Lawrence Livermore National Laboratory

Science & Technology REVIEW

December 2013

Safety in the Skies

Also in this issue:

- **Preventing Asteroid Collisions**
- **A Forensic Bomb-Pulse Date**
- **Forecasts for an Efficient Grid**

About the Cover

The article beginning on p. 4 describes the Laboratory's multidisciplinary research to help the Department of Homeland Security and Transportation Security Administration stay one step ahead of terrorists who want to detonate homemade explosives onboard airplanes. By combining computer modeling and simulation, controlled experiments, and nondestructive evaluation, Livermore research teams are working to better understand how homemade explosives are made and how destructive a particular formulation might be if detonated on a pressurized jetliner. Laboratory scientists are also focused on improving detection capabilities to ensure that airport scanning systems can detect explosives in smaller and smaller quantities and mitigate potential threats.

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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NNSA National Nuclear Security Administration

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Feature

Research Highlights

Departments

Bret Knapp Selected as Livermore's Interim Director

Bret E. Knapp (center) has been named as the Laboratory's acting director and as acting president of Lawrence Livermore National Security, LLC (LLNS), which manages Lawrence Livermore for the Department of Energy. Knapp replaces Penrose "Parney" C. Albright, who stepped down as director on October 31, 2013, to pursue his broader interests and contributions to the U.S. national security enterprise. Albright had served as Laboratory director since December 2011.

A recognized expert in national security, Knapp began his career at Livermore and spent more than 25 years at the Laboratory, working in nuclear weapons design and testing and leading programs in defense and nuclear technology development. In 2006, he joined the senior management team at Los Alamos National Laboratory, serving as principal associate director for the Weapons Program.

In addressing Livermore employees, Knapp said, "I am honored to be selected by the LLNS Board of Governors to serve during this transition period until a permanent successor is named. I would also like to acknowledge Director Albright for his hard work and dedication to the people and programs at [Lawrence Livermore]. Livermore is a vital national security institution, and I will work to continue and grow its cutting-edge science and engineering programs."

Knapp received a bachelor's degree in mechanical engineering from California Polytechnic State University in San Luis Obispo and a master's degree in mechanical engineering from the University of California at Davis. According to Norman Pattiz, chairman of the LLNS Board of Governors, a national search for a new Laboratory director will be conducted under the leadership of the University of California.

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Laser Fusion Experiments Yield Record Energy

Cryogenic experiments using all 192 laser beams on the National Ignition Facility (NIF) have achieved record yields for neutron energy generated by the implosion of a tiny target capsule filled with deuterium–tritium fuel. An early morning shot on August 13, 2013, released nearly 3×10^{15} neutrons, or approximately 8,000 joules of neutron energy—about 3 times the previous neutron yield for cryogenic implosions on the Livermore facility. A shot on September 28 surpassed that record, producing 5×10^{15} neutrons. These conditions had not been observed since the days of underground nuclear weapons testing; achieving them is an important milestone for the world's most energetic laser system.

NIF's primary mission is experimental research in support of the Stockpile Stewardship Program, which applies science-based techniques instead of underground testing to ensure the safety, security, and reliability of the nation's nuclear weapons. Results from the successful experiments provide a benchmark for validating computer simulation tools developed for stockpile stewardship. The record yields also represent a significant step along the path toward another NIF mission: to achieve fusion ignition and sustained burn in a laboratory setting.

According to Livermore physicist Omar Hurricane, previous experiments showed that the breakup of the target capsule's imploding shell (or ablator) was reducing target compression and thus degrading performance. To make the ablator more resistant to breakup, the NIF team turned up the laser power during the "picket" that occurs at the beginning of the laser pulse. The added power increased the radiation temperature in the foot or trough period of the pulse, which improved the ablator's stability and reduced compression later in the implosion. Hurricane, who led the record-setting experiments, adds that the team's results were remarkably close to simulations and provide important information for better understanding and improving NIF's performance.

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Virus Detected in Bladder Cancers

An international collaboration involving two Livermore scientists has detected a virus in bladder cancer, the seventh most common malignancy in humans. This research is believed to be the first study to demonstrate a link between Kaposi's sarcoma–associated herpesvirus (KSHV) and bladder cancers.

Scientists from the University of Split in Croatia collected bladder biopsies from 55 Croatian patients (44 men and 11 women) with different stages of bladder cancer. Livermore biologist Crystal Jaing and computational biologist Kevin McLoughlin then used the Lawrence Livermore Microbial Detection Array (LLMDA) to analyze DNA extracts from three randomly selected specimens. Results showed that all three samples had the KSHV pathogen. Team members confirmed the LLMDA analysis through KSHV-specific polymerase chain reaction (PCR) testing. PCR tests of the remaining specimens detected KSHV DNA in 30 of the 55 samples, or 55 percent of the study group.

The team, which also included scientists from the University of Jordan, published these results in the August 2013 issue of *Tumor Biology*. According to the authors, the high prevalence of KSHV infection indicates that the pathogen may play a role in the formation of bladder cancer. Jaing notes that this paper is the first to demonstrate LLMDA being used as the primary detector of a virus associated with a specific disease—findings that were then confirmed using other techniques.

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Commentary by Bruce E. Warner

Solving National Problems by Integrating Innovative Ideas, Experiments, and Simulation

In Livermore’s Global Security Principal Directorate, our job is to apply core Laboratory capabilities to address complex national security problems. We achieve this goal by anticipating what problems are evolving and applying multidisciplinary science and technology to deliver innovative and responsive solutions.

The article beginning on p. 4 provides an example of our efforts. It describes work we are doing to protect the more than 600 million passengers who pass through Transportation Security Administration (TSA) checkpoints each year. As the number of passengers traveling by air continues to grow, TSA has the daunting challenge of preventing the smuggling of weapons and explosives aboard, while allowing the freedom of movement for people and commerce.

The threats to passengers are evolving as terrorists move away from using military weapons to homemade explosives (HMEs). TSA is constantly challenged to find ways to detect a broad and growing range of HME formulations. Although some of these explosives are unstable and dangerous, they are simple enough to be mixed in a bathtub, using ingredients that could be bought in a grocery store.

Lawrence Livermore is the ideal place to address these threats because of our scientists’ deep knowledge of explosives. The Laboratory also has experimental facilities specifically designed to test explosives, computer codes to simulate explosions and mechanical deformation, and expertise in nondestructive evaluation.

At the High Explosives Applications Facility—the National Nuclear Security Administration’s Center of Excellence for Explosives—scientists can safely test a broad range of explosives that a terrorist might use. Those experiments help researchers understand x-ray signatures, material stability, and performance changes.

Laboratory researchers use experimental results to validate computer simulation codes and to develop and update complex algorithms that are used in baggage scanners. Our simulations take into account a wide variety of HME formulations and locations where a device might be placed in a plane to determine the potential impact to a pressurized aircraft. Once the various options are simulated, specific testing is done to validate the results.

Lawrence Livermore partners with Los Alamos and Sandia national laboratories in conducting this work as a part of the National Explosives Engineering Sciences Security (NEXESS) Center, established in 2006 by the Department of Homeland Security. Bringing together the expertise of the three national weapons laboratories, NEXESS studies how HMEs are synthesized and formulated so that TSA can better understand risks to the traveling public.

This issue of *Science & Technology Review* also includes three highlights that demonstrate innovative ways the Laboratory conducts national security work, the range of work we do, and the breadth of our mission. The highlight beginning on p. 12 describes a collaboration that is developing computational models to evaluate potential methods for preventing large asteroids from hitting Earth. This work builds on the Laboratory’s expertise in simulations and knowledge of nuclear-explosives effects.

The second highlight, which begins on p. 16, explores a novel application for radiocarbon bomb-pulse dating—a technique pioneered by Livermore researchers at the Center for Accelerator Mass Spectrometry, which was founded 25 years ago. Using this technique to determine the age of biological materials has become a valuable forensics tool for law enforcement and is helping to advance medical research.

The third highlight, beginning on p. 20, focuses on energy security and helping California balance the state’s supply and demand for electricity. With funding from the California Energy Commission, the Laboratory is using its supercomputing resources to address grid optimization problems and determine whether new energy storage technologies and demand response initiatives might help balance the load on the state’s electricity generators.

As these articles show, the Laboratory works to make the world a safer place by leveraging our multidisciplinary capabilities to ensure national security—the driver behind all of our efforts.

■ Bruce E. Warner is principal associate director for Global Security.

Physicist Harry Martz checks a case used to acquire x-ray signature data on reference standards and explosives specimens after the case enters a baggage screening system maintained at Livermore's High Explosives Applications Facility (HEAF).

Understanding Homemade to Enhance

Researchers combine computer modeling and simulation, controlled experiments, and nondestructive evaluation to protect U.S. airline passengers from onboard explosives.

WITH more than 600 million passengers boarding U.S. airliners yearly, protecting the flying public from onboard explosives is a critical responsibility for the Department of Homeland Security (DHS) and its Transportation Security Administration (TSA). Keeping travelers safe requires that airport security quickly and accurately identify any credible threat posed by

Explosives Aviation Security

explosives hidden in checked and carry-on baggage or on passengers themselves. “We must be right every time,” says materials scientist Amy Waters, who leads the Explosives and Infrastructure Security Program in Livermore’s Global Security Principal Directorate.

Waters notes that U.S. air transportation has never been safer, but threats continue to evolve. Despite the multiple layers of security at U.S. airports, terrorists still find aircraft tempting targets. “A plane going down is psychologically terrifying and would be a huge propaganda victory,” says Waters. She adds that any disruption to air transportation would be damaging to the U.S. economy.

Lawrence Livermore currently leads and participates in several efforts to enhance aviation security, all centered around better understanding and detecting the threat from explosives carried aboard aircraft. This work builds on decades of nonnuclear explosives research—expertise the Laboratory has applied to address the needs of various government agencies, including the Departments of Energy, Defense, and Justice; the Federal Aviation Administration; DHS; and TSA.

About 35 Livermore chemists, engineers, structural analysts, physicists, and computer scientists contribute to these projects, which combine computer modeling and simulation, controlled experiments, and nondestructive evaluation. Ultimately, the goal of this coordinated effort is to develop a predictive capability to improve detection and mitigation of explosives threats.

From Military to Homemade

Historically, the explosives threat to aviation has been primarily limited to military and commercial devices, which are designed to be relatively safe to handle. Over the past decade, homemade explosives (HMEs) have become the material preferred by terrorists, a change in tactic that has challenged the capabilities of existing detection systems. As a result, providing increased knowledge about HMEs and developing advanced systems to detect them are increasingly important.

Livermore research efforts to enhance aviation security focus on three sets of questions regarding HMEs: First, what HMEs might terrorists use, how easy and safe are those materials to manufacture and transport, and what are their detonation and performance characteristics? Second, how destructive would a particular formulation be if detonated on a pressurized aircraft, what quantity would be required to bring down a jetliner, and to what extent could high-performance computing simulations replace experiments conducted on the ground? And finally, can the screening systems used at airports detect the growing list of HMEs so they never get on board?

Tapping the National Labs

In 2006, DHS established the National Explosives Engineering Sciences Security (NEXESS) Center to apply advanced science and engineering toward reducing the risks to aviation. The center relies on the expertise available at Lawrence Livermore, Los Alamos, and Sandia national laboratories to better understand how HMEs are synthesized and formulated—critical information for deploying detection technologies that still meet the demands of the traveling public. Chemical engineer Jon Maienschein, former NEXESS leader and current director of Livermore's Energetic Materials Center, says, "In the past few decades, the use of so-called homemade or improvised explosives in attacks by terrorists has led to many questions, such as how these devices are made, what threat they pose to aircraft, how to handle them safely, and most importantly, how to detect them." (See *S&TR*, July/August 2012, pp. 4–11.)

NEXESS projects are focused on characterizing the performance of HMEs and understanding the vulnerability of aircraft to these threats. Researchers at NEXESS have provided an important science base for aviation security, for example, by evaluating various explosives formulations including HMEs and determining each one's detonability, method of initiation, detonation velocity, and impulse energy. NEXESS teams have combined sophisticated computer modeling with small- and large-scale experiments to assess the catastrophic damage threshold for aircraft as a function of the amount and location of the explosives and the flight conditions at the time of detonation. They also have evaluated the performance of emerging detection systems and their application at airport security checkpoints.

HMEs, which typically contain both a fuel and an oxidizer, can be dangerous to handle, and no surrogates are currently approved for experimental testing. "We are faced with applying a strict set of safety standards and practices to materials whose reaction chemistries and initiation mechanisms differ from those we have worked with more extensively," says Maienschein.

He adds that HMEs do not follow the standard detonation theories for military and commercial explosives. For example, HMEs often react much more slowly than conventional explosives. While military explosives release energy in tens of microseconds, HMEs take hundreds to thousands of microseconds. Such "slow" chemical reactions may lead to incomplete detonations and a possible delayed energy release through a phenomenon called afterburn, which involves the combustion of unreacted ingredients with ambient air.

"Very slow energy releases are not well understood," says Maienschein. "Current theoretical and modeling approaches cannot accurately account for them. We must extend 50 years of experience with military and commercial formulations to this new class of explosives. As a result, the anticipated damage caused by detonating a specific amount of HME is less certain than, say, TNT [trinitrotoluene]."

Livermore chemists test formulations found in terrorist manuals on the Internet and those used in conflicts around the world. Although military explosives are manufactured to tight tolerances, terrorist

production methods are less stringent; a terrorist might resort to mixing an explosive in a bathtub, for example. As a result, the ratio of ingredients in HMEs may vary considerably. "We test and model fuels and oxidizers in different proportions to obtain a general understanding of HMEs," says Maienschein. The goal is to deduce the characteristics of a family of related chemicals instead of determining the exact characteristics of every possible formula.

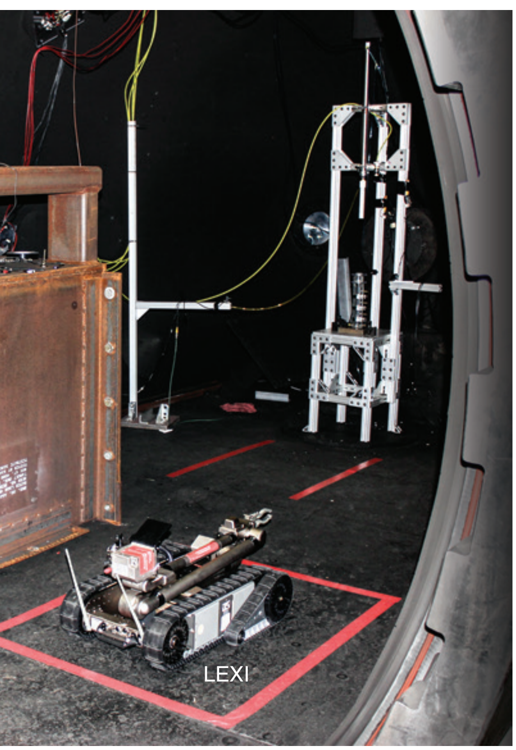
Robotics to Maximize Safety

Typically, HME ingredients are benign when handled individually, but mixed together, they become dangerous, particularly if they contain additives such as sulfur or aluminum. Explosive experts often turn to robotic and pneumatic systems to synthesize and test liquid and solid formulations that are too dangerous or unstable to mix or handle safely. At the Laboratory's High Explosives Applications Facility (HEAF), personnel use the iRobot Packbot 510. Dubbed LEXI (Livermore Explosives iRobot), the robot is manufactured by the same company that makes the Roomba vacuum-cleaning robot. "Before we acquired LEXI, we couldn't study some of these explosives because of safety concerns," says Livermore chemical engineer Sabrina DePiero.

DePiero prepares the materials by layering two or three ingredients including a fuel and oxidizer in a plastic cylinder. The ingredients are safe to handle at this stage because they have not been mixed. She then carries the cylinder to a walk-in HEAF firing tank and inserts it into an acoustic mixer called LabRam. After she leaves the area, the tank and secondary doors are closed and LabRam is started by remote control. LabRam mixes the materials using sound waves. When this step is finished, LEXI rolls to the mixer and removes the cylinder, which contains the now dangerous mixed explosive, and transports it to the tank's firing table. LEXI rolls out the door, the door closes, and the explosive is detonated.

Data collected from experiments are added to the Laboratory's online database of explosives, explosive properties, and potential materials from which terrorists could build a bomb. About 1,000 federal and state scientists, engineers, and emergency responders can access the database, which includes information on potential safety hazards involved in manufacturing and handling the different materials, the degree of difficulty a terrorist would face in attempting to destroy a plane with a particular device, and the energy output and power (how fast energy is released) from a detonation.

Test data also help scientists validate computer codes to ensure that calculations accurately simulate an HME's destructive performance. In particular, explosives chemists rely on Livermore's CHEETAH thermochemical code to predict detonation properties for any mixture, including its pressure, temperature, detonation energy, and rate of energy release.



Livermore Explosives iRobot (LEXI) works in a firing tank at HEAF. Shown to the left of LEXI is the metal container that houses the acoustic mixer called LabRam.

Simulating Airborne Detonations

"Airplanes are more vulnerable to explosives than other structures such as subway tunnels because their frames are manufactured to be as light as possible," says Maienschein. To analyze the susceptibility of airframes to HMEs, NEXESS experts combine computer analyses made with several Livermore codes and data from experiments on airframe components conducted by DHS at its Transportation Security Laboratory in Atlantic City, New Jersey.

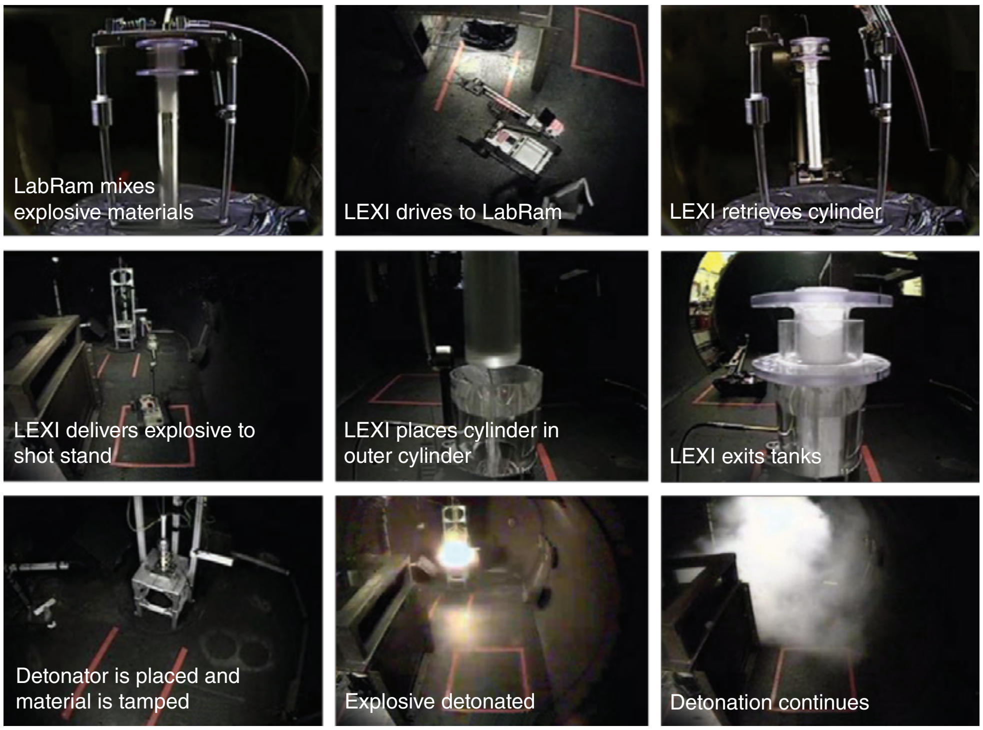
The traditional method for determining the threshold mass of an explosive is subjecting retired aircraft to controlled internal explosions and monitoring the extent of damage. This approach has several limitations. Retired aircraft may have compromised physical structures, and their designs are not representative of newer planes in the commercial fleet. Also, because of costs, only a limited set of explosive parameters is tested. Moreover, a critical factor in the response of aircraft structural components is internal pressurization while a plane is in flight because it magnifies the effect of an onboard explosion. However, pressurized tests are more expensive than experiments at room pressure, and an aircraft can generally be used only once for such experiments.

DHS managers recognized that modern computational tools might overcome these limitations. If supercomputers could accurately illustrate how aircraft would respond to onboard explosions from HMEs, scientists would have a cost-effective tool to better understand and mitigate this threat to commercial aircraft. DHS thus sponsored a demonstration project at NEXESS laboratories aimed at applying the capabilities of high-performance simulation and modeling to explosions on aircraft.

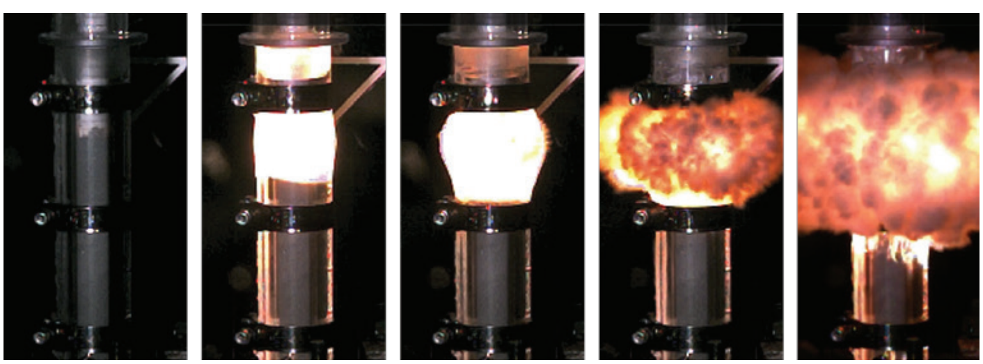
For this project, the Laboratory's simulation team, led by computational engineers Lee Glascoe and Steve Alves, developed a structural computer model of a common commercial aircraft and subjected it to simulated explosive detonations. Their goal was to determine the threshold amount of certain explosives that would catastrophically impact the plane. Many parameters are relevant to this complex calculation, including the age and type of aircraft, its altitude at the time of detonation, and the shape of the explosive. The explosive's location—for example, whether it is in an overhead compartment or bathroom or near a window—also affects the calculation because objects surrounding the charge may increase or decrease its destructiveness. This work leveraged modeling and simulation capabilities developed at Livermore to evaluate explosive threats to critical infrastructure, such as research led by Glascoe that examined ways to limit damage to underwater structures from destructive blasts.

At the start of the DHS project, NEXESS researchers developed a structural model of a commercial aircraft for which explosives test data were available. The simulations were "informed" by data generated by small- and large-scale experiments conducted by the Transportation Security Laboratory, Los Alamos, and Sandia. The team then applied these modeling approaches to another commercial aircraft for which no live-fire test data were available. The simulation tools calculated the threshold mass of an HME that would cause catastrophic failure in flight when placed at different locations inside the plane. The team also investigated multiple scenarios of varying quantities and formulations of explosives.

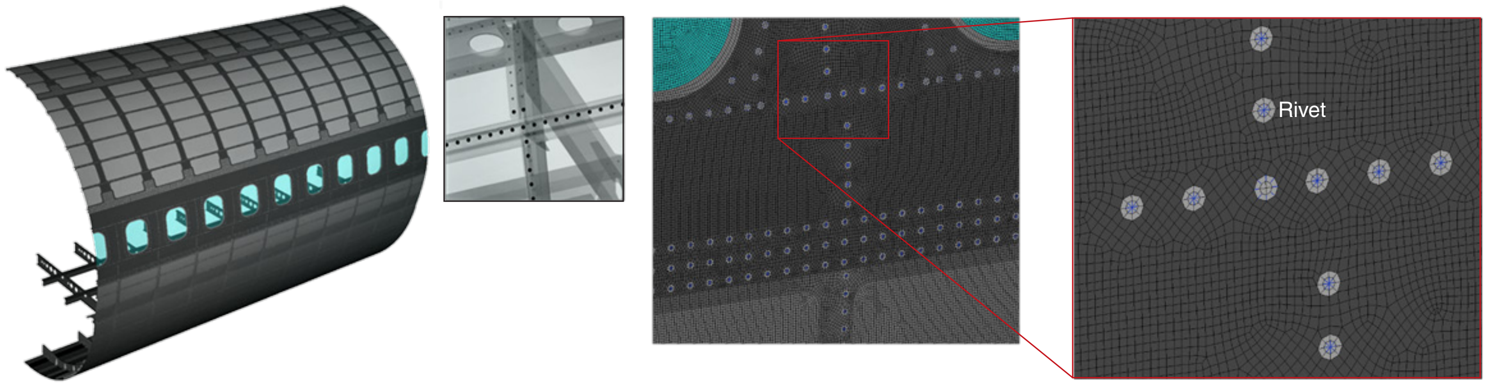
To simulate the high-pressure shock waves caused by detonating a selected HME, the researchers integrated the hydrodynamic code ALE3D and longtime workhorse code DYNA3D with thermochemistry data supplied by CHEETAH. ALE3D is a high-fidelity numerical simulation tool for analyzing the elastic, or plastic, response of materials under extreme conditions. CHEETAH results coupled with ALE3D predict the size and other characteristics of the blast. The time and spatially varying pressure from the blast were then mapped to determine damage to the aircraft's frame on a fine three-dimensional (3D) grid.



These images show the sequence of operations (from left to right, top to bottom) performed by LEXI in testing homemade explosives (HMEs) in the HEAF gun tank.



After LEXI positions an explosive test assembly in the gun tank at HEAF, high-speed cameras record details of the explosion. This image sequence shows a detonability test of an aluminized explosive, where elapsed time is in milliseconds (ms).



A finite-element model tested with the Laboratory's DYNA3D and ALE3D codes revealed details of an airplane's fuselage down to the stringers (horizontal elements) and rivets.

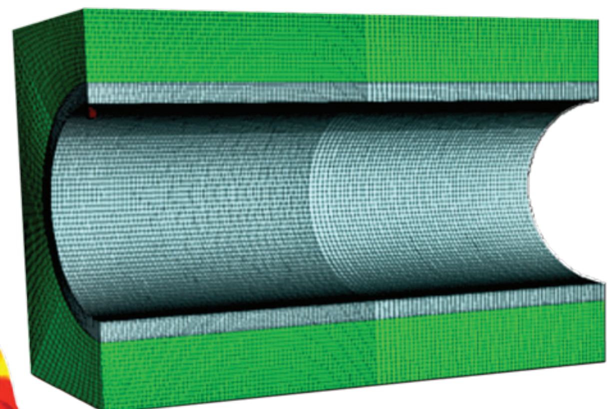
Simulations Validate Tests

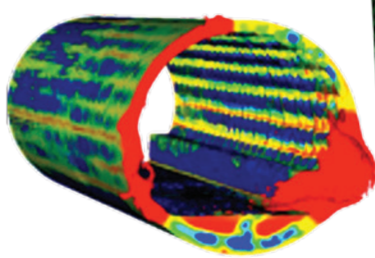
The simulations ran on a Livermore supercomputer with between 512 to 1,024 processors working in tandem. Simulating a detonation event that lasted a relatively long 40 milliseconds required about a day of computing time. The simulations revealed in three dimensions—and millisecond by millisecond—what is likely to take place when the selected HME is detonated inside an aircraft, in particular the blast's effects on the aircraft's aluminum skin and the degree to which the plane's interior components and objects near the explosive mitigated the blast. Effects ranged from minor interior damage to cracks in the aluminum skin to sections of the fuselage blown out. "The numerical models were built to accommodate a large but necessary amount of structural detail about an aircraft," says Glascoe. "Our simulations compare well with available experimental data at both the component and system level."

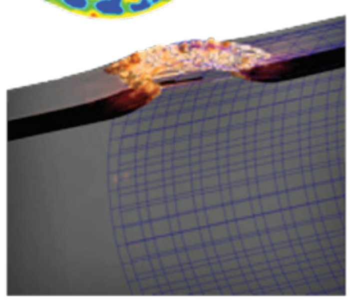
Glascoe notes that data from physical experiments on aircraft components are particularly valuable because they provide "ground truth" for simulations. He compares the experiment–simulation linkage to the National Nuclear Security Administration's Stockpile Stewardship Program, in which scientists ensure the safety and effectiveness of the nation's nuclear weapons through simulations and physical component testing without resorting to underground nuclear tests. "Small-scale tests help determine how well our model works," he says. "We learn details about how an aircraft might fail down to individual rivets."

The project, which concluded in early 2013 with a final report to TSA, demonstrated the utility of computer simulation. Says Maienschein, "We showed that our modeling and simulation tools can provide useful assessments of aircraft vulnerability and determine the threshold explosive masses for catastrophic damage at selected locations inside a specific aircraft."

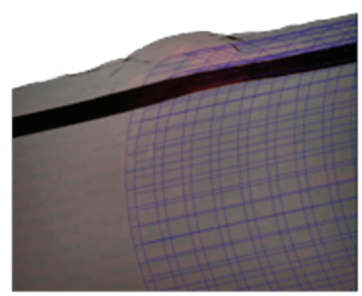
Supercomputing models help scientists understand how enclosed structures made of complex materials such as steel-reinforced concrete will respond to an HME detonation.



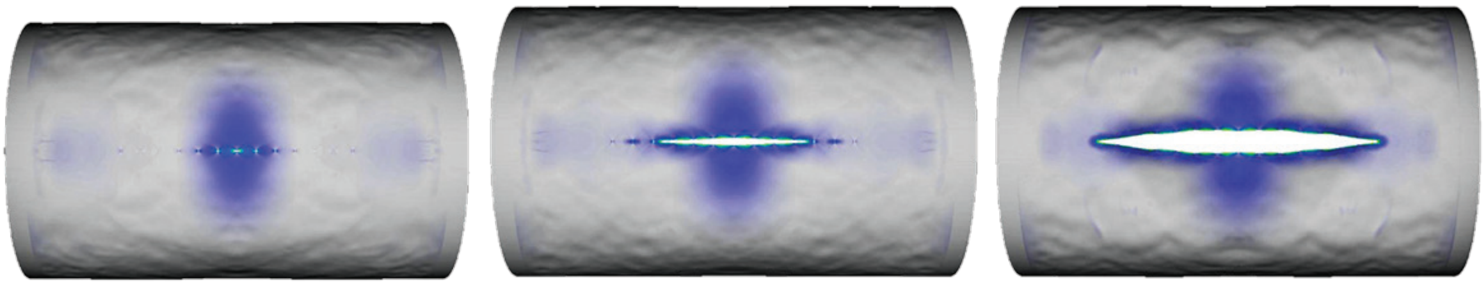




Breach



No breach



Snapshots from three simulations using ALE3D and DYNA3D show the damage caused by different quantities of HMEs detonated inside a small, thin-walled pressure vessel. Testing objects that are far less complicated than an airplane fuselage helps scientists validate the ability of larger computer models to capture important details.

3D Imaging at Every Airport

TSA has deployed a wide range of technologies to address known and emerging security threats to air transportation. X-ray computed tomography (CT) and radiography machines at every airport analyze the contents of all checked and carry-on baggage, searching for hidden explosives and other prohibited items. Additional layers of security include explosives detection canine units and techniques to screen baggage and passengers for traces of explosives. Scanners also examine bottled liquids at security checkpoints primarily to test medically exempt liquids, which may be transported in quantities greater than 100 milliliters (3.4 ounces).

Livermore experts have worked closely with government agencies and private industry to strengthen existing detection tools and commercialize new technologies. One example is a Livermore-developed device called ELITE, for Easy Livermore Inspection Test for Explosives. (See *S&TR*, October 2006, pp. 16–17.) This pocket-sized detector, which tests for a broad range of explosives, is now licensed to Field Forensics, Inc., and has been sold to law-enforcement agencies and the U.S. Army.

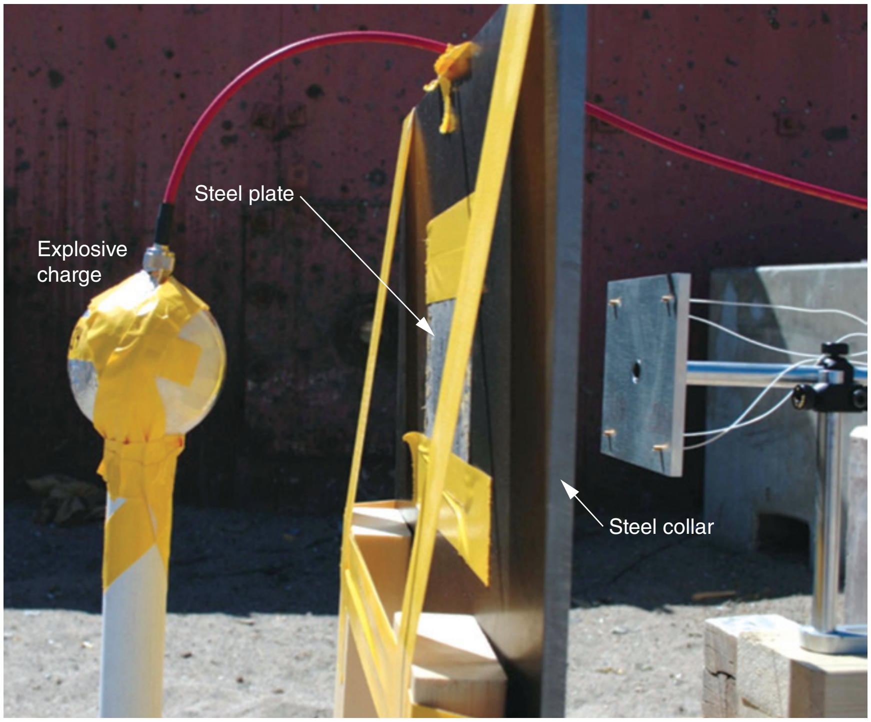
To meet TSA's screening requirements, physicist Harry Martz is leading a team of explosives and nondestructive evaluation experts to enhance the performance of airport x-ray CT and radiography machines and to recommend improvements for future devices. Martz is head of the Laboratory's Center for Nondestructive Characterization, which has pioneered ways to use x rays and other forms of radiation for noninvasive imaging of everything from nuclear warhead components to bridge decks. (See *S&TR*, June 2011, pp. 19–21.) The goal of the Livermore Explosives Detection Program is to simultaneously enhance the machines' sensitivity to the expanding range of explosive threats without increasing the number of false alarms. Martz notes that any time an alarm is generated, security personnel must review the images or manually verify the bag's contents, which can slow airport operations.

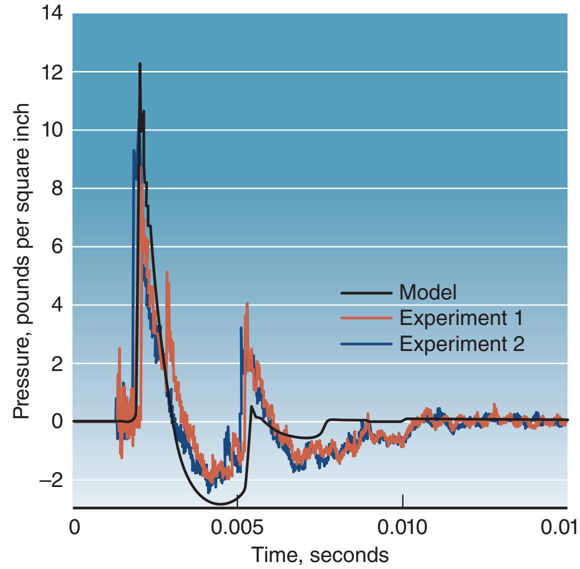
The Livermore team is enhancing two types of algorithms (data-processing strategies) that analyze the x-ray images produced by the machines. The first task is to improve the complex reconstruction algorithms that turn numerous two-dimensional x-ray projections into a detailed 3D representation of the items inside a piece of luggage. Says Martz, "Reconstructed 3D radiographic images provide a clearer picture of a bag's contents."

Martz's team is also improving threat-detection algorithms, which automatically interpret the 3D CT images produced by the first set of algorithms. Threat-detection algorithms extract relevant characteristics such as a material's x-ray attenuation, density, atomic number, and mass and compare these data to values of known explosives, including HMEs. As baggage is scanned, the algorithms automatically classify each item inside as either a threat or a nonthreat. If an alarm signals a potential threat, TSA staff screen the item further. Computer simulations play an important role in improving signal accuracy. The Laboratory's HADES code, for example, can predict changes in radiographic signatures that are associated with explosives of different elemental content or density.

In a related effort, Livermore researchers are working on algorithms to advance dual-energy detection technology for use by TSA. With this technique, the detector measures the linear attenuation coefficients of materials at two energy spectra, one low and the other high. The measurements provide a stronger basis for interpreting an object's elemental composition and density. If dual-energy technology is adopted by TSA, it would enhance detection capabilities and overall efficiency.

The Livermore researchers have created a database with detailed information on the x-ray properties of explosives threats and nonthreats. These data help TSA and scanner manufacturers develop performance standards for screening checked and carry-on baggage. "We need an extremely high detection rate and a very





The photo shows the experimental setup used at Los Alamos National Laboratory to test the close-in effects of an explosive charge and to characterize the blast wave as it travels through air. The graph plots measurements from two Los Alamos experiments versus a Lawrence Livermore simulation of the same test.

low false-alarm rate to mitigate evolving threats," says Martz. Another challenge is that some benign materials share similar characteristics with actual HME threats and thus could generate a false alarm.

Staying Ahead of the Next Threat

The team's investigations to enhance the performance of existing or next-generation technologies should improve explosives detection systems, reduce false-alarm rates, and increase system operational efficiencies. "Advancing the technologies used at airports to screen for dangerous materials is a challenging task," says Martz. "TSA and manufacturers are doing a good job, but we must continue to improve our capabilities." The urgency of the task was underscored in July 2013 when TSA chief John Pistole discussed a next-generation device called Underwear 2—a successor to the underwear bomb Umar Farouk Abdulmutallab attempted to detonate on a flight near Detroit on December 25, 2009. According to Pistole, the new and improved bomb, identified in May 2012, was designed to evade current TSA detection systems.

While counterterrorism officials are tracking down the latest generation of bomb makers, TSA and a small group of scientists and engineers are advancing their understanding of explosives and the methods to detect and mitigate these devices. Waters is optimistic. "For the first time, we're developing a predictive capability to determine what a bad guy could do and how we could detect it," she says. "This predictive understanding will enable us to help DHS stay ahead of the evolving threat to air travel."

—*Arnie Heller*

Key Words: ALE3D code, aviation security, CHEETAH code, computed tomography (CT), DYNA3D code, Easy Livermore Inspection Test for Explosives (ELITE), Energetic Materials Center, HADES code, High Explosives Applications Facility (HEAF), homemade explosive (HME), LabRam, Livermore Explosives iRobot (LEXI), National Explosives Engineering Sciences Security (NEXESS) Center.

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Averting Impact

Modeling Solutions to Prevent Asteroid Collisions

THE story is common in science fiction: A large asteroid is on a collision course with planet Earth, and scientists are working to save the world. In February 2013, the scenario became a little less fictional when a meteor nearly 20 meters in diameter streaked through the sky above Russia. The midsized object packed quite a wallop, exploding in an air burst over the city of Chelyabinsk. The resulting shock wave damaged more than 7,000 buildings in six cities across the southern Ural region. About 1,500 people were treated for injuries, many caused by glass shards from shattered windows. The atmosphere absorbed most of the object's energy, equivalent to about 440 kilotons of TNT (trinitrotoluene), nearly 30 times more energy than was released by the atomic bomb detonated at Hiroshima.

The 2013 event demonstrated that an asteroid impact, although unlikely, is a real threat. Since the mid-1990s, scientists at Lawrence Livermore have been supporting government agencies such as the National Aeronautics and Space Administration (NASA) by evaluating different methods for preventing such a catastrophe. (See *S&TR*, December 2009, pp. 12–14.) Results from a project led by Livermore physicist Paul Miller are helping researchers better understand how an astronomical object headed toward Earth can be deflected or disrupted.

Disrupt or Deflect

"Many strategies have been examined for dealing with a hazardous asteroid or comet that has the potential to impact Earth and significantly damage a region," says Miller. One proposal involves colliding a spacecraft into the asteroid to deflect its course. Another approach would use lasers to melt and ablate portions of the object's surface, with the resulting jets of material providing a thrust to change the object's orbit.

Of all the mitigation strategies, the most effective approach is using a nuclear explosive to either disrupt or deflect the asteroid. In disruption, the explosive acts like a hammer blow, smashing the asteroid into pieces that then fly off course or are too small to cause damage. In deflection, the energy deposited by the nuclear blast heats the asteroid's surface to a temperature that vaporizes material, thus nudging the asteroid in the opposite direction. According to Laboratory astrophysicist David Dearborn, a nuclear explosive would impart 10 to 100 times more momentum to the object than other proposed methods. Says Miller, "For scenarios with little warning time before impact or when the object is large, nuclear explosives often are the only option."

This project, which is funded by the Laboratory Directed Research and Development Program, draws on the expertise of nearly a dozen Livermore scientists and includes collaborators from NASA, University of Colorado, University of California at Santa Cruz, Jet Propulsion Laboratory, and other national laboratories. The team is focused on developing the modeling capability to evaluate nuclear approaches that will deflect and break up an incoming asteroid. By better understanding the available threat-mitigation options and their outcomes, the researchers will improve confidence in the effectiveness of a nuclear response should the need arise.

"The Laboratory is one of a few places worldwide with the simulation capability and the knowledge of nuclear-explosives effects to conduct this research," says Miller. The scenarios considered include deflecting a dense solid asteroid by striking it at the apex of its orbit or dispersing a "rubble-pile" asteroid—an agglomerate of boulders, rocks, and dust. By applying uncertainty quantification techniques, radiation hydrodynamics codes, and advanced algorithms, the team is modeling energy coupling to an asteroid, how that object's material composition affects energy deposition, and what path the debris will take as it is dispersed.

Analyze the Threat

Asteroids and comets vary in size, density, composition, dynamics, and internal structure. The Livermore team is thus considering cases that span observed behavior and properties. "Asteroids are notoriously nonspherical," says Kirsten Howley, a postdoctoral researcher working on the project. "Different shapes and materials can affect how and where the energy from an explosion is deposited and distributed." Characterizing an object's surface material helps researchers determine how deeply energy would be deposited and to accurately model what happens to that material once heated with energy from a nuclear explosive. "We are dealing with complicated phase changes, material that is solid, liquid, and vapor at different times and depths," says Howley. "The more we know about an asteroid's composition, the better our results."

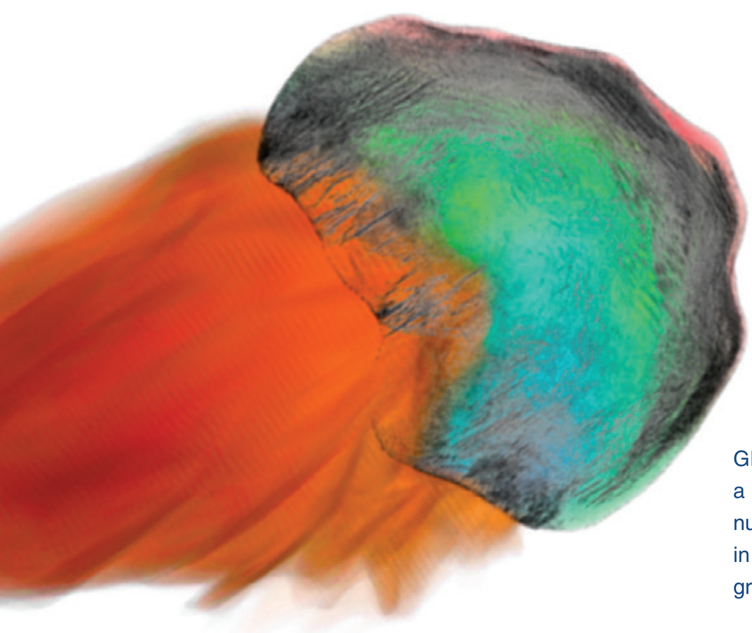
Density is another important variable. "The asteroid's response to an explosive push depends on its internal structure, its density, and how that density is dispersed," says Laboratory scientist Joseph Wasem. "Density can vary from 1 gram per cubic centimeter—which is like pumice—to over 2 grams per cubic centimeter—which would be more of a rubble-pile asteroid. An asteroid with a density of 7 grams per cubic centimeter would be a relatively solid chunk of iron. A rubble pile or fractured rock will not hold up to the same stresses as would a monolithic block of the same material."

Bring on the Computers

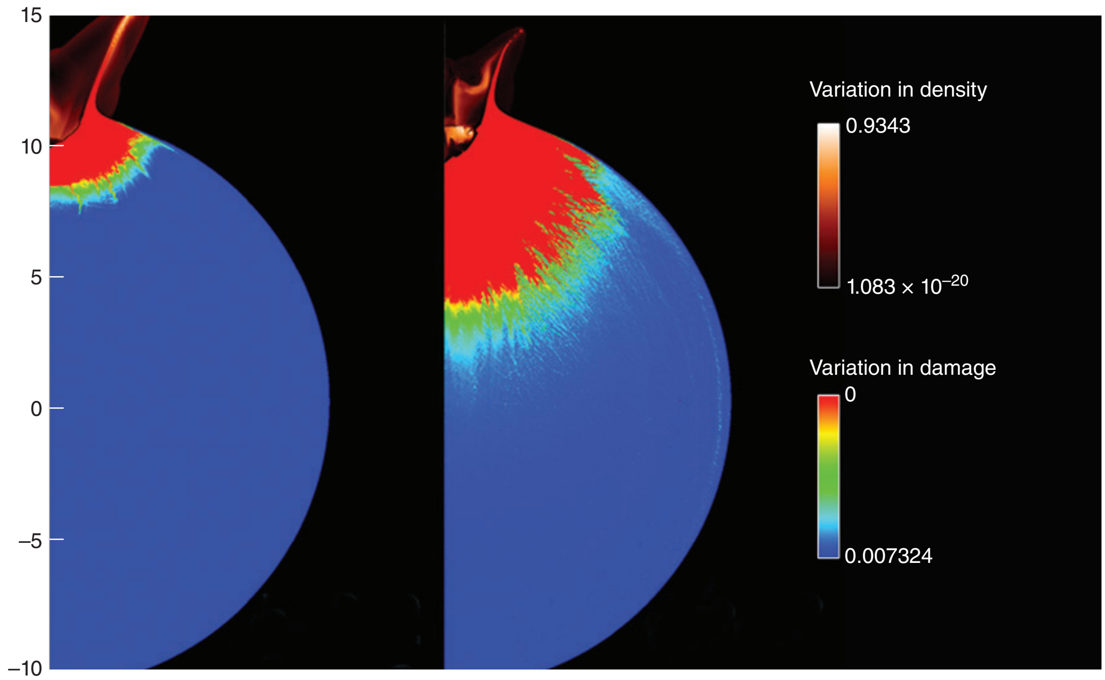
The team is using different simulation capabilities to examine the physical processes involved in a nuclear detonation, the subsequent energy production and deposition, and the material's response. Says Miller, "We are faced with a wide range of length and timescales, and the behavior we are modeling is described by plasma physics, fluid dynamics, and solid mechanics. We also need to link the code results, so we can track what happens through the various stages."

One of the team's early simulations made by Ilya Lomov modeled a 500-meter-diameter asteroid with a realistic shape as it was deflected by a 750-kiloton nuclear explosion, which deposited 150 kilotons of energy. "Most of the energy output in a nuclear detonation comes in the form of neutrons and x rays," says Laboratory astrophysicist Seran Gibbard. "We are especially interested in neutrons because they penetrate deep into material."

She notes that the dominant force in a deflection attempt would come from the surface material that is melted or vaporized. The momentum generated for the deflection would be closely tied to energy-coupling issues and the material's equation of state. Results from the team's simulations indicate that bulk porosity, which affects a material's strength, is an important factor in the amount of damage and cratering induced on an asteroid's surface by a hypervelocity impact.



GEODYN simulated this scaled model of the Geographos asteroid, which shows a realistically shaped object about 500 meters in diameter, driven by a 750-kiloton nuclear explosion that deposited 150 kilotons of energy. Orange indicates variations in the ejecta's energy density, the blue–green hues show deviatoric stress levels, and gray represents damage.



GEODYN simulations show the effect of bulk porosity on an object's response to a hypervelocity impact. The blue–red color scale depicts the degree of damage inflicted on an object with bulk porosity of (left) 20 and (right) 30 percent. A material's strength decreases as porosity increases, which affects the amount of damage and cratering.

"We want to estimate the minimum momentum in various scenarios to know how much push a nuclear device can deliver in different situations," says Livermore scientist James Elliott. "For these calculations, we considered the size, shape, and composition of the asteroid and the energy from the explosive."

The researchers began with a one-dimensional simulation using quartz (silicon dioxide), a relatively well-understood mineral with high melting and vaporization energies. Determining the proper mesh size for the hydrodynamics simulation is important to avoid large uncertainties while keeping the run time reasonable. A mesh resolution of less than 0.2 centimeters to a depth of at least 1 meter covered most energy density scenarios. Once the researchers determined the lower bounds on the blowoff momentum in one dimension, they extended the results to two and three dimensions and to other materials. "We are now expanding the work to include various sources, such as photons, and a range of asteroid compositions," says Howley.

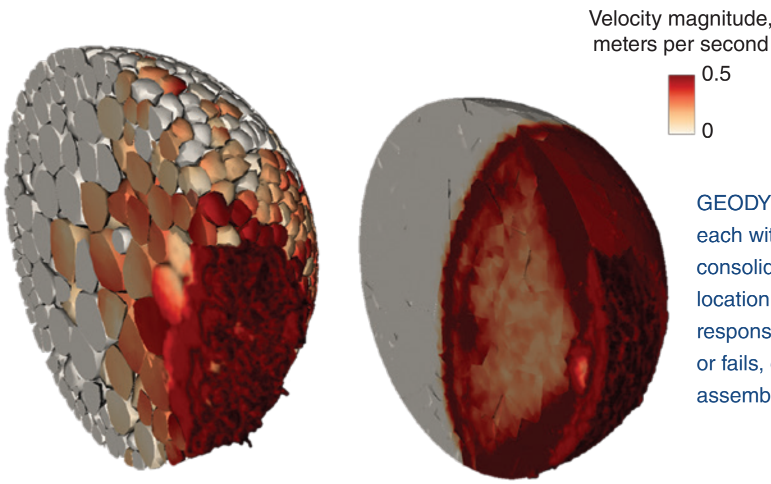
An alternative to deflection is disruption, or blasting the object to bits—an approach that would work well with small asteroids or those composed of loosely bound rock fragments. When the team modeled the disruption of a monolithic iron sphere 50 meters in diameter and with 5 percent porosity, the cloud of fragments expanded so much that few of them impacted Earth, and no pieces larger than 3 meters in diameter remained. Fortunately, Earth's atmosphere protects the planet from objects less than about 10 meters in diameter.

When a simulated blast was applied to a rubble pile, the shock set the loosely aggregated boulders in motion. "Our simulation captured the behavior inside each boulder as well as its interaction with its neighbors," says computational physicist Eric Herbold. Material near the energy-deposition site vaporizes, melts, or fails, contributing to blowoff that imparts momentum to the assembly of boulders.

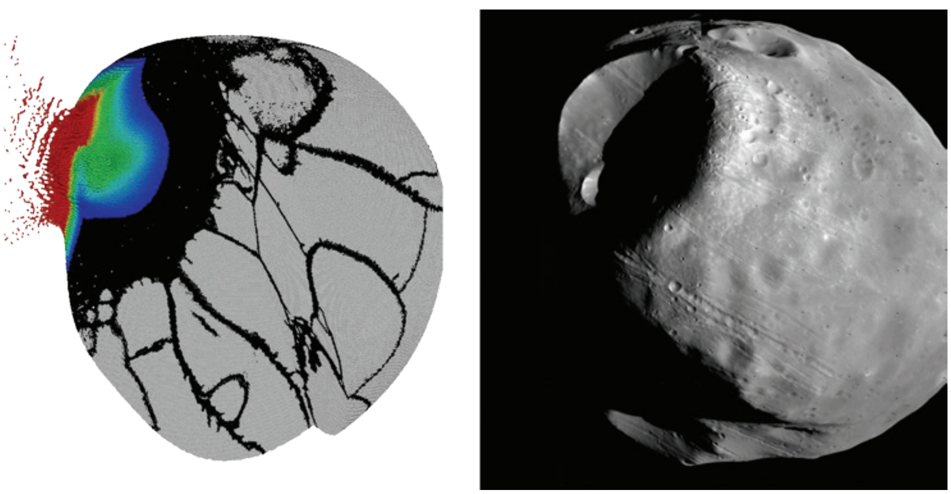
Compounding Uncertainties

Simulations also modeled debris dispersal after the disruption, allowing researchers to observe how fragments spread over time and space. The object's orbit is crucial in determining the time available, the difficulty involved in sending a spacecraft to the object, and the debris dispersal paths following the explosion. "We also have to pin down uncertainties in the deflection velocity after the disruption event because they determine the probability that fragments might impact Earth," says Wasem. He notes that an actual deflection attempt would have multiple sources of uncertainty. "We may not have accurate information on the object's composition or its total mass. These factors increase uncertainty in the calculated deflection velocity delivered to the object, which can create a final positional error associated with the attempt."

To evaluate the propagation of errors, the team created a fictitious scenario using the orbital parameters of 2011 AG5, a 140-meter-diameter near-Earth asteroid. Simulation results showed that deflection attempts are more effective at certain points in the object's orbit, for example, when an asteroid is closest to the



GEODYN-L simulations compare two realizations of porous asteroids, each with 2,380 individual pieces in a (left) rubble pile and (right) fractured consolidated configuration. The incident wave is at approximately the same location at (left) 7.1 and (right) 0.9 seconds, indicating a large contrast in response. Material near the energy deposition region vaporizes, melts, or fails, contributing to blowoff that imparts momentum to the remaining assembly of boulders.



Researchers used the SPHERAL code to model a high-speed impact such as the one that created the large Stickney crater on Phobos, a moon orbiting Mars. (left) Results from the simulation compare well with (right) a photo of the crater.

Sun. Varying a spacecraft's orbital parameters or launch date also changes the confidence level for mission success.

Validation with Impact

The research team extensively tested the algorithms and codes used in the work. A large-scale validation problem integrated several aspects of nuclear deflection and disruption to model the impact that created the large Stickney crater on Mars's moon Phobos. "The problem is challenging," says Miller. "Previous attempts to simulate the crater formation resulted in completely destroying the virtual Phobos." Using SPHERAL, Livermore scientist Mike Owen and Jared Rovney, a summer student from Yale University, modeled the interaction of a high-speed impactor with Phobos. The results compared well with photos of the crater, thus helping to validate the methodology.

Future work will consider comets, which tend to be much bigger than near-Earth asteroids. "Comets are less likely to impact Earth than an asteroid, but they are still a serious concern," says Miller. "Because of their size, they have the potential to cause global devastation or even extinction. And they are typically discovered with little warning time."

The asteroid deflection and disruption project has been made possible by the Laboratory's broad science, technology, and engineering expertise. Says Miller, "We have the capabilities necessary to address this problem. Should the world be faced with an impact event, the question will be how best to stop it. Our work will provide decision makers with options they can consider to help them meet the challenge."

—Ann Parker

Key Words: asteroid impact, comet, deflection, disruption, GEODYN code, GEODYN-L code, nuclear explosive, Phobos, SPHERAL code, Stickney crater.

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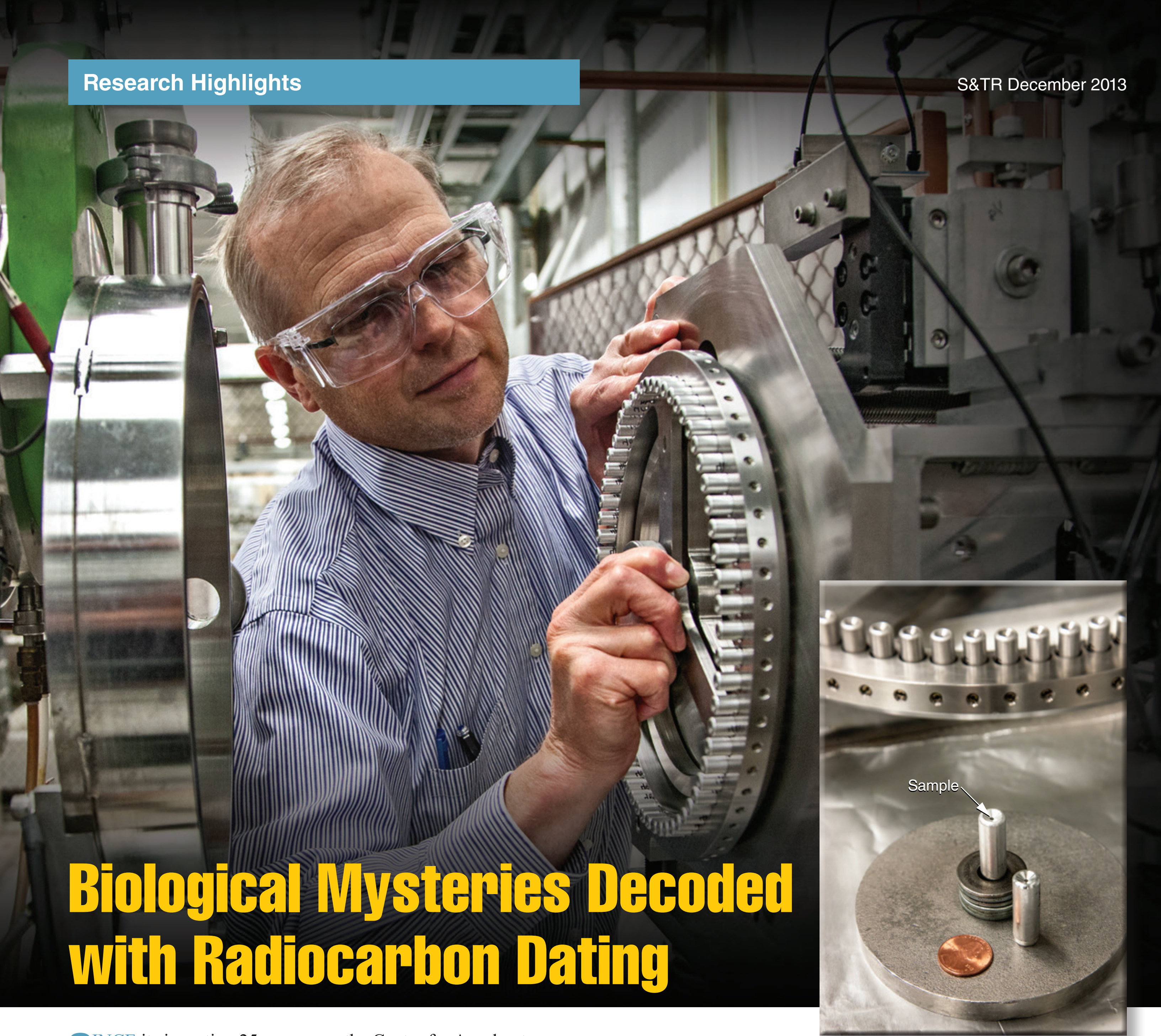


Biological Mysteries Decoded with Radiocarbon Dating

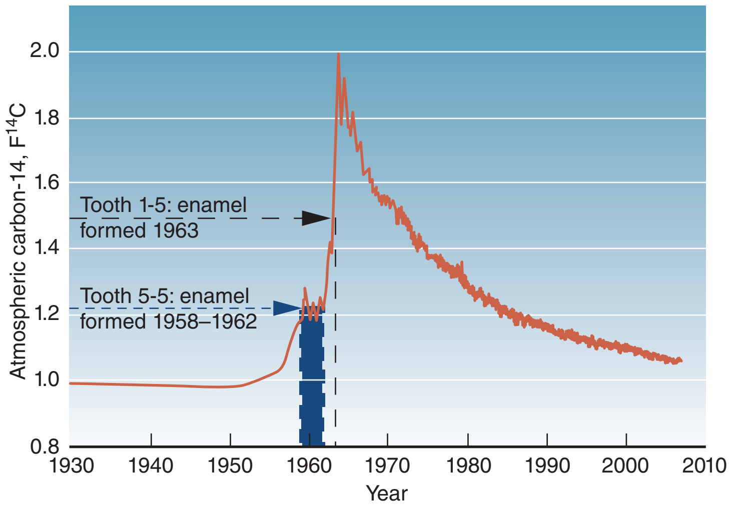
Bruce Buchholz loads a wheel of samples into the spectrometer at the Laboratory's Center for Accelerator Mass Spectrometry (CAMS) to determine the materials' concentration of carbon-14. The inset shows a closeup of a sample holder.

SINCE its inception 25 years ago, the Center for Accelerator Mass Spectrometry (CAMS) at Lawrence Livermore has supported scientific research for a diverse range of disciplines. The precise measurement capabilities at CAMS allow researchers to identify the isotopic composition of a given sample. Continued efforts to improve the center's sample preparation techniques and detection methods have ensured that CAMS can help address important scientific challenges in fields ranging from archaeology and geophysics to pharmacology and nonproliferation.

One important research endeavor involves determining the precise age of biological material generated in the past 60 years by measuring the ratio of radiocarbon (or carbon-14) to the carbon-12 and carbon-13 in samples. Scientific forensics using radiocarbon bomb-pulse dating is possible because of the isotopic signature created by aboveground nuclear testing between 1955 and 1963, which nearly doubled the amount of carbon-14 in the atmosphere. When the aboveground test-ban treaty took effect in 1963, atmospheric levels of radiocarbon began to decline as carbon-14 migrated into the oceans and biosphere. Living organisms naturally incorporate carbon into their tissues as the element moves through the food chain. As a result, the concentration of carbon-14 leaves an indelible time stamp on every biological molecule when it comes into being.

To extract carbon for measurement, researchers at CAMS turn a sample into carbon dioxide through either combustion or a chemical process and then reduce the carbon dioxide to graphite—a form of carbon—on an iron catalyst. "The graphite is what we measure," says Livermore scientist Bruce Buchholz, who helped pioneer this technique at CAMS. "A full-size sample is about the size of a grain of salt, weighing between 100 micrograms to 1 milligram, although we often measure amounts as small as 20 micrograms."

Any sample that contains enough carbon to measure—dental enamel, proteins, or DNA, for example—can be dated using the highly accurate spectrometer at CAMS. (See the box on p. 18.) Recent projects have applied bomb-pulse dating to help resolve three biologically based mysteries involving a missing-person's cold case, neuron growth in the human brain, and proteins in the lens of the human eye.



Researchers at CAMS helped solve a missing-person's cold case by analyzing teeth from a skull fragment found in Canada in 1968. The orange line shows the ratio of atmospheric carbon-14 to carbon over time (measured in a concentration unit called $F^{14}C$). Results indicated that the baby tooth (5-5) formed between 1958 and 1962, whereas the premolar (1-5) formed in 1963 or later.

Tooth Leads to Truth on Cold Case

Cold cases are seldom solved at the speed shown in a TV crime drama. However, recent breakthroughs have resulted from the combined use of modern forensic technology and analysis methods. One such case involved a skull fragment found in 1968 on the banks of a Canadian river. In 1969, an anthropological assessment of a tooth in the fragment placed the age of the deceased at 7 to 9 years. No local children within this age range had been reported missing, so the evidence was placed in storage.

In 2005, the remains were shipped to the Ancient DNA Laboratory at Simon Frazier University in Canada for analysis with newer techniques, including radiocarbon dating. "The measurements we make at CAMS don't necessarily solve a case, but they can help authorities narrow the possibilities," says Buchholz.

For the cold case, the Livermore team analyzed the enamel of two teeth from the skull fragment: a fully formed deciduous molar (a baby tooth) and a partially formed premolar (an adult tooth). Buchholz notes that once tooth enamel has developed, it does not incorporate new carbon, making it a remarkably accurate indicator of a person's age. Because the teeth from the fragment would have formed at different times in the child's growing cycle, the amount of carbon-14 in each tooth would indicate whether the deceased was born before or after the peak of aboveground nuclear testing. Enamel from the baby tooth corresponded to a birth year between 1958 and 1962. The premolar enamel formed around 1963, and because this tooth was incomplete, researchers concluded that the child died in 1963 or later.

The team's collaborators also analyzed the sample using newer anthropological techniques, for example, determining the amount of skeletal ossification and the head circumference. Those results yielded an age at death of 4.4 years ± 1. The combined measurements suggested the child was born between 1958 and 1962 and died between 1963 and 1968. More detailed DNA analysis led authorities to a local child who had been missing since early 1965 and was presumed to have drowned, allowing them to close the case.

"This is just one example of how we assist law enforcement," says Buchholz. "In the U.S. alone, there are thousands of unidentified remains, and those John and Jane Doe cases might benefit from analysis using such a combination of techniques."

Neurons Keep on Growing

Buchholz also worked with a CAMS team on an international collaboration to study neuron growth in the human brain. For most of the 20th century, scientists thought that neurogenesis stops shortly after birth. In the 1990s, however, studies of rodents showed that neuron growth continues in the olfactory bulb region associated with smell. Although this growth was not found in nonhuman primates, researchers wondered if the human brain generated neurons in appreciable numbers throughout life, and if so, what areas of the brain were involved.

CAMS researchers measured the concentration of carbon-14 in genomic DNA of neurons from the hippocampus to help collaborators in Europe develop a model for exploring how and how often different types of hippocampal cells regenerate. The team then took cells from the hippocampus of human cadavers, isolated the nuclei from neurons and nonneuronal cells, and extracted the DNA for analysis. Results showed that, in nonneuronal cells, the turnover rate declines with age. That is, as

Celebrating 25 Years of Teamwork and Collaboration

It makes perfect sense that, 25 years ago, the Center for Accelerator Mass Spectrometry (CAMS) began as a joint effort. From the beginning, CAMS has been about collaboration, bringing excellent people and excellent science together in an environment that encourages teamwork. In 1985, the University of California Regents joined Lawrence Livermore and Sandia national laboratories as equal partners to fund the Multi-User Tandem Laboratory, with Livermore physicist Jay Davis as the facility's first director.

The Multi-User Tandem Laboratory initially focused on using accelerator mass spectrometry (AMS) to diagnose fission products of atomic tests and to conduct research in materials science, nuclear astrophysics, nuclear spectrometry, and neutron physics. Academic collaboration was encouraged from the very first, and in 1988, Lawrence Livermore established the Center for Accelerator Mass Spectrometry to coordinate the increasing number of experiments with academic users.

Today, CAMS is the world's most versatile and productive AMS facility. The center operates around the clock, performing up to 25,000 measurements per year. The research made possible by CAMS covers areas as diverse as archaeology, atmospheric chemistry, biomedicine, carbon-cycle dynamics, earth system processes, cell biology, alternative fuels, forensic dating, and forensic reconstruction of radiation doses.

AMS is an exceptionally sensitive technique for measuring concentrations of isotopes in small samples, typically less than 1 milligram, and the relative abundance of isotopes at low levels. For example, it can identify one carbon-14 isotope among a quadrillion other carbon atoms. In the CAMS spectrometer, negative ions made in an ion source are accelerated in a field of hundreds of thousands of volts. The accelerated ions smash through a thin carbon foil or gas that destroys molecular species. After passing through a high-energy mass spectrometer and various filters, the ions slow to a stop in a solid-state or gas-ionization detector. The system identifies individual ions by the rate at which they slow down.

In 1988, Lawrence Livermore established the Center for Accelerator Mass Spectrometry to diagnose fission products from nuclear tests and study climate and geologic records. Shown here is Laboratory physicist Jay Davis, who served as the center's first director.

"It's amazing to see the variety of problems brought in for analysis," says CAMS director Graham Bench. By measuring the carbon-14 isotopes in various samples, CAMS researchers have helped solve cold cases and plumb the mysteries of the human brain and eye (this highlight), tested the efficacy of cancer drugs (*S&TR*, September/October 2008, pp. 12–18), and established the age of a potential Mayan codex. Challenges come from near and far. "We have strong ties to research communities worldwide in academia, private industry, and government agencies," says Bench. "We also continue to support the Laboratory's programs. For instance, we have become a leader in biological AMS research, and we have generated isotopes to calibrate sample recovery instruments for the National Ignition Facility." (See *S&TR*, December 2012, pp. 18–20; September 2011, pp. 4–10.)

In addition, CAMS offers research opportunities for graduate students and postdoctoral fellows. According to Bench, in the past 15 years, the center has generated data for more than 300 graduate-level theses and annually supports the work required for 20 PhDs—a number that even a first-flight academic department would envy. Bench notes that several Lawrence scholars have crossed the center's threshold. "Throughout its history, CAMS has helped prepare and train the next generation of scientists," he says. Some of these scientists launch long-term careers at the Laboratory, such as geochemist Tom Guilderson. In 2011, Guilderson won the Department of Energy's E. O. Lawrence Award for groundbreaking radiocarbon measurements of corals, helping researchers to better understand the ocean's paleohistory and how oceanic processes affect the global carbon cycle. Other early-career researchers from CAMS have become senior scientists at facilities worldwide, such as Susan Trumbore, the current director of Biogeochemical Processes at the Max Planck Institute for Biogeochemistry in Germany.

"We provide an environment for extremely bright people to be creative, take initiative, and truly collaborate," says Bench. "CAMS has been successful because of this culture. It's the kind of place where people will stop what they are doing on their own projects to help others. We have a group focus, a community of true team players. This innovative culture makes CAMS and Lawrence Livermore a great place to work and to deliver breakthrough discoveries on important scientific challenges."

humans grow older, their brains create fewer nonneuronal cells. The measurements in neuronal genomic DNA told a different story. The oldest subjects studied (who had died at age 90 or older) had higher carbon-14 levels than would have been present in the atmosphere before 1955, indicating neuron growth continued in the hippocampus at least into the subjects' fifth decade. These markers and others showed no dramatic decline in hippocampal neurogenesis with age.

The team is still exploring the exact role of hippocampal neurons, in particular, because neuron growth is important for healthy aging. New neurons are required for efficient pattern separation and allow the brain to process and store similar experiences as distinct memories. Older cells are necessary for pattern completion, helping people to associate similar memories with each other. Studies also indicate that reduced neurogenesis plays a role in psychiatric diseases such as depression, but questions remain about the processes involved. Knowing that neuron growth continues could even lead to therapies for regenerating brain tissue lost to trauma or disease.

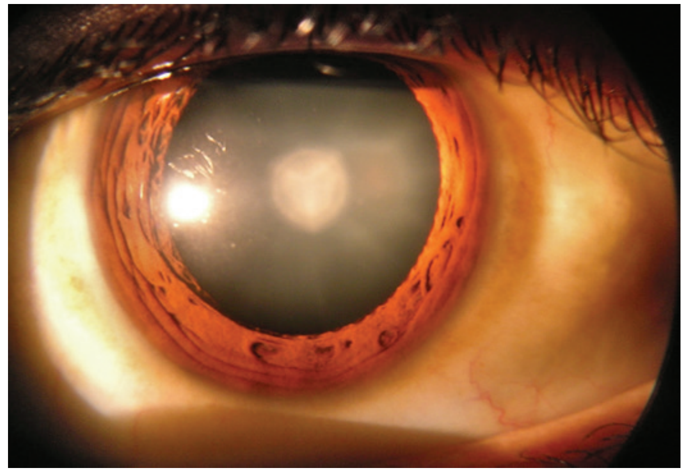
An Eye on Renewal

Another CAMS collaboration studied proteins in the lens of the human eye to better understand how cataracts form and how best to treat them. Cataracts are caused by a clouding in the eye's crystalline lens and, if left untreated, can lead to blindness. According to the Centers for Disease Control and Prevention, about 20.5 million Americans age 40 or older have cataracts. By 2020, that number is expected to increase to 30.1 million.

At the core of the eye lens are highly specialized, long-lived cells made of crystalline, transparent proteins. The structural and functional integrity of lenticular proteins helps keep the cells transparent, allowing for proper vision. "How these lenses cope with a lifetime of stress and aging, without any capacity for protein turnover and repair, is not completely understood," says Buchholz. In the mid-2000s, CAMS researchers collaborated with Paul FitzGerald, a professor at the University of California at Davis, to determine whether proteins in the core are made from cells of differing ages. "If they are, we'd know there is a process for protein turnover and renewal," says Buchholz.

Using samples from cadavers, researchers removed the cell layers of adult human eye lenses to reach the core. They then separated the core proteins into water-soluble and water-insoluble fractions, which were analyzed at CAMS to determine the average age for each sample. The water-insoluble samples—which contained the membrane proteins—had ratios of carbon-14 to carbon consistent with the age of the cells, whereas the water-soluble crystalline protein samples contained carbon that was younger.

"Our study provided the first direct evidence of carbon turnover in this type of protein in adult humans," says Buchholz.



Cataracts are a national health problem, growing in proportion with the aging population. CAMS research on proteins in the eye lens could lead to better treatments for this debilitating condition.

The findings suggest that the lens nucleus is a dynamic system, maintaining health and resisting injury through unknown protein transport mechanisms and possibly protein repair. "If scientists can understand protein transport, they may eventually find ways to delay the onset of cataracts or even prevent or heal this debilitating condition," says Buchholz.

The Curve of the Future

As time passes, the bomb-pulse curve continues to flatten. However, carbon-14 has a half-life of nearly 6,000 years, so traces of it will linger. Livermore researchers are working to improve the analysis capabilities at CAMS so that smaller and smaller traces of the isotope can be measured. The CAMS team is contributing to other biological research as well, including a study on the formation of aneurysms.

Using the bomb pulse from aboveground nuclear tests to date biologically based materials has grown from a novel technique into an integral part of many scientific endeavors. This innovative spin-off from the Laboratory's primary national security mission is helping to advance law-enforcement efforts and medical research. Twenty-five years in and still counting, CAMS continues to offer its unique capabilities to help solve important scientific mysteries.

—Ann Parker

Key Words: bomb-pulse radiocarbon dating, carbon-14, cataracts, Center for Accelerator Mass Spectrometry (CAMS), cold case, hippocampus, neurogenesis, scientific forensics.

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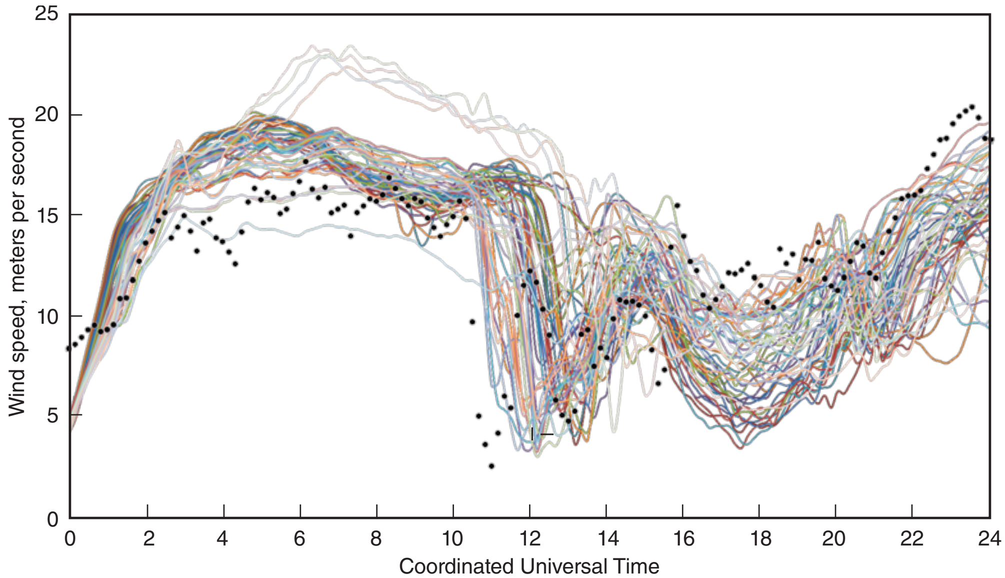
2020 Vision for California's Electric Grid

SCHEDULING the electric generators that supply the grid with power is a balancing act. Each day, system operators evaluate the supply-and-demand conditions forecast for the electric grid for the following day and prepare a generation schedule to satisfy projected demand. (See *S&TR*, June 2013, pp. 4–12.) If operators turn on too many generators, the units will run at only partial capacity, which is inefficient and more expensive than running at full capacity. But if too few are operating when demand spikes, operators will have to engage more generators at the last moment, which also increases costs. If available generators cannot start up quickly enough, power interruptions may result.

California could face more frequent last-minute capacity corrections or even power interruptions as the state implements the ambitious Renewables Portfolio Standard (RPS). This standard requires the state to derive at least 33 percent of its electricity from eligible renewable energy resources by 2020. (See *S&TR*, March 2009, pp. 13–16.) Meeting the RPS goals will involve a sizable boost in wind and solar power generation, but integrating a large number of these intermittent energy resources into the power grid could challenge both generation planning and system reliability.

In 2011, the California Energy Commission funded research at Lawrence Livermore to determine whether new energy storage technologies and demand response initiatives might help balance the load on generators as more solar and wind resources are added to the grid. (See *S&TR*, December 2011, pp. 4–11.) Energy storage systems allow grid operators to more effectively manage the power



A Weather Research and Forecasting multiphysics ensemble of wind speed forecasts (colored lines) and lidar measurements (black dots) over a 24-hour period demonstrate the value of generating multiple forecasts using different physics configurations to capture the uncertainty inherent in wind generation. Only a few of the outlier trajectories capture the early drop in wind speed measured at hour 11, illustrating how a single forecast will often mistime an extreme event. Large-scale ensemble weather modeling is enabled by Livermore's high-performance computing and weather forecasting resources and expertise.

supply when demand is high but wind and solar resources are not generating much electricity. Demand response initiatives offer customers financial incentives to reduce or shift their electricity usage when there is a shortage of power generated.

For this project, a multidisciplinary research team led by computational engineer Thomas Edmunds combined atmospheric forecasting, scheduling optimization, and production simulation to create a comprehensive planning system for electric grid research. By tapping the Laboratory's supercomputing resources to run thousands of simulations, the researchers determined the value of using increased storage and demand response initiatives to keep California's complex grid system operating affordably and reliably.

More Is Better

Efficient scheduling hinges on accurate next-day renewable forecasting, but the generation potential of wind and solar resources is harder to predict than it is for other energy sources. The role of demand response and storage depends on which units are providing electricity at any given time. Addressing uncertainties in both forecasting and scheduling was thus essential to accurately estimate the value of implementing these options.

For this effort, the Livermore team created a multiscale atmospheric model of the western U.S. for use in generating forecasts with the Weather Research and Forecasting (WRF) modeling system. The study year was 2020, but weather data recorded in 2005 provided a starting point for the forecasts. A single day-ahead forecast may not accurately predict the changes in atmospheric conditions that actually occur throughout the day. The team accounted for this uncertainty with a multiphysics modeling approach, running 30 different atmospheric simulations for every 24-hour period. The result was an ensemble of physically plausible weather scenarios for each day of the year.

The simulation predicted weather conditions at 15-minute intervals to capture the precise timing of changes such as wind speed and cloud cover. Completing the daily ensemble forecasts for all of 2020 took approximately 840,000 computational hours on Livermore's supercomputing systems and produced over 500 terabytes of data.

"Our ensemble technique looks at the many ways weather could evolve," says Edmunds. "Other analyses use a statistical model with one weather forecast for each season, which is derived from historical data. Our representations of uncertainty are many orders of magnitude richer than those produced by standard analysis methods." In fact, these computationally intensive approaches have demonstrated a reduction in errors of up to 22 percent in predictions for day-ahead wind generation.

The team used the WRF model and the sets of weather trajectories to calculate next-day generation forecasts for about 5,000 wind and solar generators located throughout the western region. Each day's 30 weather forecasts became 30 solar and wind generation forecasts, each of which was then subtracted from the energy demand. The amount remaining, the net demand, was the portion that needed to be met through unit scheduling of other resources.

Calculations quantified an important relationship between demand and temperature. Starting at 100°F (38°C), each 1° rise in temperature across the territory serviced by California ISO increases electricity demand by 1 gigawatt—equivalent to the output of a large power plant. Because demand changes so quickly at high temperatures, forecast accuracy is especially important on the hottest days. "By running an ensemble of forecasts instead of only one scenario, we are more likely to capture an extreme event," says atmospheric physicist Matthew Simpson.

Intelligent Decision Making

The production simulation model used by California ISO incorporates 2,400 generators and 120 transmission lines and is designed to optimally allocate energy resources for the state's residents. The Livermore team worked with the same WRF model, PLEXOS modeling platform, and CPLEX optimization algorithms as the system operator, but with two additional software features—optimization across multiple timescales and stochastic unit commitment.

"What makes our study special is that we're modeling at multiple timescales," says Livermore mathematician Carol Meyers. "PLEXOS handles all these different scales intelligently." The software simultaneously optimized weekly scheduling for hydroelectric resources, day-ahead and hourly unit commitment for slow-starting generators, and real-time commitment and power-level decisions for quick-starting generators.

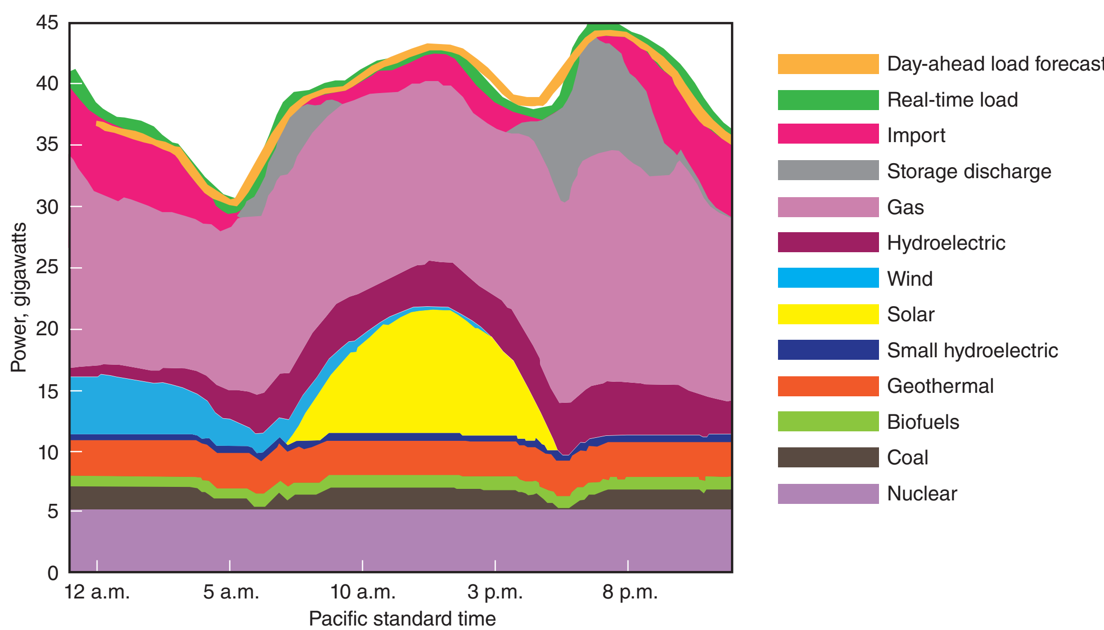
Rather than minimizing cost for a single supply-and-demand trajectory, stochastic unit commitment finds the most economic schedule across a set of probability-weighted forecast scenarios for renewable generation. Resource scheduling involves specifying for every hour of a day whether each generator should be on or off. Problems of this nature, called integer optimization, are computationally intensive, and the calculations balloon when multiple net demand scenarios are considered. To reduce problem size and computing time, the team grouped each day's 30 forecasts using statistical methods and chose five or six representative paths for stochastic unit commitment input.

The California ISO simulation model optimized system operation at 5-minute intervals for each day of 2020, both with and without storage and demand response, to determine which combination of the two options represented the best investment. The solution detailed the operational costs and revenues generated by all resources in the California grid system. In total, the team simulated 3,000 days of electric grid operations. On a high-end workstation, those simulations would have taken more than 8 years, but Livermore's high-performance systems compressed the computing time by a factor of 100, generating results in just 1 month.

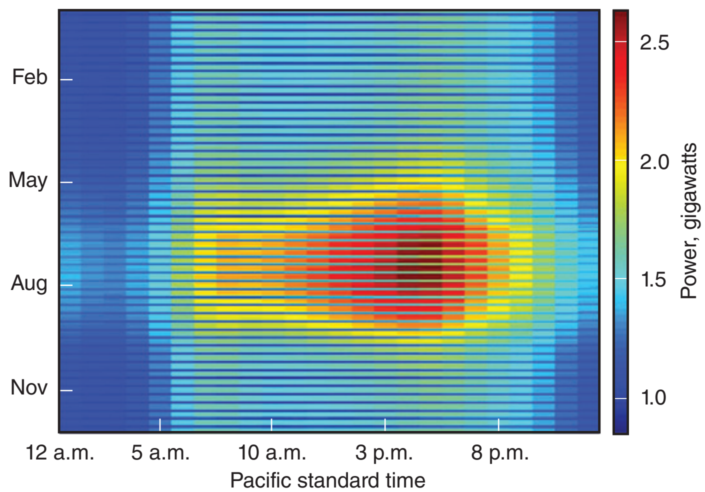
The team's results indicate that either approach alone or in combination will effectively balance resources, but neither one significantly affects revenue. Demand response initiatives reduce total annual operating costs by a little less than 1 percent. The high costs to build storage systems outweigh the revenue provided by storing energy when the price is low and selling it when the price is high. One cause of the low revenues from energy storage is California's mild weather. "Storage value depends on the difference between the lowest and highest cost during the day," says energy economist Alan Lamont. "Most of the time, the differential is not all that large in California."

A Resilient System

The team also analyzed how high quantities of renewables might affect grid performance—specifically, the grid's ability to regulate alternating current frequency second by second under normal operating conditions and to compensate for unexpected events such as loss of a generator or transmission line. Researchers worked with DNV KEMA Energy and Sustainability to develop a simplified version of the company's KERMIT software. The revised software analyzed performance of frequency regulation resources over an entire year and on a sample of days to



Production simulation results for a winter day in 2020 highlight the utility of energy storage systems when demand is high but wind and solar resources do not generate much electricity.



This snapshot of a simulation input shows the demand response capacity available in a given year. In the summer, large amounts of demand response are available to help alleviate energy demands during peak periods. Weekends have low availability (as shown by the "striping" pattern) because the primary program participants, large businesses, are typically closed.

examine how different resource combinations affected system performance overall.

The stability analysis examined potentially challenging periods throughout the year, such as when an especially large fraction of energy was provided by renewables. For this analysis, researchers introduced a 2,000-megawatt loss of generation capacity into the system and compared two scenarios: one without any storage capacity to regulate frequency and a second with 200 megawatts of storage available for regulation. These tests helped determine the effectiveness of various technologies at maintaining a stable and adaptable grid.

The performance study found no significant problems for the range of options considered. "It appears that California's current technology can withstand short-term variations in renewable power generation and delivery," observes electrical engineer Philip Top. "This finding is what we expected, but it was important to see confirmation through the study." The simulations did suggest that grid stability could be compromised if renewable energy sources were to reach levels significantly above the RPS goals. The team's analysis also showed that both demand response programs and flywheels, a type of energy storage, are effective and economically viable options for frequency regulation. In addition, providing regulation using a combination of storage and conventional generation units reduces overall maintenance costs.

Storage systems can make the grid more resilient to shocks as well. A sudden loss of power lowers the frequency throughout the system. Periods when renewables are supplying a large proportion of electricity tend to produce more extreme frequency drops. The Livermore modeling demonstrated that storage systems reduce the severity and duration of such deviations.

Weathering Changes in the Grid

Results from the study indicate that California's electric grid can accommodate a large increase in capacity from renewables, even if energy storage is not widely deployed. The data should also help policy makers determine the best path for achieving the state's RPS goals.

According to Edmunds, the Livermore project is the first to combine physics-based uncertainty modeling of renewable generation with stochastic planning methods to simulate the operation of a highly renewable system. "We are in the vanguard of organizations applying supercomputing to grid optimization problems," he says. "We've shown that our platform can be used to evaluate complementary technologies such as demand response and storage. But what truly made this effort unique was its scope." Modeling a full year of system behavior and accounting for forecasting and energy production uncertainty compounded the project's complexity, but it provided more confidence in the resulting data.

In future studies, Livermore scientists will use this end-to-end planning system to analyze scenarios with more variables and in greater detail than ever before. "Our goal is to evaluate refinements in planning and atmospheric forecasting methods and determine how different configurations of renewable generators affect the energy available throughout the grid system," says Edmunds. "We also are expanding the study to examine geothermal energy as a method of frequency regulation."

Another significant outcome of the project is that it demonstrated the value of ensemble modeling for optimizing complex operations. "Running the California electric grid with 33 percent renewable generation introduces a great deal of uncertainty that needs to be managed effectively," says Lamont. "Current methods of forecasting, scheduling, and dispatching do not account for such high levels of fluctuation. As a result, grid operators could over- or undercommit energy-generation resources on any given day, which might either increase operating costs or lead to power shortages. More sophisticated methods for measuring and incorporating uncertainty will improve the system's efficiency and reliability."

—Rose Hansen

Key Words: California Energy Commission, California ISO, CPLEX code, demand response initiative, energy storage, frequency regulation, integer optimization, KERMIT code, multiphysics modeling, PLEXOS code, renewable energy generation, Renewables Portfolio Standard (RPS), stochastic unit commitment, weather forecast ensemble, Weather Research and Forecasting (WRF) modeling system.

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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

Aerosol Mass Spectrometry Systems and Methods
David P. Fergenson, Eric E. Gard
U.S. Patent 8,513,598 B2
August 20, 2013
In this system, a particle accelerator directs a succession of polydisperse aerosol particles along a predetermined particle path. Multiple tracking lasers generate beams of light across the particle path, and an optical detector adjacent to that path detects the light beams impinging on individual particles. A desorption laser generates a beam of desorbing light across the particle path about coaxial with the light beam produced by one of the tracking lasers. The desorption laser is manipulated by a controller that is responsive to detection of a signal produced by the optical detector. Additional systems and methods are also disclosed.

Compositions of Corrosion-Resistant Fe-Based Amorphous Metals Suitable for Producing Thermal Spray Coatings
Joseph C. Farmer, Frank M. G. Wong, Jeffery J. Haslam, Xiaoyan (Jane) Ji, Sumner D. Day, Craig A. Blue, John D. K. Rivard, Louis F. Aprigliano, Leslie K. Kohler, Robert Bayles, Edward J. Lemieux, Nancy Yang, John H. Perepezko, Larry Kaufman, Arthur Heuer, Enrique J. Lavernia
U.S. Patent 8,524,053 B2
September 3, 2013
This method can be used to spray an amorphous metal coating on a surface. The amorphous metal is composed of 1 to 3 atomic percent manganese, 0.1 to 10 atomic percent yttrium, and 0.3 to 3.1 atomic percent silicon. It also contains the following elements in the composition range specified in parentheses: chromium (15–20 atomic percent), molybdenum (2–15 atomic percent), tungsten (1–3 atomic percent), boron (5–16 atomic percent), carbon (3–16 atomic percent), and the balance iron.

Three Dimensional Microelectrode System for Dielectrophoresis
Dietrich A. Dehlinger, Klint A. Rose, Maxim Shusteff, Christopher G. Bailey, Raymond P. Mariella, Jr.
U.S. Patent 8,524,064 B2
September 3, 2013
This apparatus is designed to separate particles from a sample. The device includes a dielectrophoresis channel in an apparatus body, and the channel has a central axis, a bottom and top, and two sides. A first mesa projects into the dielectrophoresis channel from the bottom and extends from the first side across the dielectrophoresis channel to the second side. The first mesa extends at an angle to the central axis of the channel, and a first electrode extends along the first mesa. A second mesa projects into the dielectrophoresis channel from the bottom and extends from the first side across the channel to the second side. The second mesa also extends at an angle to the central axis of the dielectrophoresis channel. A space is placed between at least one of the first or second electrodes and the second side, and the two electrodes have a gap between them.

Method for Fabricating Apatite Crystals and Ceramics
Thomas F. Soules, Kathleen I. Schaffers, John B. Tassano, Jr., Joel P. Hollingsworth
U.S. Patent 8,529,859 B2
September 10, 2013
This method of crystallizing ytterbium-doped fluorapatite [Yb^{3+}:$Ca_5(PO_4)_3F$, or Yb:C-FAP] dissolves Yb:C-FAP in an acidic solution and then neutralizes the solution. The method also forms crystalline Yb:C-FAP by dissolving the component ingredients in an acidic solution, followed by forming a supersaturated solution.

Cermets from Molten Metal Infiltration Processing
Richard L. Landingham
U.S. Patent 8,530,363 B2
September 10, 2013
New cermets with lower density and/or higher hardness than boron carbide (B_4C) cermet are made by incorporating new ceramics into B_4C powders or as a substitute for B_4C. The ceramic powders have a much finer particle size than those previously used, which significantly reduces the grain size of the cermet microstructure and improves the cermet properties.

UWB Delay and Multiply Receiver
Gregory E. Dallum, Garth C. Pratt, Peter C. Haugen, Carlos E. Romero
U.S. Patent 8,532,235 B2
September 10, 2013
An ultrawideband (UWB) delay-and-multiply receiver has a receive antenna with a variable gain attenuator, a signal splitter, and a multiplier with one input connected to an undelayed signal from the signal splitter and another input connected to a delayed signal from the splitter. The delay between the splitter signals is equal to the spacing between the transmitter pulses received by the antenna. A peak detection circuit controls the variable gain attenuator to maintain a constant amplitude output from the multiplier, which has a digital output circuit connected to it.

Speech Masking and Cancelling and Voice Obscuration
John F. Holzrichter
U.S. Patent 8,532,987 B2
September 10, 2013
This nonacoustic sensor measures a user's speech and then broadcasts an obscuring acoustic signal to diminish the user's vocal acoustic output intensity or to distort the voice sounds, thus making the sounds unintelligible to persons nearby. The sensor is positioned proximate to or contacting the skin tissue on a user's neck or head so that it can sense the speech production information.

Selective High-Affinity Polydentate Ligands and Methods of Making Such

Sally DeNardo, Gerald DeNardo, Rodney Balhorn
U.S. Patent 8,536,133 B2
September 17, 2013
This invention provides polydentate selective high-affinity ligands (SHALs) that can be used in a manner analogous to antibodies for various applications. SHALs typically comprise a multiplicity of ligands, each of which binds different regions on the target molecule. The ligands are joined directly or through a linker, thereby forming a polydentate moiety that typically binds the target molecule with high selectivity and avidity.

Radio-Nuclide Mixture Identification Using Medium Energy Resolution Detectors

Karl Einar Nelson
U.S. Patent 8,538,728 B2
September 17, 2013
According to one embodiment, this method for identifying radionuclides includes receiving spectral data and extracting a feature set from the data comparable to a plurality of templates in a library. A branch-and-bound method is then used to determine a probable template match based on the feature set and templates in the library. In another embodiment, a device for identifying unknown radionuclides includes a processor, a multichannel analyzer, and a memory coupled to the processor. Computer-readable code stored on the memory is configured so that, when executed by the processor, it receives spectral data and extracts a feature set that is comparable to a plurality of templates in a library. The code then uses a branch-and-bound method to determine a probable template match based on the feature set and the templates.

Printed Circuit Board Impedance Matching Step for Microwave (Millimeter Wave) Devices

Hsueh-Yuan Pao, Jerardo Aguirre, Paul Sargis
U.S. Patent 8,547,187 B2
October 1, 2013
An impedance-matching ground-plane step, in conjunction with a quarter-wave transformer section, in a printed circuit board provides a broadband microwave-matching transition from board connectors or other elements that require thin- to thick-substrate (greater than quarter wavelength) broadband microwave (millimeter-wave) devices. A method is provided for constructing microwave and other high-frequency electric circuits on a substrate of uniform thickness. The circuit is formed of multiple interconnected elements with different impedances. Individually, these elements require substrates of different thicknesses. A substrate of uniform thickness is achieved with the composite or multilayered elements. A pattern of intermediate ground planes or impedance-matching steps is formed by vias placed under various parts of the circuit where components of different impedances are located so that each part has the optimum ground-plane substrate thickness while the entire circuit is formed on a substrate with uniform thickness.

Method and System for Homogenizing Diode Laser Pump Arrays

Andy J. Bayramian
U.S. Patent 8,547,632 B2
October 1, 2013
An optical amplifier system includes a diode-pump array with multiple semiconductor diode laser bars placed in an array configuration with a periodic distance between adjacent bars. This distance is measured in a first direction perpendicular to each of the semiconductor diode laser bars. The diode-pump array provides a pump output propagating along an optical path and characterized by a first intensity profile measured as a function of the first direction and having a variation greater than 10 percent. A diffractive optic along the optical path has a photothermorefractive glass member. An amplifier slab with an input face is also positioned along the optical path and separated from the diffractive optic by a predetermined distance. A second intensity profile measured at the input face of the amplifier slab as a function of the first direction has a variation less than 10 percent.

Engineered Setpoints for Autonomous Distributed Sensors and Actuators

Thomas A. Edmunds
U.S. Patent 8,548,636 B2
October 1, 2013
Loads on an electric power system are configured with underfrequency relays in which the frequency set points and delay times for reclosure are uniformly distributed. If demand exceeds supply in the system, frequency will decrease. The decrease in frequency will actuate relays and reduce load so that demand will meet the available supply. After an engineered delay time, each relay will attempt to close contact and reestablish the load.

Methods and Devices for In Situ Determination of a Vitamin-D Synthesizing Amount of Natural and Artificial UV Irradiation

Iryna P. Terenetska, Tetiana M. Orlova, Eugene K. Kirilenko, Grygory A Galich, Anna M. Eremneko
U.S. Patent 8,552,391 B2
October 8, 2013
A matrix with a biologically active substance is exposed to ultraviolet (UV) radiation. The biologically active substance is selected to initiate photoconversions that originate vitamin D synthesis. A dosimeter measures the change that occurs to an optical parameter of the substance when it is under UV irradiation, thus measuring the amount of radiation that caused vitamin D synthesis through photoconversion.

Awards

Jim Hammer, a physicist in the Laboratory's Weapons and Complex Integration Principal Directorate, received the **2013 Edward Teller Medal** from the **American Nuclear Society Fusion Energy Division**. Hammer was cited for "outstanding, innovative research in inertial confinement fusion and high energy density physics using both high-powered lasers and Z-pinch machines."

Hammer joined the Laboratory in 1979, working first on magnetic fusion research and moving to inertial confinement fusion in the early 1990s. He is recognized for inventing and demonstrating new fusion and high-energy-density concepts as well as groundbreaking science.

The Edward Teller Medal recognizes pioneering research and leadership in the use of lasers, ion-particle beams, or other high-intensity drivers to produce unique high-density matter for scientific research and to conduct investigations of inertial fusion. The medal was established in 1991 in honor of the late Edward Teller, a director emeritus of Lawrence Livermore, senior research fellow at the Hoover Institution, and pioneer in inertial fusion science.

Former Lawrence Fellow **David Lobell** is one of 24 people to receive a **2013 MacArthur Fellowship** from the **John D. and Catherine T. MacArthur Foundation**. He was cited "for unearthing richly informative, but often underutilized sources of data to investigate the impact of climate change on crop production and global food security." Each year, the MacArthur Fellows Program awards unrestricted fellowships to talented individuals who have shown extraordinary originality and dedication in their creative pursuits and a marked capacity for self-direction.

Lobell is an agricultural ecologist and assistant professor at Stanford University. While working at Livermore from 2005 to early 2008, he served as coinvestigator for a Laboratory Directed Research and Development project that studied the environmental consequences of deploying new energy sources on a large scale. His multidisciplinary background in remote sensing, statistics, ecosystem modeling, and land use enables him to draw insights from enormous data sets on weather, agricultural practices, and natural resources such as soil and water.

Livermore chemist **Phil Pagoria** received the **2013 Munitions Safety Award for Technical Achievement** from the **North Atlantic Treaty Organization** (**NATO**) in recognition of his work in developing the energetic molecule LLM-105, which has the potential to enhance the safety of nuclear and conventional weapons. A Laboratory employee for 27 years, Pagoria serves as the deputy scientific capabilities leader for the Energetic Materials Center. He also chairs the Explosives Safety Committee and leads the Energetic Materials Synthesis Group for Livermore's Physical and Life Sciences Directorate.

The NATO Munitions Safety Award for Technical Achievement is given annually to an individual or team to acknowledge significant advances in munitions safety technology. Pagoria was nominated for the 2013 award by scientists from the U.S. Army and the Office of the Undersecretary of Defense for Acquisition, Technology, and Logistics.

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Abstract

Understanding Homemade Explosives to Enhance Aviation Security

Despite multiple layers of security at U.S. airports, terrorists still find aircraft tempting targets, and the threat from homemade explosives (HMEs) hidden in baggage or on passengers continues to evolve. To help protect U.S. airline passengers from onboard explosives, multidisciplinary research teams at Lawrence Livermore are combining computer modeling and simulation, controlled experiments, and nondestructive evaluation to better understand these threats and improve detection technologies. The researchers are determining what materials terrorists might use to make HMEs and how easy and safe those devices are to manufacture and transport. They also are using high-performance computational models to evaluate how destructive a particular HME formulation would be if detonated on a pressurized aircraft and what quantity would be required to bring down a jetliner. Another effort is focused on improving detection capabilities to ensure that airport scanning systems can detect explosives in smaller and smaller quantities. Through this multidisciplinary effort, Livermore researchers are helping the Department of Homeland Security and its Transportation Security Administration stay one step ahead of terrorists.

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Coming Next Issue

Shining a Light on New Physics

Livermore and Czech scientists are building a high-repetition-rate, short-pulse laser with performance far in advance of any laser system worldwide.

Also in January/February

- *Unexpected experimental results open a door to understanding and even customizing high-strength, high-conductivity metals.*

- *Ultrashort betatron x rays, produced on a tabletop system at Livermore, will help researchers probe the nature of matter at femtosecond timescales.*

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