that were monitored.

With MPDV, scientists can make hundreds of velocity measurements between 0.001 to 30 kilometers per second that are both economical and logistically feasible. The portable MPDV system requires no special laser safety requirements.

Proof-of-concept experiments were conducted in early 2011. The technology was first demonstrated at Los Alamos in August and September of that year. MPDV was then fielded on two multimillion-dollar experiments in October and December at Lawrence Livermore and Los Alamos, respectively. On March 7, 2012, a record 96 channels were demonstrated using three MPDV units.

By providing scientists with much more high-quality data, MPDV improves the ability to predict shock and material conditions and allows detailed comparisons between computational and experimental results. In this way, the technology helps ensure the safety and security of the nation's nuclear stockpile.

The new capability has potential applications to pulsed-power experiments as well as low-velocity commercial applications such as noncontact measurements of vibration. The team plans to continue development with an eye on increasing channel count, improving cost-effectiveness, and enhancing measurement capabilities.

—Arnie Heller

Key Words: fiber-optic interferometer, hydrodynamics test, multiplexed photonic Doppler velocimetry (MPDV), R&D 100 Award, shock physics.

For further information contact Natalie Kostinski (925) 423-1890 (kostinski1@llnl.gov).

Simulation and Precision Engineering Lead to Extraordinary Results in Experiment

A multidisciplinary international team, led by Livermore physicist Don Roberts, designed and conducted the first subscale integrated weapons experiment in the U.S. since the 1980s. What made this test truly remarkable was that the entire experiment was designed using an advanced, three-dimensional (3D) supercomputer software code.

The Laboratory conducts scores of hydrodynamics experiments, or hydrotests, such as integrated weapons experiments (IWEs), which re-create the exact specifications of a nuclear device except for the special nuclear material. Conducted as part of the Stockpile Stewardship Program, which ensures the safety, security, and reliability of the nation's current weapons stockpile without nuclear testing, IWEs address performance- and safety-related questions and are also used to improve computer simulations.

Hydrotests are set up to understand what happens to metal adjacent to a high-explosive detonation. An experiment involves first detonating insensitive high explosives (IHEs) that surround a pit made of inert (nonfissile) material. Except for the nonfissile materials, experiments use parts and materials similar to those in stockpile devices, including the same high explosives. (See *S&TR*, September 2007, pp. 4–11.)

In the early years of the Laboratory, Livermore conducted hydrotests in a trial-and-error fashion, particularly when new diagnostics were developed. Scientists would design a diagnostic,

and if the experiment didn't work, they would modify it and conduct another experiment. As computer simulation power has increased, researchers can better model diagnostic features, thus requiring fewer hydrotests.

Several features of the multimillion-dollar test conducted in October 2011 were extraordinary. First, in preparation for possible follow-on subcritical experiments using special nuclear material, the experiment was done at subscale—that is, at a smaller scale than an actual nuclear device. Second, the experiment included new diagnostics, scaled detonators, and boosters developed specifically for this IWE but that had not been tested. Finally, the experiment required unprecedented precision in the engineering and assembly of the device because of its subscale size.

A key goal of this experiment was to obtain as much information as possible about the continually changing velocities of materials as they implode. Photonic Doppler velocimetry (PDV), a technique invented by Livermore scientists, can measure particle velocities up to 30 kilometers per second, with a precision of 1 meter per second. (See *S&TR*, July/August 2004, pp. 23–25.) The team used PDV to precisely measure the response of the materials to shock waves.

Designing Experiments by Computer

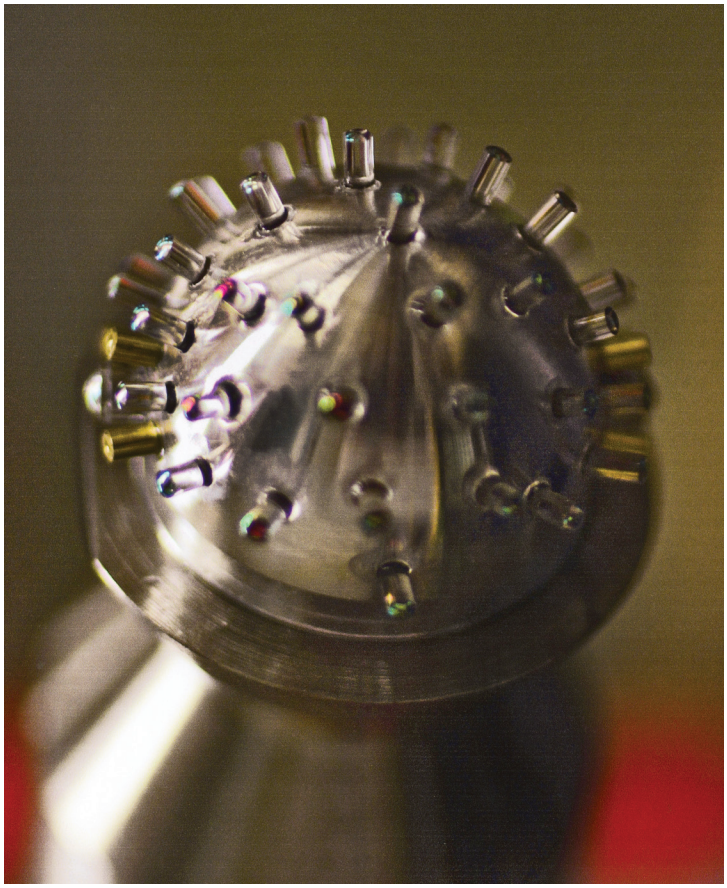
This experiment was ambitious because the device had many original pieces of equipment that were designed to an unprecedented level of precision. Traditionally, any of these design features would have required a number of expensive preparatory experiments to ensure successful data collection.

To avoid the financial costs and schedule delays of preparatory experiments, Roberts assembled a team that included computer-modeling experts who developed 3D simulations that showed the functioning of the experiment from the lighting of the detonators through data collection. Much of the trial-and-error process was accomplished with simulations rather than with a series of expensive—often $5 million—hydrotests.

Still, the accuracy of the simulations was a concern. For example, the team used IHE computer models to simulate the implosion, but devices that use IHE are difficult to model accurately. IHE is more resistant to fire or accident, but it is also harder to detonate than conventional high explosives. The team performed small-scale experiments at Livermore's High Explosives Applications Facility (HEAF) to test the models, which led to improved simulations and a modified design of the detonators. (See *S&TR*, July/August 2012, pp. 4–11 for more information about research and development of explosives, propellants, and pyrotechnics at HEAF.)

All-Optical Probe Dome

Historically, Livermore scientists used pin domes to obtain data about the temporal and spatial uniformity of an implosion. Pin domes, which are small spheres with hundreds of protruding radial pins of different lengths, send signals as the implosion strikes the dome, and the data from each pin reflect a snapshot at that point in space and time.



The Livermore-designed all-optical probe dome is studded with outlets for fiber optical lines. The new diagnostic provided continuous photonic Doppler velocimetry data during a subscale integrated weapons experiment performed at the Laboratory's Contained Firing Facility in October 2011.

In the continual search for better equipment to measure extreme velocities, Roberts's team designed a diagnostic called the all-optical probe dome. The dome is studded with outlets for fiber optical lines leading to recording instruments, and it provides 60 channels of continuous PDV data using both Livermore and National Security Technologies, LLC, multiplexers. An additional 12 channels provide exterior data. (See the related article on p. 14, which describes the R&D 100 Award-winning multiplexers.) Mike Dunning, program director for Livermore's Primary Nuclear Design, says, "The all-optical probe dome provides continuous data versus snapshots—akin to replacing 10 snapshots of a horse race with a full movie. We have much more detailed information about the response of the metal. This hydrotest featured the most PDV channels ever used at the Laboratory."

Precision Engineering

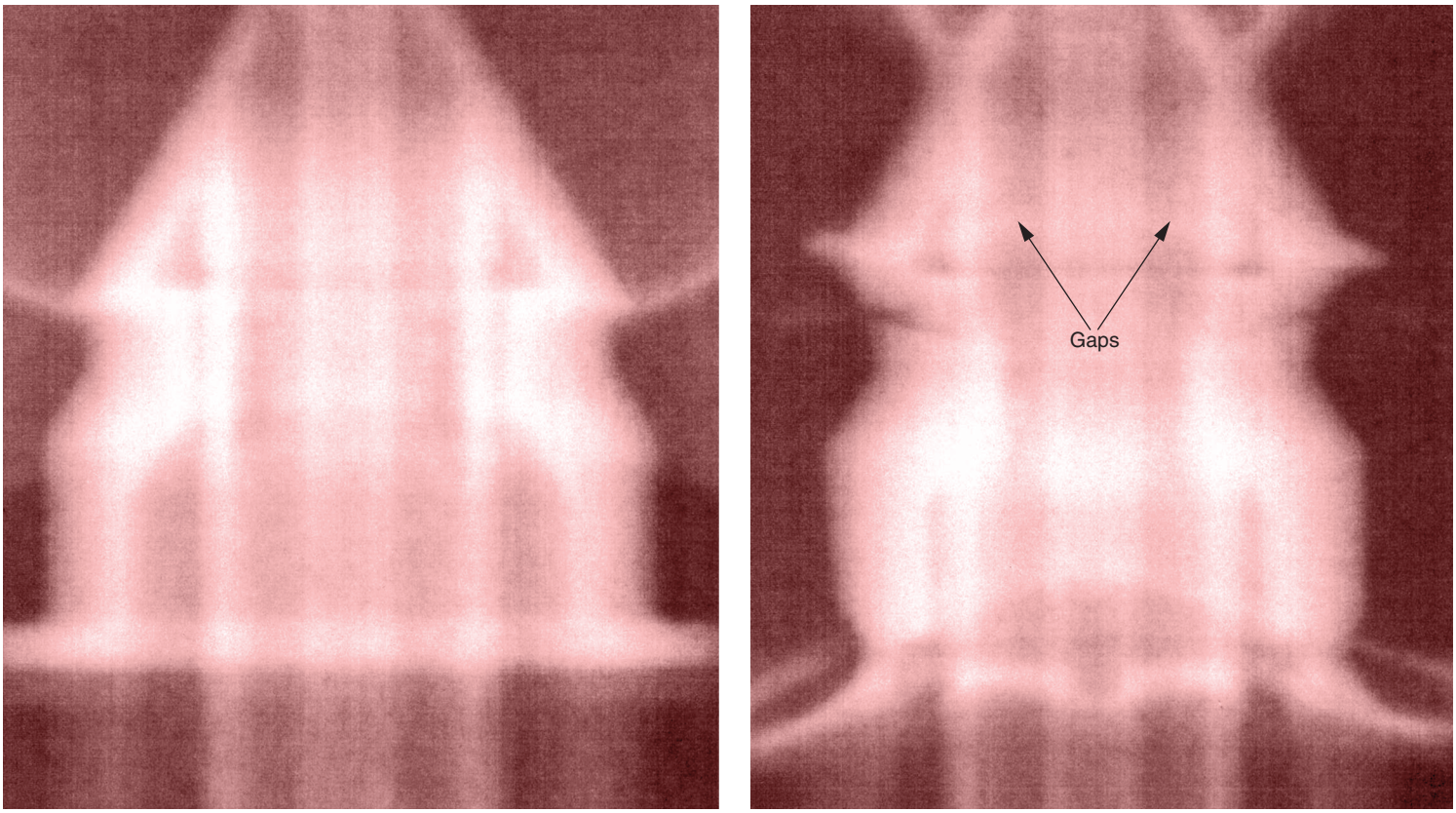
Once the experiment was simulated in 3D, the team had to build the device. "The real trick was to capture the available information

within the few microseconds before the diagnostics were destroyed by the explosion," says Matt Wraith, Livermore engineering team leader. "All the months or even years of setup go to waste if we don't obtain the data." To prevent the destruction of the probe dome before the data could be captured, former Livermore hydroengineer Ryan Krone designed gaps around each of the fibers, which allowed them to transmit information in the tiny fractions of a second before their destruction by the implosion.

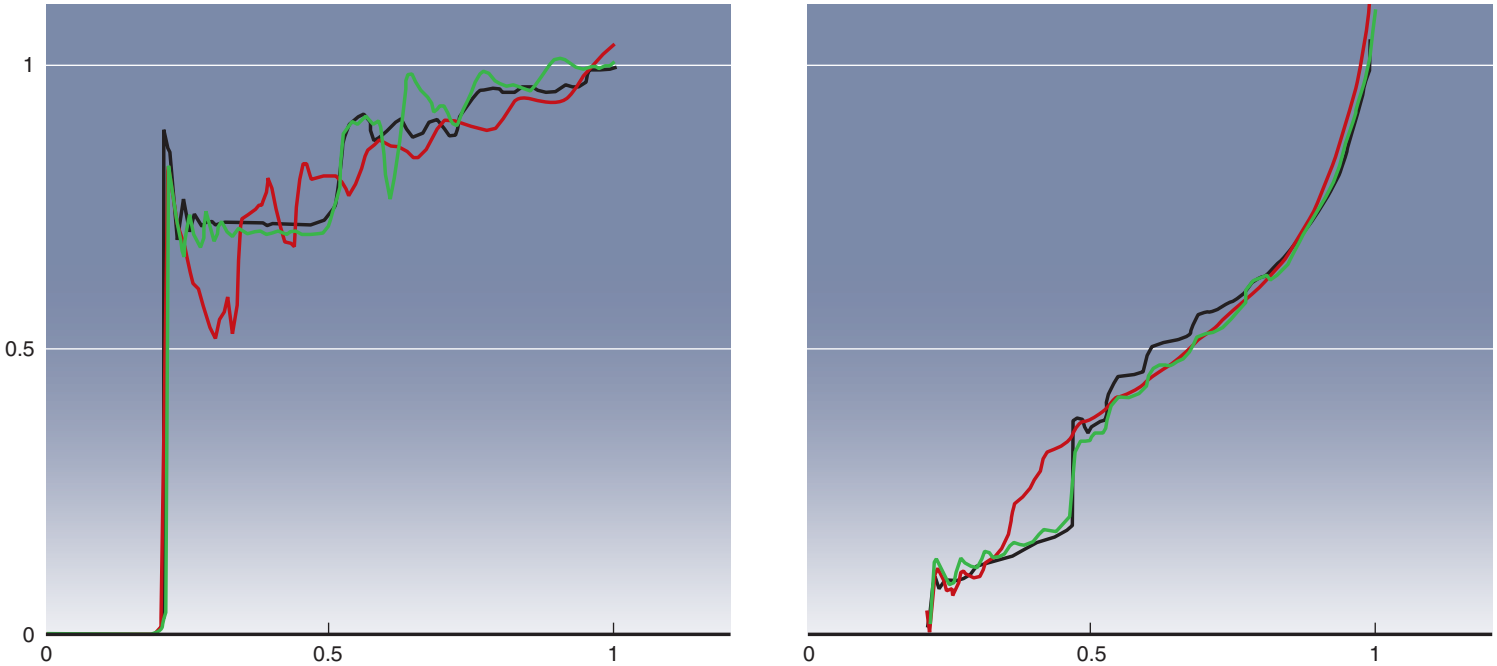
To ensure that the researchers could extract as much data as possible, the engineers, drafter–designers, specialized experimental physicists (called ramrods), and technicians were responsible for building components that matched the simulations exactly. These components required high-precision machining and had to be manufactured to unprecedented tolerances, a task made even more difficult because of the small size of the device.

Once the components were fabricated and the parts were carefully inspected, the device had to be assembled at the same level of precision as each individual part had been manufactured. As in watchmaking, it is not enough to just have precise parts—they must be assembled perfectly. The experimental device was even more difficult to assemble than an actual nuclear device because of its small scale. To ensure successful assembly, the team used Livermore's emerging rapid prototyping capability to fabricate practice parts, which were then used to refine assembly techniques. (See *S&TR*, March 2012, pp. 14–20.)

This hydrotest, which was the culmination of three years of work, took place at the Contained Firing Facility (CFF) at the Laboratory's Experimental Test Site located 24 kilometers southeast of Livermore. CFF, the only one of its kind in the Department of Energy complex, allows the Laboratory to conduct nonnuclear high-explosives



Radiographs of the probe dome taken (left) before and (right) during detonation show the central cylinder, which contains optical fibers. The dark lines show the precisely engineered gaps that delay the implosion long enough to allow the optical fibers to send data to the multiplexers located outside the firing chamber.



(left) The original material failure (spallation) model (red line) does not correspond well to the experimental spallation data (black line). The model was then updated (green line) and now corresponds more closely with the experimental data. (right) This postshot model of explosives performance (red line) still fails to capture some features in the experimental data (black line). After the model was improved (green line), the simulation corresponds more closely with the experimental data.

experiments indoors, minimizing noise and reducing the emission of hazardous materials. It provides a controlled environment for experiments to optimize data capture. In addition to the firing chamber, the facility includes a staging area, diagnostic equipment rooms with radiographic capabilities and ports to the firing chamber, and a control room from which the shot is fired.

Results Pay Off

The experimental data help validate computer modeling of test-device performance and support upcoming milestones for predictive capabilities. Results led to improved high-explosives and material failure (spallation) models. (See the figure above.) Simulations now correspond more closely to experimental results.

"Bringing together diverse teams of experts to accomplish our programmatic objectives is a hallmark of this Laboratory," says Dunning. "In this case, Don assembled a team that spans multiple organizations inside and outside Livermore." The team included 44 people from the Laboratory, three from the Nevada National Security Site (formerly known as the Nevada Test Site), one from Los Alamos National Laboratory, and six from Great Britain's Atomic Weapons Establishment. Disciplines encompassed physicists, experimentalists, computer scientists, diagnosticians, engineers, drafter–designers, ramrods, machinists, inspectors, and technicians.

Despite all the innovative technology and the higher level of precision engineering, the team obtained full results with a single high-risk, high-payoff experiment. The high-fidelity, continuous temporal measurements not only provided more information about the actual test but were also used to further improve computer simulation codes.

—Karen Rath

Key Words: all-optical probe dome, hydrodynamics experiment, hydrotest, integrated weapons experiment (IWE), multiplexer, photonic Doppler velocimetry (PDV), precision engineering, three-dimensional (3D) computer simulation.

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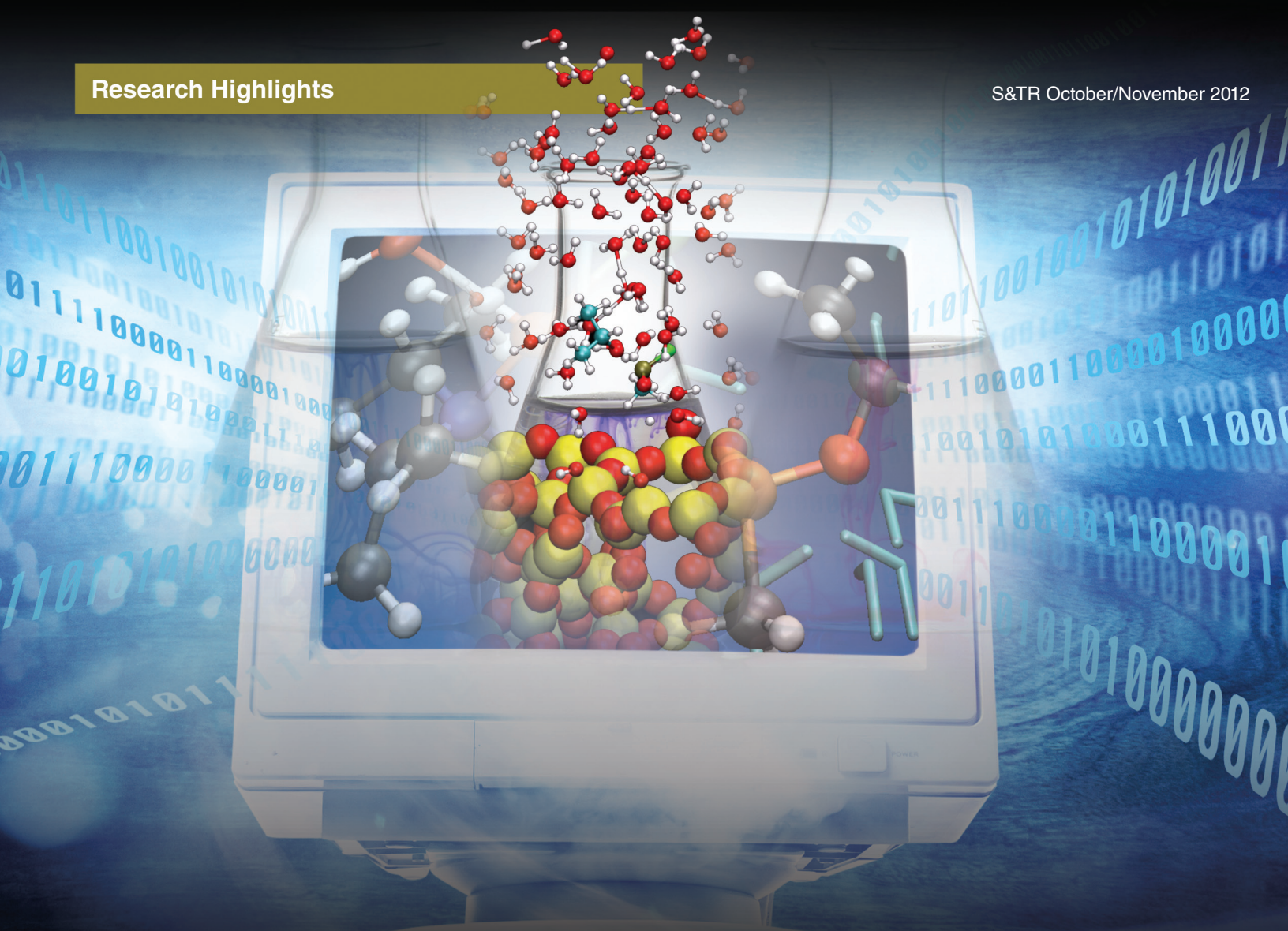


Breaking Down Nerve Agent Behavior

CHEMISTRY research immediately conjures imagery of scientists in lab coats mixing colorful reagents in flasks and beakers. It is becoming increasingly common, though, for traditional chemists to work side by side with computational chemists to probe the world at the atomic scale. Today's computational chemists are performing similar tasks to laboratory chemists, albeit in a virtual environment. As computing power increases and scientists are able to model the world around them with increasing fidelity, computational chemistry is emerging as an effective complementary approach to traditional laboratory experiments for better understanding of complex chemical behavior.

One area benefiting from these insights is the study of toxic substances such as nerve agents. Among the more dangerous components of humankind's destructive arsenal, nerve agents are potent chemical warfare agents that, if inhaled, swallowed, or absorbed through the skin or eyes, will inhibit the transmission of nerve impulses and swiftly cause death. In a post-9/11 world, with the lingering threat of terrorism, researchers have been working to supply national security personnel and emergency responders with reliable information on how best to remediate an area contaminated with a nerve agent, if such a dire situation were to occur. Restoration and remediation efforts will dramatically benefit from a molecular understanding of how nerve agents react chemically with potential decontaminants as well as adjacent surfaces. Computational chemistry offers an opportunity to study nerve agents without the risk incurred from handling these toxic chemicals.

Today, computer simulations allow researchers to perform fewer and more targeted laboratory experiments. Experimental chemist Bradley Hart, director of Livermore's Forensic Science Center (FSC), observes, "With laboratory experiments, it can be difficult to get at the mechanisms behind the chemical reactions. We see the reaction products and the reaction rates, but understanding the reaction process at an atomic level is more difficult. For example,

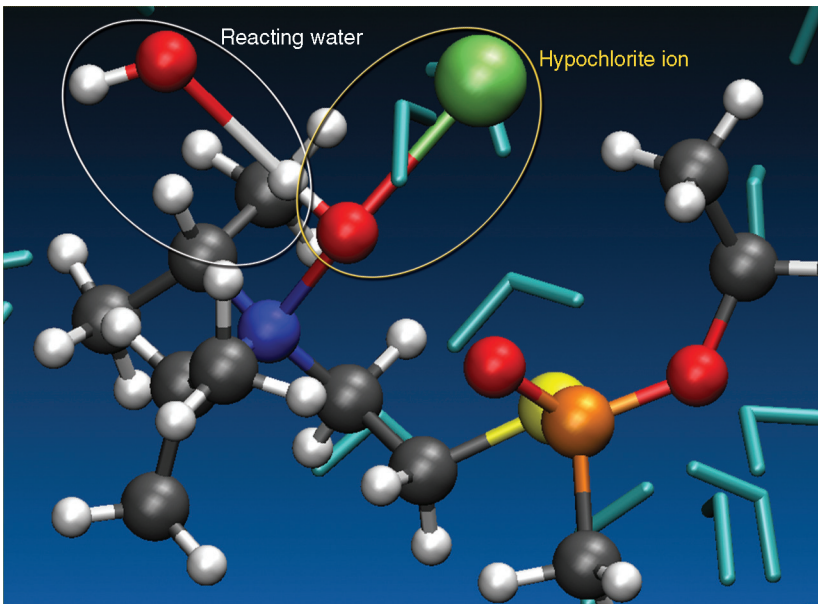
sometimes multiple reaction paths can lead to the same result." Computational chemistry is well suited for peering beneath the surface of reactions. Computational chemist Richard Gee says, "Experimentalists have to make many inferences, but computationalists can observe what's happening at an atomic level."

Saving Time

Gee and computational chemist William Kuo have led a successful effort to demonstrate a computational approach to decontamination research by characterizing how the nerve agents VX and sarin chemically degrade. Using the simulation suite CP2K on Livermore's 360-trillion floating-point operations per second (teraflops) BlueGene/L supercomputer, the researchers modeled the complex interactions between nerve agents and decontaminant molecules within a first-principles framework. Unlike most simulation techniques, first-principles simulations build models directly from quantum-mechanical principles and fundamental physical properties such as atomic mass and charge. This technique eliminates potential biases and assumptions about how atoms and molecules interact by calculating the forces dictating these reactions directly from a system's electronic structure and nature's basic laws. First-principles methods are ideal for modeling chemical processes where bonds can form, alter, or break. (See *S&TR*, October 2005, pp. 12–18.)

In a prototypical chemical reaction, a reactant is converted to a product at a rate determined by the activation energy barrier. With a low activation barrier, the chemical reaction can proceed quickly, while a high activation barrier impedes the reaction, causing it to proceed more slowly. Many chemical reactions can take microseconds to many seconds to occur, depending on the activation barrier involved. Unfortunately, even fast chemical reactions are computationally expensive to model with first-principles methods. Using BlueGene/L, it is only possible to directly simulate the interactions of hundreds of atoms for a span of picoseconds. Were researchers to run such a simulation, they would require an incredible stroke of luck to observe a chemical reaction of interest.

Bridging the temporal gap between chemical reaction and computer simulation necessitates improvements in simulation efficiency. By using a rare-event sampling method known as metadynamics to artificially accelerate the simulation time, the Livermore researchers were able to study many potential chemical degradation pathways. Metadynamics is a powerful and flexible algorithm for enhancing molecular-dynamics simulations and determining the free-energy surface—the multidimensional energy landscape of a reaction pathway—for a chemical reaction. For this technique, the researchers define a set of reaction possibilities to describe a multitude of potential reactions. Ideally, these variables examine a variety of potential reaction sites, including the surrounding medium.



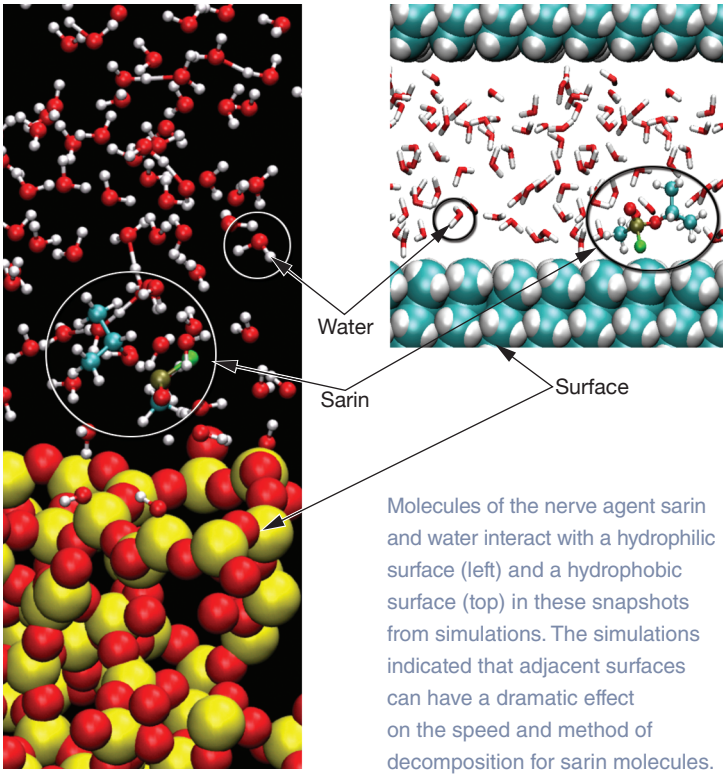
In this snapshot from a simulation of the nerve agent VX, an incoming hypochlorite ion (bleach) interacts with the nitrogen (blue) atomic center of VX. As the hypochlorite oxygen atom is displaced from the chlorine (green atom), the nitrogen also reacts with an adjacent water molecule. Water molecules not directly involved in the reaction are displayed as L-shaped objects. Computational chemists are using a metadynamics algorithm to efficiently examine potential reaction sites, such as VX's nitrogen atomic center.

A Close Match

Experiments have demonstrated that for the nerve agents VX and sarin, the most important chemical reactions are likely to occur at the phosphorus atomic center. It is here that the nerve agent molecule is most susceptible to a bond rupture, possibly resulting in a nontoxic product. The formation of the product can be accelerated by increasing temperature or adding a strong oxidizing agent, such as hypochlorite ions from bleaching powder. To provide a computational comparison, Gee and his team modeled VX behavior in the presence of bleach and water. Tracking the results in half-femtosecond intervals, they examined a variety of decontamination mechanisms and chemical-reaction energy barriers. They also examined how both the water and the bleach might affect the decontamination reactions, something that had not previously been studied computationally.

The degradation of nerve agents can occur through multiple reaction pathways. By leveraging computer resources and the metadynamics algorithm, the researchers could independently simulate each possible reaction pathway, not only at the phosphorus atomic center but also at the sulfur, nitrogen, and carbon atomic centers. Each potential pathway requires an independent simulation, which takes approximately 100,000 computing hours to execute.

VX had already been extensively studied in the laboratory, and the researchers found a solid match between the computed and



Molecules of the nerve agent sarin and water interact with a hydrophilic surface (left) and a hydrophobic surface (top) in these snapshots from simulations. The simulations indicated that adjacent surfaces can have a dramatic effect on the speed and method of decomposition for sarin molecules.

experimentally measured results. Gee says, "Our modeling results were surprisingly accurate and precise when compared with the experimental data." Kuo adds, "This modeling would not have been possible without fast computers and rare-event calculation methods."

In a related study, the researchers modeled the decontamination of sarin and compared their results to experiments conducted at FSC. Through reliable, efficient chemical modeling of the interactions between nerve agents, water, and bleach, Gee, Kuo, and their colleagues demonstrated the efficacy and precision of simulations for decontamination research.

Love–Hate Relationship

In a real remediation situation, nerve agents, water, and bleach interact within a complex chemical environment. Previous laboratory research has shown that sarin has only one path for decomposition in a standard liquid solution, but whether this holds true when sarin is adjacent to surfaces such as dirt, concrete, or linoleum has been unknown. Kuo notes, "Experiments have indicated that interfaces can have a profound effect on the chemistry for sarin, but it has been hard to pinpoint the effect." Different surfaces could potentially accelerate or retard decontamination. Building on their successful VX simulations, the researchers investigated potential degradation pathways for sarin in the presence of a hydrophilic (water-loving) or a hydrophobic (water-hating) surface.

For the hydrophilic surface, researchers modeled a slab of glass. The simulations revealed that when sarin was near the glass surface, the most probable decomposition mechanism was similar to that of a standard liquid solution, but the sarin broke down more quickly. The thin film of water in contact with the glass surface adopted a distinctive molecular arrangement, which likely helped lower the activation barrier by 30 percent. The hydrophobic surface, vinyl, produced the opposite effect. It not only raised the energy barrier by 20 percent but also changed the reaction path for molecular degradation.

These simulations involving extremely hydrophilic and hydrophobic surfaces effectively demonstrated the extent to which surfaces can influence sarin degradation. Gee is quick to note that the surfaces used in the simulations were idealistic, involving perfectly smooth crystals. "In the real world, at an atomic level, the topology of common materials is complex, containing many nonideal features," he says. "Such features may provide many places for a sarin molecule to hide from being chemically degraded." Still, the models are sufficiently realistic in that they provide a means to obtain useful information regarding how possible nerve agent degradation chemistry may change depending on the encountered surface. The simulations confirmed that surfaces within bonding distance of sarin could fundamentally affect its reaction rates and decomposition processes.

The ideal investigation of the chemical behavior of nerve agents should combine both modeling and experiments. As home to simulation experts, powerful computers, and scientists who can validate degradation mechanisms experimentally (see *S&TR,* May 2003, pp. 4–11; April 2002, pp. 11–18), Lawrence Livermore is uniquely qualified for such work. While this effort is still in its early stages, the research performed thus far supports using simulations to understand relevant reaction mechanisms. The results also indicate that computational chemistry could provide a viable means for screening decontamination formulations, with the goal of prioritizing promising substances and reducing the number of hazardous laboratory experiments required. Simulations examining the role of surfaces could also help guide Homeland Security and Defense Department personnel in customizing decontamination solutions to specific surfaces. Amassing reliable information on chemical weapon remediation methods enables a timely and effective response should a chemical attack ever come to pass.

—Rose Hansen

Key Words: BlueGene/L, computational chemistry, CP2K, energy barrier, first-principles simulation, metadynamics, nerve agent, rare-event sampling, sarin, transition state, VX.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Method of Remote Powering and Detecting Multiple UWB Passive Tags in an RFID System

Farid Dowla, Faranak Nekoogar, David M. Benzel, Gregory E. Dallum, Alex Spiridon
U.S. Patent 8,188,841 B2
May 29, 2012
A radio-frequency-identification (RFID) tracking and powering system uses coded ultrawideband (UWB) signaling. The proposed hardware and techniques use passive UWB transponders in the field of an RFID-radar system. The radar system enables multiple passive tags to be remotely powered (activated) at about the same time frame via predetermined-frequency UWB-pulsed formats. Once such tags are activated, UWB radar transmits specific interrogating codes to awaken the tags, which then communicate with a unique response code. A UWB system detects the tags using radar methods.

Signal Enhancement Using a Switchable Magnetic Trap

Neil Reginald Beer
U.S. Patent 8,189,186 B2
May 29, 2012
This system for analyzing a sample has a microflow channel. The system associates the sample with magnetic nanoparticles or magnetic polystyrene-coated beads, moves the sample with these nanoparticles or beads into the channel, and holds it there in a magnetic trap in the channel. The sample is then analyzed to obtain an enhanced analysis signal. The apparatus for sample analysis consists of magnetic particles connected to the sample, a microchip with a flow channel, and a carrier-fluid source connected to the flow channel for moving the sample. An electromagnetic trap connected to the flow line selectively traps the sample and the magnetic particles for analysis.

Portable Laser Synthesizer for High-Speed Multidimensional Spectroscopy

Stavros G. Demos, Miroslav Y. Shverdin, Michael D. Shirk
U.S. Patent 8,190,242 B2
May 29, 2012
This portable, field-deployable laser synthesizer is designed for multidimensional spectrometry and time-resolved or hyperspectral imaging. The device includes a coherent light source that simultaneously produces a broad, energetic, discrete spectrum spanning through or within ultraviolet, visible, and near-infrared wavelengths. The light output is spectrally resolved, and each wavelength is delayed with respect to the others. A probe enables light delivery to a target. For multidimensional spectroscopy applications, the probe can collect the resulting emitted light and deliver this radiation to a time-gated spectrometer for temporal and spectral analyses.

Assembly for Electrical Conductivity Measurements in the Piston Cylinder Device

Heather Christine Watson, Jeffrey James Roberts
U.S. Patent 8,193,823 B2
June 5, 2012
This assembly apparatus measures electrical conductivity and other properties of a sample in a piston cylinder device. The device applies pressure and heat to the sample. The assembly apparatus includes a body with an electrode that connects to the sample, an electrical conductor that connects to the electrode, a washer constructed of a hard conducting material that surrounds the electrical conductor, and a second electrode. The second electrode also connects to the sample, and a second electrical conductor connects to the second electrode.

Detecting Fission from Special Nuclear Material Sources

Mark S. Rowland, Neal J. Snyderman
U.S. Patent 8,194,814 B2
June 5, 2012
This neutron-detector system discriminates fissile material from nonfissile material and includes a digital data-acquisition unit that collects data at a high rate. The unit processes in real time large volumes of data directly into information that a first responder can use to discriminate materials. The system counts neutrons from an unknown source and detects excess grouped neutrons to identify fission in the unknown source. The system includes a graphing component that displays the plot of the neutron distribution from the unknown source over a Poisson distribution as well as a plot of neutrons from background or environmental sources. The system further includes a known neutron source placed in proximity to the unknown source to actively interrogate the unknown source and accentuate differences in neutron emission between the known and unknown sources.

Laser Diode Package with Enhanced Cooling

Robert J. Deri, Jack Kotovsky, Christopher M. Spadaccini
U.S. Patent 8,199,787 B2
June 12, 2012
A laser diode package includes a reservoir filled with a fusible metal in close proximity to a laser diode. The fusible metal absorbs heat from the laser diode and undergoes a phase change from solid to liquid during the laser's operation. The metal absorbs heat during the phase transition. Once the laser diode is turned off, the liquid metal cools and resolidifies. The reservoir is designed such that the liquid metal does not leave the reservoir even when in a liquid state. The laser diode package also includes a lid with one or more fin structures that extend into the reservoir and are in contact with the metal in the reservoir.

Method of Producing an Electronic Unit Having a Polydimethylsiloxane Substrate and Circuit Lines

James Courtney Davidson, Peter A. Krulevitch, Mariam N. Maghribi, William J. Benett, Julie K. Hamilton, Armando R. Tovar
U.S. Patent 8,202,566 B2
June 19, 2012
This metal system is contained in an integrated polymer microsystem. Conductive ink is applied to a flexible polymer substrate made of either silicone or polydimethylsiloxane.

Awards

Two Laboratory researchers received **Presidential Early Career Awards for Scientists and Engineers** (PECASE) for work in computational science and physics. This honor is the highest bestowed by the **U.S. government** on outstanding scientists and engineers, who are early in their independent research careers.

Heather Whitley, a design physicist, was chosen for her work using path-integral Monte Carlo techniques to produce accurate quantum statistical potentials for use in molecular-dynamic codes and for applying these methods to first-principles understanding of thermal conductivity in ignition capsules for the National Ignition Facility (NIF). Whitley was also selected for her service to the Laboratory Postdoctoral Association.

Jeffrey Banks, a computational scientist, was selected for his work in computational physics, scientific computation, and numerical analysis. In particular, he pioneered contributions in numerical approximations to hyperbolic partial differential equations that focus on the development and analysis of nonlinear and high-resolution finite-volume and finite-difference methods. Banks was also selected for his service in high schools and the scientific community.

PECASE winners receive $50,000 a year over five years to pursue research in their field. Both researchers have been able to pursue the science for which they were honored thanks to Livermore's Laboratory Directed Research and Development Program.

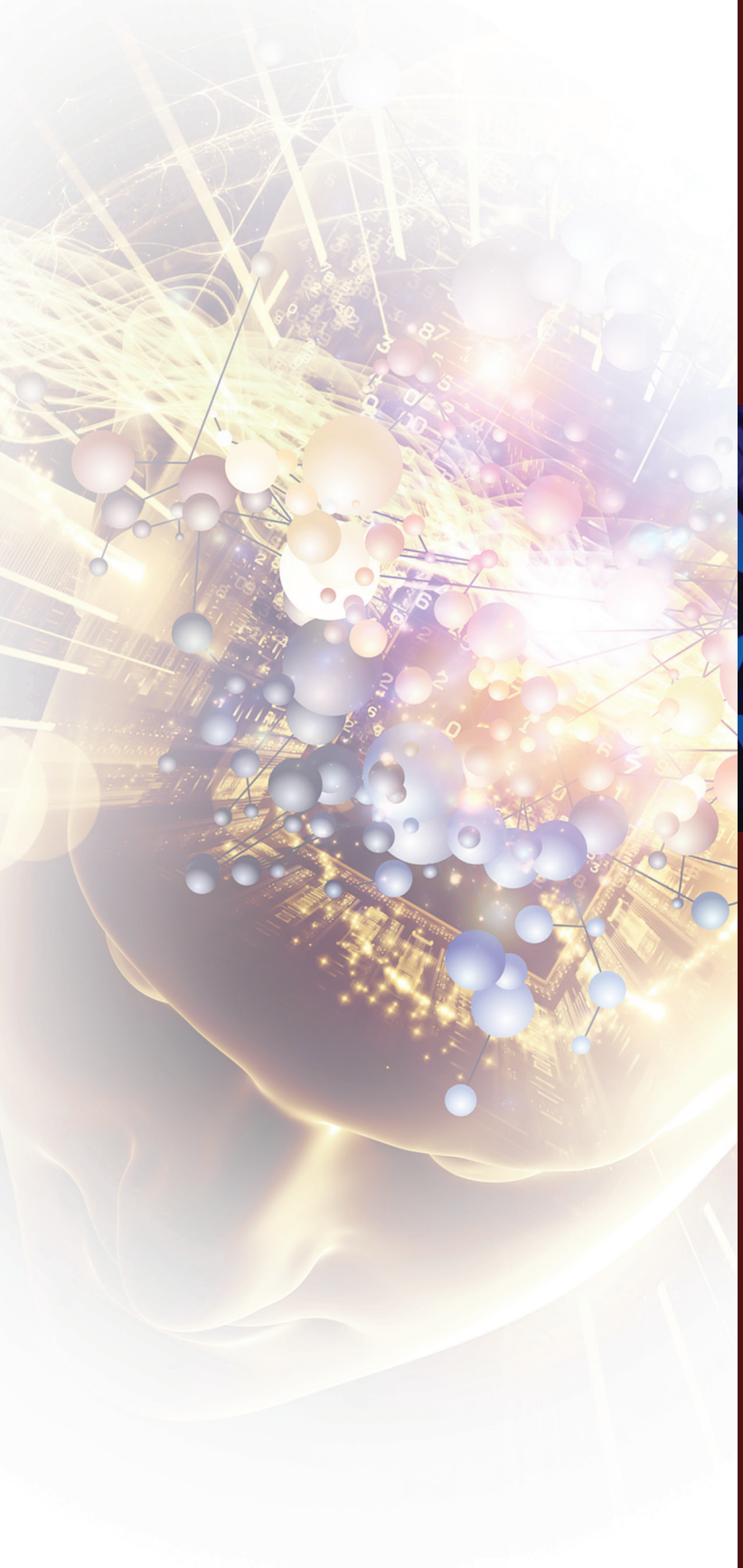
Mike McCoy, whose pioneering work in high-performance computing (HPC) established Lawrence Livermore as a world-renowned supercomputing center, was honored with the **National Nuclear Security Administration**'s (NNSA's) **Science and Technology Award**. McCoy received the award for "16 years of dedicated and relentless pursuit of excellence" from NNSA Administrator Thomas D'Agostino. Calling HPC "the lifeblood of NNSA science and technology," D'Agostino says McCoy's leadership in HPC "has had a global impact." McCoy leads the Laboratory's effort to develop and deploy the HPC systems required for the three national nuclear design laboratories (Lawrence Livermore, Los Alamos, and Sandia) to fulfill their mission to ensure the safety, security, and reliability of the nation's nuclear deterrent without nuclear testing. The newly created award is the highest recognition for science and technology achievements in NNSA.

A far-reaching discovery about laser–matter interaction with important implications for NIF has led to the selection of a team of researchers to receive the **2012 John Dawson Award for Excellence in Plasma Physics Research**. The award, established by the **American Physical Society**, will be presented in October to Livermore's **Debra Callahan**, **Edward Williams**, **Nathan Meezan**, **Laurent Divol**, **Robert Kirkwood**, and **Pierre Michel** as well as **George Kyrala** of Los Alamos National Laboratory.

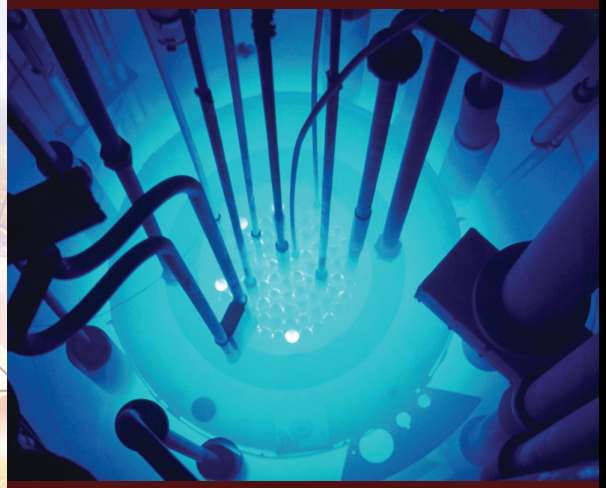
Their accomplishment had its genesis in the late 1990s, when physicists noted that laser beams crossing paths in a plasma could exchange energy. This phenomenon could potentially degrade the implosion symmetry of implosion targets, a crucial requirement for fusion ignition. Over the following 15 years, the researchers conducted experiments at the University of Rochester's OMEGA laser. They also developed new physics models, run on Livermore's Atlas and Hera supercomputers, to better understand the phenomenon. The researchers concluded that the energy-transfer process could be controlled with slight adjustments to the laser beams' wavelengths.

Yu-Hsin Chen, a Livermore postdoctoral researcher in the NIF and Photon Science Principal Directorate, was selected to receive the **2012 Marshall N. Rosenbluth Outstanding Doctoral Thesis Award** by the **American Physical Society**'s **Division of Plasma Physics**. The award, sponsored by General Atomics, was established to recognize "exceptional young scientists who have performed original thesis work of outstanding scientific quality and achievement in the area of plasma physics." Chen was honored "for measurements and theory of the ultrafast, high-field, nonlinear response of gases near the ionization threshold; characterization of femtosecond plasma filaments; and demonstration that femtosecond filamentation requires plasma stabilization."

The Laboratory received the **FY 2011 M&O Small Business Achievement of the Year Award** from the **Department of Energy** (DOE). The award, given by the DOE Office of Economic Impact and Diversity, Office of Small and Disadvantaged Utilization, recognizes the Laboratory's efforts and commitment as a small business advocate that "takes every opportunity to utilize small business concerns to meet its requirements." According to Michelle Quick, Livermore's Small Business Program Manager, the award reflects the Laboratory's achievement of a 2011 NNSA performance goal of 45 percent of total estimated subcontracting efforts toward small businesses. Quick says that promoting small business benefits everyone, as it is "essential in stimulating the economy." In 2011, more than $573 million in Laboratory procurements were awarded to a diverse group of businesses in California and across the nation, including more than $333 million in procurements to small businesses.



Detectors Reveal Neutral Particle Interplay



Ultrasensitive detectors that identify rare particle interactions are advancing fundamental physics research and improving nuclear reactor monitoring worldwide.

Also in December

- *A new diagnostic for the National Ignition Facility resides inside the experimental target.*
- *Experiments show that plutonium is still aging gracefully in the nation's nuclear stockpile.*
- *Livermore researchers develop more user-friendly biological accelerator mass spectrometry.*

Coming Next Issue

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