NATIONAL SECURITY

SCIENCE

MOVING FROM EMPIRICAL OBSERVATION TO **PREDICTIVE DESIGN AND CONTROL**

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Los Alamos
NATIONAL LABORATORY

About the Cover

Amy Bauer, Improvised & Foreign Design Group scientist, illustrates how LANL's advanced computing and simulation are transforming materials. Predictive-design-and-control developments aid Bauer's group to better understand or forensically diagnose nuclear threats.

CHARLES McMILLAN

2010 has been an exceptional year for the Los Alamos nuclear weapons programs.

This year, President Obama requested a significant increase in funding—$624 million; if approved, a portion of the funds will be used to redress LANL's crumbly plutonium infrastructure, support the aging stockpile, and recruit a new generation of scientists and engineers. The administration unveiled the Nuclear Posture Review Report. *Combined with the bipartisan Congressional Commission on the Strategic Posture of the U.S., this development provides a solid policy foundation for nuclear deterrence.*

In January, Lawrence Livermore and Los Alamos co-hosted the Strategic Weapons in the 21st Century meeting in D.C. The forum covered national security policy, defense programs, technical advances, international developments, and the impact of these issues on the nation's strategic weapons.

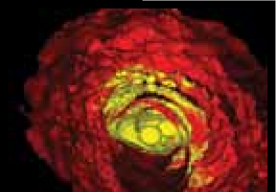
In April, the U.S. and Russia signed the New START to reduce the number of strategic warheads. Laboratory Director Anastasio appeared before the Senate and testified, "New START emphasizes the importance of the laboratory's mission and the need for a healthy and vibrant science, technology, and engineering base to be able to continue to assure the stockpile into the future."

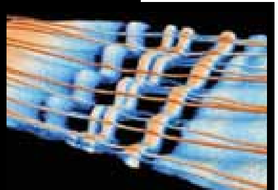
LANL hosted a number of distinguished visitors, including, Secretary of Defense Gates, the commander of STRATCOM, six members of the U.S. Senate, and several members of the House. The visitors were briefed on B61 work, pit manufacturing, actinide science, and nonproliferation activities. Deputy Administrator for Defense Programs Cook noted this is an "exceptional time." Cook proclaimed that Los Alamos continues to play a vital role in a national-security duality that involves modernizing the U.S. nuclear deterrent and ensuring effective arms control. Cook also said renewing human talent is vital. He presented NNSA's Defense Programs Awards of excellence to staff members from across the laboratory.

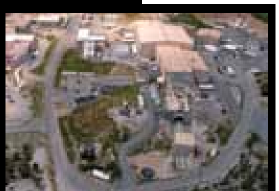
In July, Los Alamos scientists won five R&D 100 Awards, bringing the lab's total to 117. Our winning technologies span x-ray science, safer explosives, semiconductors, and biofuels. Capturing transient events is essential in science, especially the science of nuclear weapons and energetic materials. The MOXIE camera system reveals the behavior of explosives and pressure waves.

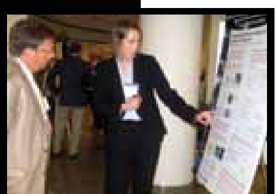
After last year's shots, our Dual-Axis Radiographic Hydrodynamic Test facility completed three more tests this year. The tests provided superior-quality material radiographs. The first phase of the Chemistry and Metallurgy Research Facility Replacement project was completed with the Radiological Laboratory/Utility/Office Building. We are nearing completion of work on W88 WR pits. Early September brought the first installment of Cielo, our newest capability-platform supercomputer.

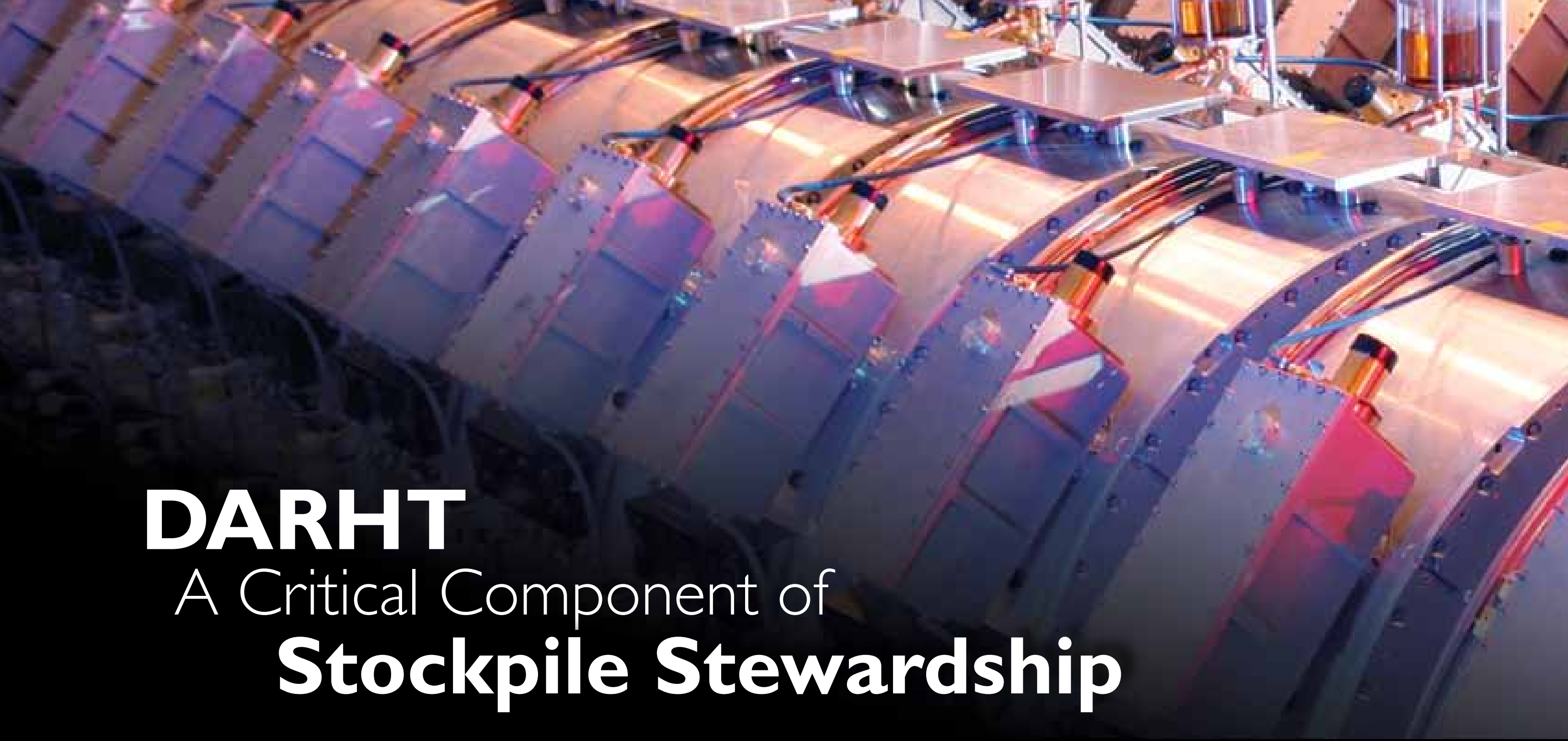
In closing, I would like to thank my colleagues at LANL. Our success would not have been possible without your commitment and pursuit of excellence in support of our nation.











DARHT
A Critical Component of **Stockpile Stewardship**

The weapons programs at Los Alamos have one principal mission: ensure the safety, security, and effectiveness of nuclear weapons in our nation's enduring stockpile. One critical component of this mission is DARHT, the Dual-Axis Radiographic Hydrodynamic Test facility.

DARHT consists of two large x-ray machines that produce freeze-frame radiographs (high-powered x-ray images) of materials that implode at speeds greater than 10,000 miles an hour. Such radiographs help scientists ensure that weapons in the stockpile are safe and effective and that—if ever necessary—they will perform as designed.

Ten years ago, Los Alamos personnel brought DARHT's first axis online. And in December 2009, after surmounting technical challenges, DARHT achieved its first dual-axis, multiframe hydrodynamic test (hydrotest), following a preliminary test in November. The facility has now completed three successful two-axis multiframe hydrotests. Data from the December experiment provides the technical information needed to close a Significant Finding Investigation (SFI) on the W78 warhead.

With DARHT fully operational and producing successful dual-axis hydrotests, scientists can now study full-scale mockups of how nuclear primaries explode.

"You could say that in fiscal year 2010 we finally put the 'D' in DARHT," said Mary Hockaday, LANL's Deputy Associate Director for Weapons.

Overcoming Complex Technical Challenges

Although the first axis of DARHT functioned well for more than 10 years, the second axis experienced monumental challenges. The challenges arose essentially because the second axis was an operational prototype of the world's longest pulsed-electron linear accelerator.

One challenge consisted of fitting the accelerator prototype into the DARHT facility. To reduce the accelerator's size, designers and engineers turned to a novel material, Metglas, which possessed an exceptionally high magnetic suscepti-bility. By using this novel material, designers fabricated an accelerator five times smaller than the original prototype.

Other challenges included designing a cathode injector system to supply enough electrical current to the accelerator and developing a target robust enough to survive four pulses from the second axis' extremely high energy electron beam. The injector system produces electrons that are drawn from the cathode and are accelerated through a potential of several million electron volts. A magnetic field guides the electrons into the accelerator.

The first-axis injector uses a five-centimeter cathode covered with velvet cloth. Velvet is used because the whiskers perpendicular to the cloth's surface are favorable to electron emission. This simple cathode is only suitable for beams that are shorter than 100 nanoseconds.

DARHT's second axis requires a more complex cathode because its pulse durations last 1,600 nanoseconds—27 times longer than the pulse in the first axis. The injector for this axis uses a 16.5-centimeter-diameter thermionic cathode. This larger-diameter thermionic cathode is

maintained typically at 1,150°C, with electrons literally boiled off the cathode's surface.

The technical demands of the second axis are unique. For example, the axis is designed to produce a 17-million-volt electron beam that lasts for 1.5 millionth of a second. The beam is sliced into four pulses, each of which lasts less than 100 billionths of a second, to create four x-ray pulses. Making multiple x-ray pulses from a single-pulse induction accelerator requires creating a single electron pulse of approximately 1,600 nanoseconds. The x-ray dose from just one DARHT pulse is as high as 1,000 roentgens—the equivalent of 60,000 chest x-rays.

The resultant x-rays create images of materials with densities that exceed those at the center of the Earth. Moreover, one of the pulses from the second axis can be synchronized with that of the first axis, so that three-dimensional information can be reconstructed.

Maintenance Worth the Investment

DARHT was shut down this summer to complete a months-long maintenance and upgrade project. As part of this maintenance, workers refurbished the second axis at the 88-stage Marx bank, which consists of a series of large capacitors that can be charged in parallel but can be discharged in series, thus yielding extremely high voltage pulses.

DARHT's accelerator and execution control rooms also underwent extensive upgrades. Workers built a fiber-optic timing and firing communication system, which greatly improved reliability. In addition, the facility incorporated energy-efficient, high-definition video monitors.

"The recent technical upgrades and facility maintenance at DARHT were important investments to NNSA's infrastructure to help solve tough national challenges," said Don Cook, NNSA's Deputy Administrator for Defense Programs. "We congratulate the Los Alamos lab for a job well done."

2010 Yields Three More Successful Hydrotests

In July 2010, DARHT completed a successful two-axis, multiframe hydrotest. This data will allow LANL to close another SFI. Two additional successful tests—one of which was designed by Lawrence Livermore National Laboratory—were performed this year.

"Once again, the people supporting DARHT have demonstrated their exceptional professionalism in facility operations," noted Charles McMillan, Principal Associate Director for Weapons Programs at Los Alamos. "Their focus continues to be the delivery of high-quality data, effectively dealing with complex technical questions as they arise and consistently seeking ways to advance the scientific and technical capability at DARHT."

During a hydrotest, scientists detonate a "mockup" of a pit, the primary stage of a nuclear weapons system. The mockup consists of actual high explosives and most other ingredients, except for plutonium. Instead of plutonium, scientists use a nonfissile substitute material that has similar, weight, density, and other metallurgical properties so that it behaves much like the plutonium. The one thing the mockup does not do is produce a nuclear explosion when detonated.

Hydrotest Results and Application

With both beams now operational, DARHT can take four sequential radiographs on one axis and one radiograph along a perpendicular axis, providing the first-ever simultaneous views of an implosion from two directions. The exposure time of such radiographs—60 billionths of a second—freezes the action of an imploding mockup to much less than a millimeter.

To do this, DARHT orients the two linear-induction accelerators at right angles to one another. A linear-induction accelerator uses magnetic cores to enable better coupling of electrostatic fields, thus accelerating electrons or other particles to extremely high energies. At DARHT, such electron beams are focused on a metal target. As the high-energy electrons hit the target, the electrons are deflected, converting the beam's kinetic energy to powerful x-rays.

Along with other tools, such as advanced laser interferometers and electronic position indicators, DARHT produces data sets during these hydrotests that are used to verify computer codes for nuclear weapons. The data sets of full-scale implosions are compared to simulations derived from the computer codes.

Current and Future Camera Technology

Capturing such transient events requires special camera systems. DARHT's current camera system converts x-rays to visible light with a scintillator (a material that exhibits the property of luminescence when excited by ionizing radiation). The second-axis scintillator is made from a dense, exotic manmade crystal known as bismuth germinate, which is highly sensitive to x-rays. To prevent lateral blurring of light, the scintillator is made up of 137,000 one-millimeter square rods, each covered with a metal sleeve. For the second axis, this material exhibits a rapid (50 nanoseconds) decay between flashes, thus ensuring that light from one image does not corrupt succeeding frames in the sequence.

The resultant light from a scintillator is recorded on astronomy-grade charged-couple devices (CCDs). CCDs are the most sensitive optical-recording devices available. The DARHT camera systems (one on each axis) are 100 times more sensitive than film and 40 times more efficient at absorbing x-rays.

To obtain multiple images with the second axis, scientists use a unique CCD architecture that records four images at a rate of two million frames per second. Because there is insufficient time to transfer data off the chip at this high frame rate, the information for each frame must be stored locally on each pixel and then slowly read off after the explosive experiment comes to an end.

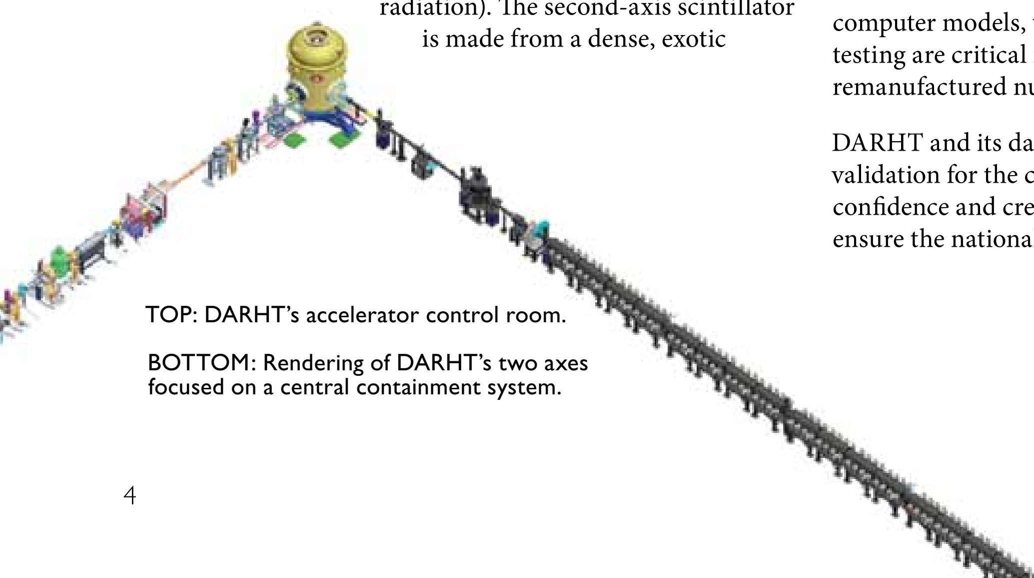
In the future, DARHT may take advantage of a new type of camera, known as the Movies of eXtreme Imaging Events, or MOXIE. Known as the world's fastest camera, MOXIE can take pictures closely spaced in time (much like a motion-picture camera), which enable researchers to "see" into the unseen, imaging transient events from start to finish. MOXIE's x-ray images could allow scientists to measure quantities such as velocity, acceleration, and voriticity. This year, MOXIE's inventors received an R&D 100 Award, which *R&D Magazine* gives to the world's 100 most technologically significant new products each year.

Bolstering the Nuclear Deterrent of the United States

The DARHT program has proposed to increase the rate of hydrotests in the coming year. DARHT personnel also plan to improve its multi-image capability. Such improvement could potentially increase the number of radiographs possible with each test.

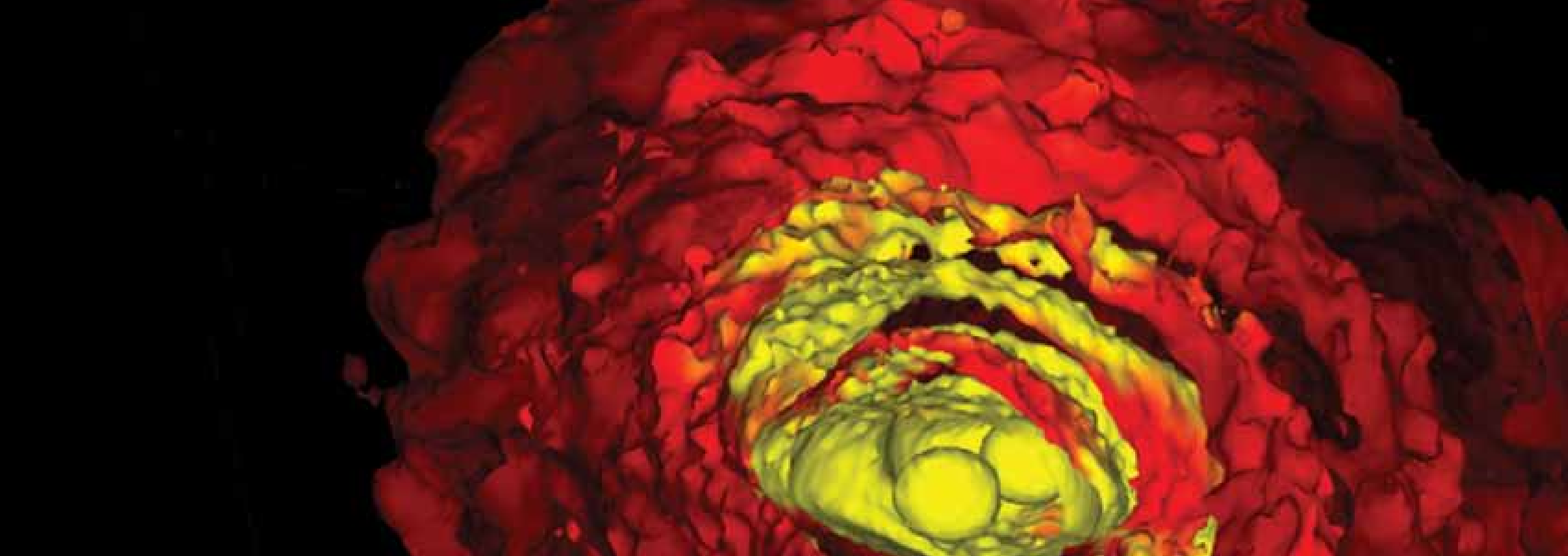
The results of these studies will help improve and verify computer models, which in the absence of actual nuclear testing are critical in assessing the effects of aging and remanufactured nuclear weapons.

DARHT and its data-rich radiographs supply real-world validation for the codes and thus effectively enhance the confidence and credibility of stewardship efforts designed to ensure the national security of the United States.



TOP: DARHT's accelerator control room.

BOTTOM: Rendering of DARHT's two axes focused on a central containment system.



LDRD Day

Cultivating Next-Generation Science

Los Alamos National Laboratory scientists and engineers participated in the Laboratory's second annual Laboratory-Directed Research and Development (LDRD) Day, at which the public viewed advanced research currently underway. This year's LDRD Day, held near Santa Fe on September 28, consisted of poster presentations that covered subjects spanning global security, space science, and biofuels development. Materials science—a focal point in several research fields—and its reliance on computers was highlighted in many of the presentations.

Advancing Our Understanding of Materials and Achieving Exascale Supercomputing

Charles McMillan, featured speaker at LDRD Day and head of LANL's weapons program, noted that sustaining the nation's nuclear deterrent over the long term requires investing in advanced science and technology. He highlighted how nanoscale materials synthesis and advanced simulation are transforming materials science, which has broad applications (including energy independence). Initially funded by LDRD, LANL researchers discovered new mechanisms for substantially increasing materials strength and radiation resistance. According to McMillan, two elements of interest to LDRD researchers are better understanding of materials in extreme environments and achieving exascale computing—supercomputers capable of handling a million trillion calculations per second.

In addition to sustaining the nation's nuclear deterrent, exascale computing and better understanding of materials at the mesoscale have applications that can benefit the world, according to McMillan. For example, it would be possible for researchers to design technologies to better protect electric-transmission infrastructures from attack, create novel metals for industrial applications, and develop technologies that enhance energy production, transmission, and storage.

MaRIE and Cielo: Two Powerful Allies

Advanced computing capabilities or an extensive knowledge of materials often lies at the core of breakthrough science. This is a great strength for LANL and its LDRD-funded researchers. The first in a proposed new generation of scientific facilities for the materials community, MaRIE (Matter-Radiation Interactions in Extremes) will enable scientists to develop next-generation materials that will perform predictably and on demand for currently unattainable lifetimes in extreme environments.

Cielo is a new supercomputing platform at LANL with petascale capabilities—that's more that one quadrillion floating-point operations per second. The role of Cielo will be to run the largest and most demanding workloads involving modeling and simulation. Cielo will support large single jobs that can take advantage of the entire platform.

Combined, facilities such as MaRIE and supercomputers such as Cielo (in conjunction with advances in computational science and theory) will serve as tools that scientists will use to make breakthroughs in predictability that in turn will enable materials science to move from a focus on empirical observation to one of predictive design and control.

LDRD Day Presentations: Work on Scientific Breakthroughs in Predictability Already Underway

At this year's LDRD Day, scientists from Los Alamos presented 45 posters covering the projects sponsored by LDRD. Following are highlights of LDRD Day posters demonstrating efforts in predictability specific to materials science and advanced computing.

Understanding Explosives Initiation for Threat Evaluation and Mitigation

Understanding how an explosive is set off at a molecular and granular scale is critical for scientists designing safer explosives. Such knowledge may even help find ways to prevent explosives from initiating.

To determine elements such as initiation thresholds, mechanisms, and initiation pressure dependencies of relevant explosive formulations, scientists are using in situ measurements of shock and reactive-wave profiles under controlled shock-compression conditions. Liquid explosives (homogenous) display different initiation behaviors than do multicomponent (heterogeneous) explosive mixtures. Whereas homogenous explosives initiate as a result of a thermal explosion derived from bulk shock heating, heterogeneous explosives initiate with the creation of "hot spots" (localized regions of high temperature and pressure).

As a result of this LDRD project, Los Alamos researchers now have a thorough understanding of the initiation behaviors of several important liquid explosives. They have compared their relative sensitivities and have discovered that pressure dependencies of their run-distances-to-detonation appear to be similar across the series. Scientists have also learned that incorporating hot-spot "seeds" influences initiation (critical size and separations, for example).

Scientists have evaluated the relative effectiveness of solid vs. hollow particles in creating hot spots and have discovered that a balance exists between hot-spot-driven and thermal-driven burn mechanisms. By studying explosives under controlled shock conditions, scientists are establishing a foundational knowledge of the important features that dictate initiation behaviors. Predictive models derived from this knowledge will help researchers create the next-generation of explosive-modeling capabilities for the United States.

Los Alamos scientists working on this LDRD project are D. Dattelbaum (principal investigator), S. Sheffield, R. Engelke, D. Stahl, and L. Gibson.

LANL scientist Al Migliori talks with weapons director Charles McMillan and former Congresswoman Heather Wilson.

First-Principles Molecular Dynamics for Extended Length and Time Scales

Designing new materials is at best a hit-and-miss approach using traditional laboratory processes. Because such efforts waste time and effort, scientists have turned to computers, where they can analyze and experiment with materials without any experimental input. In the world of computing, it is possible to make a model of a million atoms as they move and vibrate at unimaginable speeds.

Simulations of molecular dynamics enable researchers to conduct detailed studies of fundamental material properties, such as phase transitions, chemical reactions, and molecular structures. Currently, the "gold" standard for atomistic simulations consists of molecular dynamic simulations in which the molecular motion is derived directly from the first principles of quantum mechanics.

First-principles simulations require no input from experiments, thus enabling analysis and prediction of material properties under conditions that are either too expensive or cannot be naturally achieved under laboratory conditions. Such simulations also yield more complete and detailed descriptions that can lead to a better understanding and sometimes the successful prediction of materials with new tailored properties.

Los Alamos scientists have taken a major step forward in the ability to study and predict complex material properties directly from theory. In conjunction with rapid increases in computing power, basic research conducted so far may find applications in almost every field of materials science, chemistry, and molecular biology. Applications include developing high-performance steel, new and safer explosives, nanodevices, novel polymers, and enzymes for producing new biofuels.

Los Alamos scientists working on this LDRD project are Edward Sanville, A. Niklasson (principal investigator), M. Cawkwell, D. Dattelbaum, and S. Sheffield.

Novel Materials for Detection of Radioactive Materials

A scintillator is in essence a substance that glows when struck by high-energy particles or photons. By better understanding how scintillators work, scientists can develop better detection devices and thus minimize the proliferation of radioactive materials.

Using a combined approach that consists of materials synthesis and theoretical modeling, Los Alamos scientists are designing new, more efficient optical materials and modeling their luminescent behavior. Synthesizing modular molecular and supramolecular materials containing phosphors enables researchers to control the size and dimensionality of such materials, as well as providing a better understanding of the scintillation process. By using synthesis, characterization, and theoretical modeling to better understand how molecular phosphors work, scientists can create a platform from which to design more efficient detector materials.

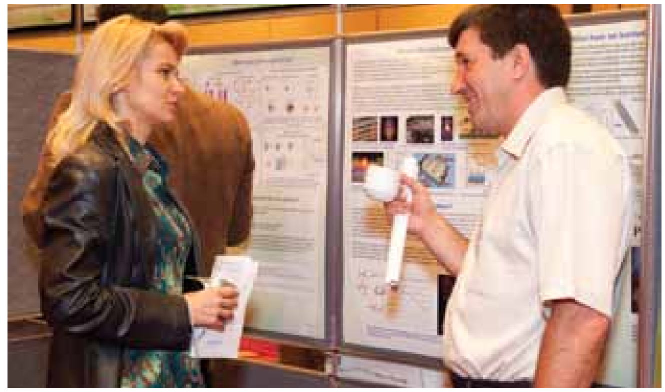
Los Alamos scientists working on this LDRD project are Rico Del Sesto (principal investigator), D. Ortiz-Acosta, and R. Feller.

Petascale Synthetic Visual Cognition: Large-Scale, Real-Time Models of Human Visual Cortex on the Roadrunner

Humans take sight as a given, but the human eye and brain—and their interactions—are extremely complex. Thus, it appears easy for a human to spot a vehicle hidden under camouflage, yet not even the fastest supercomputer in the world can analyze a similar image and reliably find the vehicle.

The goal of this LDRD project is to understand how the human visual cortex works so that researchers can teach computers to “see.” To achieve this goal, Los Alamos scientists are using one of the most powerful supercomputers, Roadrunner, to build the world’s first full-scale, real-time model of the part of the human brain known as the visual cortex. Also of interest are small mammals capable of excellent visual acuity and objective recognition with orders-of-magnitude smaller brains. New computing technology based on graphic cards could enable the widespread use of brain models for many computer vision tasks.

Los Alamos scientists working on this LDRD project are Luís Bettencourt (principal investigator), S. Brumby, G. Kenyon, J. George, C. Rasmussen, A. Galbraith, M. Anghel, and M. Ham.



Sergei Tretiak discusses his materials research. Tretiak won a 2010 LANL Fellows Prize for Outstanding Research in Science or Engineering, in part for his development of organic light-emitting diodes for flexible displays, organic lasers, and light-harvesting energy devices.

Beyond LDRD

This year’s LDRD Day posters addressed four focus areas: energy security, national security, global security, and scientific discovery.

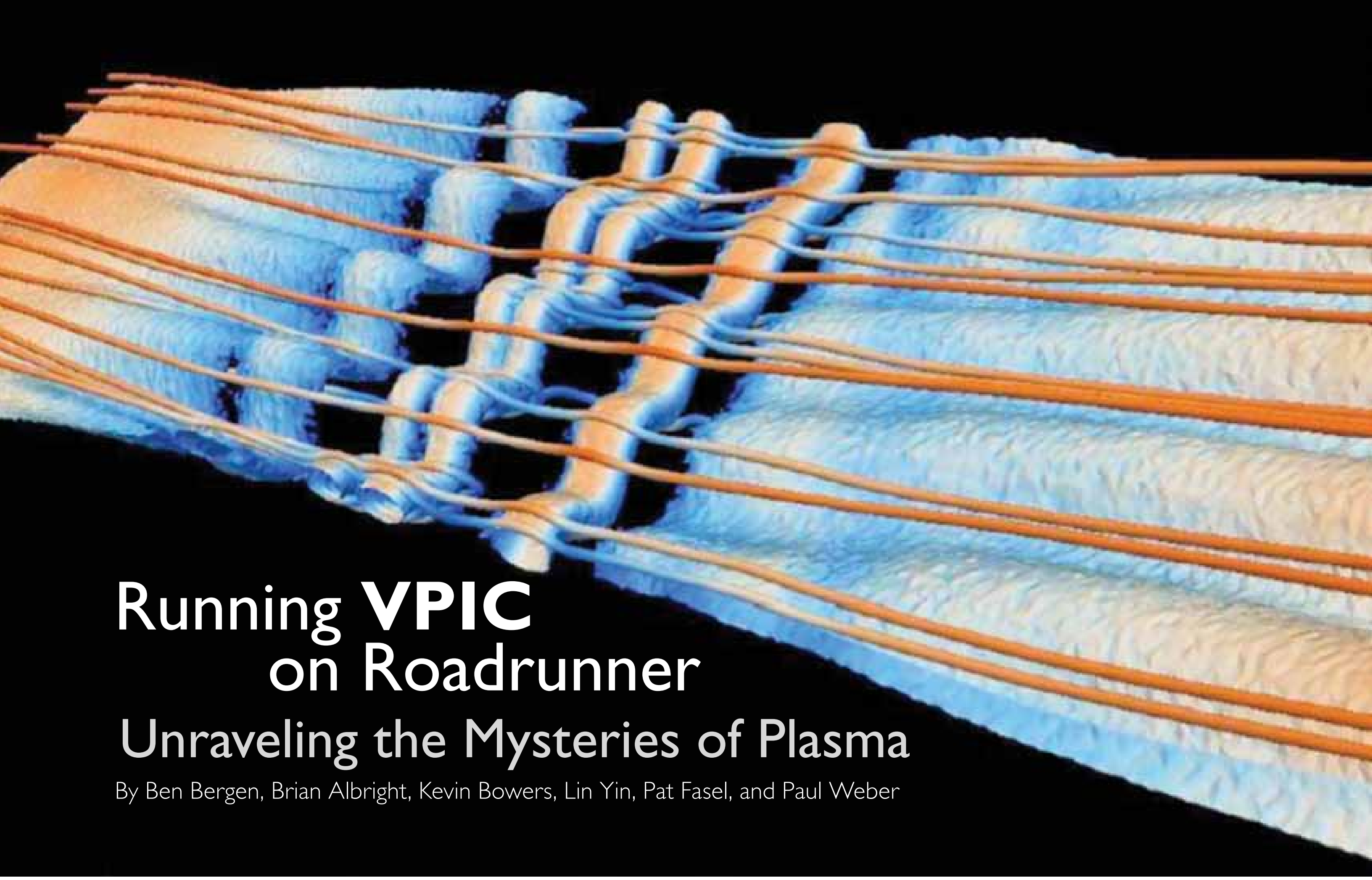
The United States is currently facing security, energy, and environmental challenges that, with respect to their scope and complexity, are perhaps unparalleled in the nation’s history. So, how does the nation go about developing long-term solutions to such challenges?

“Scientific breakthroughs seldom arise spontaneously from individual talent but from a critical mass of talented individuals who are supported by an institution committed to basic research,” noted Los Alamos LDRD Program Director William Priedhorsky.

The LDRD program is also a powerful means of attracting and retaining top researchers from around the world. Such researchers foster collaborations with other prominent scientific and technological institutions and leverage some of the world’s most technologically advanced assets.

By investing in high-risk and potentially high-payoff research, the LDRD program works to create innovative technical solutions for some of the most difficult challenges faced by the United States and the world. In many instances, projects started with LDRD funding grow into much larger projects that in some cases attract interest from other government agencies, academia, and private industry.

“Much of the Laboratory’s scientific capabilities, from energy security to large-scale infrastructure modeling, from actinide science to nuclear nonproliferation and detection, can be traced to LDRD investment,” said Priedhorsky.



Running **VPIC** on Roadrunner

Unraveling the Mysteries of Plasma

By Ben Bergen, Brian Albright, Kevin Bowers, Lin Yin, Pat Fasel, and Paul Weber

A Roadrunner simulation of magnetic reconnection, a basic plasma process in which magnetic-field energy rapidly converts into plasma kinetic energy. This simulation shows preliminary results of one type of plasma instability within the complex, three-dimensional interaction of flux ropes. Los Alamos scientists are working to understand the role such instability plays in setting the dissipation rate and accelerating electronics to high energy.

Plasma makes up 99 percent of the matter in the visible universe. Dense plasma is the stuff of stars, with tenuous plasma filling the space between stars.

Plasma is created by ionizing gas atoms—usually by heating them—to form a hot mix of positively charged atomic nuclei (ions) and negatively charged electrons. On Earth, plasmas can be seen in lightning and auroras but for the most part are not found because temperatures are relatively cool.

Common applications for plasma include neon signs and fluorescent tubes. However, artificial plasmas, those that exist only briefly during experiments, hold the key to harnessing fusion energy or in exploiting the properties of ultra-intense lasers.

To better understand the nature and behavior of plasmas, Los Alamos scientists developed VPIC (vector particle-in-cell), a computer code that simulates plasma behavior more efficiently than any other code. VPIC simulations enable researchers to study plasmas in ways that exceed conventional theory- and experiment-driven approaches.

Using VPIC, scientists at Los Alamos have conducted the following studies:

- Performed intense-laser interactions with plasmas in laser-driven fusion experiments.
- Used ultra-intense lasers to accelerate plasma electrons to produce x-rays or plasma ions, which can be used to treat cancer, detect contraband nuclear materials, or “spark” fusion in preheated and precompressed fusion fuel.
- Used high-power plasma diodes to produce intense bursts of x-rays for imaging.
- Studied magnetic-confinement fusion.
- Examined magnetic reconnection, a physical process common through the cosmos. This process produces bursts of energy-charged particles during solar flares, for example.

To further enhance VPIC, Los Alamos scientists modified the computer code to run on the supercomputer known as Roadrunner (see sidebar). Such modifications have taken VPIC to a new level, resulting in new discoveries, some of which are addressed in this article.

To simulate plasma behavior, VPIC follows the motions of simulated particles as simulated electric and magnetic force fields push the particles. Each particle represents thousands of plasma ions and electrons. The force fields can be applied externally to the simulated volume or are generated by charges or the motion of the charges in the simulated particles themselves. VPIC tracks particle motion in three dimensions, accounting for increases in particle masses as their speeds approach that of light, according to Einstein's theory of special relativity.

The Numbers Add Up

VPIC employs vector computing, in which data are operated upon in units known as vectors that contain many pieces of data (usually real numbers). The number of pieces of data in a vector makes up the vector size. In principle, a single vector can contain many thousands of pieces of data. However, most modern supercomputers have vectors that are much smaller (e.g., with four data) called "short" vectors—such a size enables the vectors to process graphics data economically.

In many modern computing architectures, the execution units—the units that actually carry out the floating-point computations—are wide enough to accommodate multiple data. These data have the same instruction applied to them simultaneously, thus increasing throughput. This is a low-energy strategy for increasing performance.

In VPIC's case, the short vectors contain only four pieces of single-precision data that add up to 16 bytes. To adapt VPIC to run on Roadrunner, scientists began by modifying the code completed in 2007. The code used an abstraction layer called "v4," written in the high-level computer language C++. The v4 abstraction layer enables VPIC to support several different architectures with a single implementation.

Using the C++ compiler, VPIC expresses algorithms in a high-level abstraction using v4 operators, which are then converted to the correct "machine language" for the given architecture. The approach gives VPIC a real advantage in handling the diversity of different architectures currently being used in supercomputing. This feature also made it easier for scientists to adapt VPIC to Roadrunner.

Waiting Games

Handling data intelligently is key in obtaining the best supercomputing performance. As the theoretical maximum number of operations that can be done in a second has steadily increased in supercomputers, the performance of memory subsystems has not kept up, specifically in terms of bandwidth and latency.

Roadrunner
An Overview of Its Architecture

On Memorial Day of 2008, the Roadrunner supercomputer broke records worldwide and exceeded a sustained speed of one petaflop per second—one million billion calculations per second. Developed by IBM in collaboration with Los Alamos National Laboratory and the National Nuclear Security Administration, Roadrunner was designed for advanced physics and predictive simulations in a classified environment.

To take VPIC to a new level, Los Alamos scientists adapted the computer code to run on Roadrunner. Roadrunner consists of 18 "connected units." Each connected unit consists of 180 "triblade" computer nodes, all of which perform calculations in parallel. Roadrunner is a hybrid supercomputer because each computer node is built with two different types of microprocessors: (1) the Opteron microprocessor and (2) the enhanced Cell Broadband Engine, or "Cell."

Each computer node includes four Opteron microprocessors and four enhanced Cells. An enhanced Cell accelerates each Opteron. The Opteron is the workhorse of many conventional supercomputers, whereas the enhanced Cell was specifically modified for use in Roadrunner. The original Cell's applications included rendering detailed graphics in real time for a video-game controller—a task mathematically similar to those involved in large-scale scientific simulations.

An enhanced Cell boosts the speed at which an Opteron processes data by as much as 25 times. However, to run at top speed on Roadrunner, a code such as VPIC must be modified carefully so that it can run optimally within Roadrunner's fairly unique hybrid architecture.

Usually given in gigabytes per second, bandwidth is the maximum rate at which a microprocessor moves data to or from memory. Latency refers to time delays associated with moving data to or from memory. Poor bandwidth and latency cause modern microprocessors to spend most of their time waiting for data.

One challenge facing VPIC will be for researchers to find innovative ways to express the physics of simulations to facilitate advanced discovery and enhance humanity's knowledge of the universe.

To circumvent bandwidth and latency limitations, VPIC reduces the number and size of data accesses. In the Roadrunner implementation of VPIC, the real numbers representing the positions, momenta, charges, and currents of all particles are stored in the local memory of a special processing element's (SPE's) core during the update of a given region of data. The storage is in contiguous blocks whose size equals the maximum size that can be directly transferred to or from local memory.

Such storage yields the highest percentage of the local memory's bandwidth, thus making it much more efficient. Once data are stored in local memory, VPIC's carefully hand-optimized algorithms can use the data as many times as necessary before they are written back to main memory, a process that takes place on the Cell Broadband Engine (Cell) chip away from the SPE.

Adapting VPIC for Roadrunner

In addition to porting VPIC's basic algorithms to the Cell architecture, scientists needed to make two primary structural enhancements to the code so that it would run on Roadrunner.

The first structural enhancement addressed Roadrunner's hierarchical nature, involving multiple layers of computing elements and memory. The goal was to enable data to remain resident on a Cell accelerator, thus avoiding the movement of large blocks of data across a slow connection between the Opterons (server and workstation processors) and the Cell chips.

To overcome this potentially serious bottleneck, scientists developed a messaging "relay" (much like a telecommunication switch relay) that forwards messages to a Cell chip's Opteron host processor and then on to the other Cell chips. This technique essentially flattens the machine's communication topology, making it seem to the Cell chips as if they are "talking" to each other (Figure 1). The code's original design made this adaptation to Roadrunner straightforward. Subsequent performance analysis has shown that any added latency in the relay is insignificant.

The second structural enhancement involved adding a data-parallel thread-management framework with abstractions that enable a single-source implementation to launch and control execution threads both on the Cell and on homogenous, multicore processors. In other words, portions of the VPIC algorithm are broken into small work units that are independent of one another and are dispatched onto separate computational "threads."

In the VPIC framework, it makes no difference if these threads run on a Cell SPE or even on separate cores of a homogeneous, multicore supercomputer. This feature is particularly advantageous on traditional supercomputers, as it yields greater flexibility in allocating node resources (Figure 2). Moreover, this feature could increase scalability by reducing the size of the communications network (reducing the number of Message-Passing Interface ranks) required to run a large simulation. Los Alamos scientists

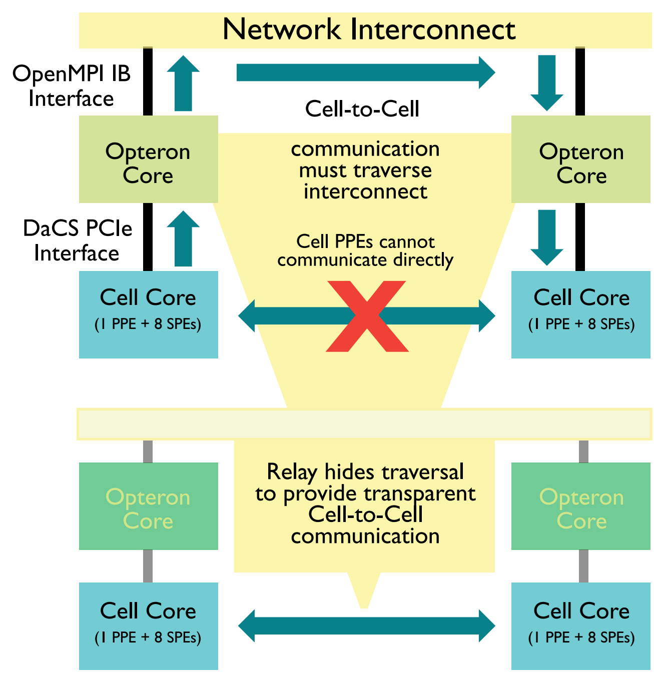


Figure 1. Roadrunner's underlying physical network structure does not allow direct communication between different Cell processors. To enable Cell-to-Cell communication, a relay forwards messages from one Cell processor to another.

have demonstrated this VPIC feature on the Cray XT5 Kraken supercomputer at Oak Ridge National Laboratory. This supercomputer uses six execution threads per chip.

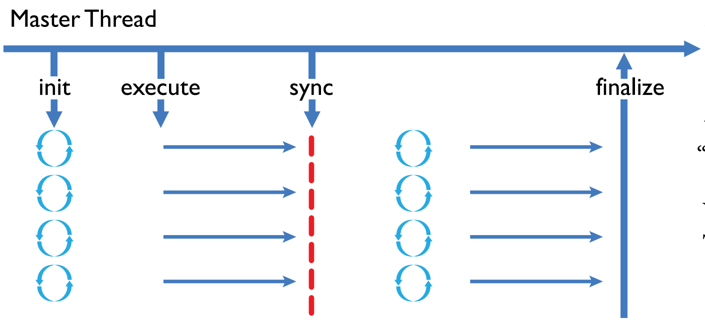


Figure 2. VPIC enables parts of the algorithm, such as the particle advance, to be broken down into small, independent work units that can be dispatched onto individual "threads" of computations. As a result, VPIC can conduct many operations in parallel.

Future Proofed

When Los Alamos scientists began this project three years ago, VPIC was already well poised to take advantage of Roadrunner's unique capabilities. This was no accident but rather the result of deep thinking about current trends in computer-architecture design, as well as careful planning in implementing a future-proofed code.

VPIC's development helped expose three principal areas for which new tools and techniques could improve the efficient use of computing resources in the future: efficient data movement, thread control for data and task-level parallelism, and the need for portable and low-level kernel specifications. An associated challenge exists in finding new programming models that are flexible enough to support a variety of architectural characteristics and capabilities.

To address these hurdles, the computer-science community has begun to develop new language standards, such as OpenCL (Open Computing Language), a cross-platform development framework for modern processors. One challenge facing VPIC will be for researchers to find innovative ways to express the physics of simulations to facilitate advanced discovery and enhance humanity's knowledge of the universe.

Simulating Plasma Behavior

A microprocessor typically stores one piece of data in a fixed amount of computer memory amounting to four bytes, for the most common representation of a number with a decimal point (as opposed to an integer). This way of storing "real" numbers is called single-precision floating-point representation (a reference to floating-point operations, or flops). Figure 3 shows how a single-precision floating-point number is stored in computer memory.

To simulate plasma behavior, a particle-in-cell plasma code first defines a three-dimensional Cartesian grid that fills the simulated volume in which the simulated plasma evolves over simulated time (Figure 4). The smallest volumes defined by the grid are known as "cells" (not to be confused with the Cell Broadband Engine). The code also defines "field states" at staggered locations on the grid.

VPIC uses a staggered (Yee) mesh to assign these locations. The field states are solutions to two of Maxwell's four electromagnetic-field equations. At the start of a simulation, the code adds small parcels—the simulated particles—to some of the cells, as dictated by the initial physical conditions of the experiment being simulated.

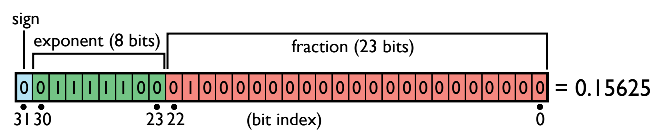


Figure 3. A microprocessor typically stores one piece of data in a fixed amount of computer memory amounting to four bytes. This way of storing "real" numbers is called single-precision floating-point representation, as illustrated here.

The code then steps through time in tiny increments. At the start of a new time step, the code uses each particle's current position, velocity, and the value of the time increment to calculate the particle's position change during the time increment. The code also uses the electric and magnetic forces acting on each particle to calculate how the particle's momentum (the product of its relativistic mass and velocity) changes.

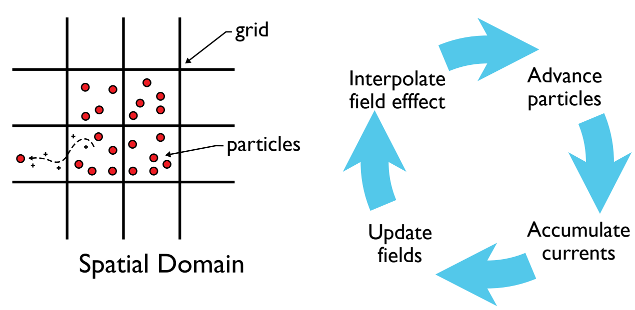


Figure 4. The particle-in-cell method evolves kinetic plasma by representing particles on a Cartesian grid.

Because the particles are charged, each one produces an electrical current as it moves through the simulated volume. The code uses the new positions and values of the charges and currents in each cell to calculate changes to the electric and magnetic fields throughout the simulated volume. The code then increases time by another time increment, with the entire process repeated again and again until the simulation is complete.

Breakthrough in Stimulated Raman Scattering

Research in inertial-confinement fusion (ICF) has both weapons and energy applications. In experiments conducted at the National Ignition Facility (NIF), 192 laser beams implode a fusion-fuel-filled spherical capsule suspended inside a cylindrical gold holhraum (Figures 5 and 6). The goal is to ignite the fusion fuel so that it releases substantially more energy than the lasers pump into it. (Read more about NIF on page 20.)

Before ignition takes place, the lasers vaporize and ionize the gas within the holhraum. Intense laser light striking the resultant plasma leads to a phenomenon known as stimulated Raman scattering (SRS), which amplifies periodic density variations in the plasma. Large density variations in the plasma reflect subsequent laser light, thereby reducing the implosion's drive energy and symmetry. Either effect significantly reduces fusion yield.

To compress the fuel capsule symmetrically requires nearly uniform laser intensity. NIF's laser beams obtain such intensity by passing each beam through a random-phase plate, which breaks the beam into an ensemble of laser speckles. To predict the effects of SRS on ICF experiments, scientists must understand the onset and saturation of SRS in a single laser speckle.

Figure 5. A closeup view of a fusion-fuel-filled spherical capsule known as a holhraum, the German word for "cavity."

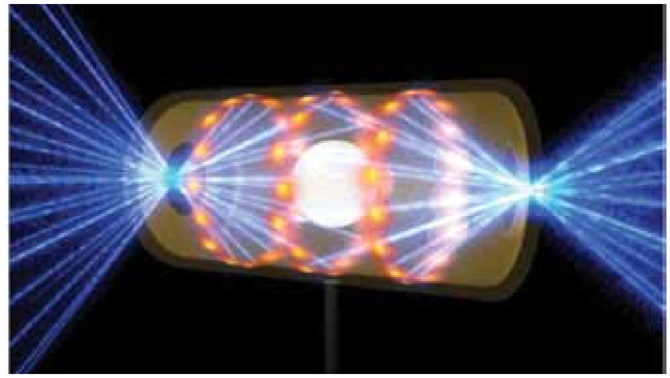


Figure 6. During NIF ignition experiments, 192 laser beams implode a fusion-fuel filled spherical capsule. Lasers striking the capsule help form a phenomenon known as stimulated Raman scattering, which reflects significant amounts of laser light. Reflection reduces the quality of the implosion and therefore the fusion yield.

Until recently, the essential nonlinear physics governing SRS growth was a mystery. Using VPIC simulations run on Roadrunner, scientists have demonstrated how nonlinear SRS physics affects laser penetration and energy deposition during a fusion experiment. These simulations modeled large, three-dimensional plasma volumes at unprecedented time and space scales and over a range of laser intensities. Each simulation typically used 4,096 processors.

During the simulations, scientists found that SRS reflectivity within a single speckle exhibited nonlinear behavior—the reflectivity quantifies how much the plasma reflects the incident laser light. A sharp onset at a threshold intensity, in which the reflectivity increased abruptly over a small range of intensity, was followed by a plateau at higher laser intensity, in which the SRS instability nonlinearly saturated (see inset in Figure 7). Single-speckle experiments at the Los Alamos Trident Laser Facility have since validated this simulated behavior.

Researchers ran the largest of the VPIC SRS simulations on 16 Roadrunner-connected units using 11,520 processors—nearly the full Roadrunner system. This simulation employed a record 0.4 trillion particles and 2 billion computational cells. It ran for 58,160 time steps (~10^{19} floating-point operations), long enough for two bursts of SRS to grow from noise levels to significant amplitudes at a laser intensity near the SRS onset.

Figure 7 shows isosurfaces of electrostatic field associated with these bursts. The wave fronts exhibit bending or "bowing" (a phenomenon arising from nonlinear electron trapping), as well as self-focusing that breaks up the phase fronts.

For the first time, these simulations have enabled researchers to understand the essential nature of the nonlinear onset and saturation of SRS. Current research focuses on determining whether neighboring speckles can interact by exchanging hot electrons—or laser or plasma waves—to better reflect laser light. This kind of study is possible only on very large (petascale-class) machines like Roadrunner, where kinetic simulations of laser-plasma interaction in three dimensions at realistic laser-speckle and multi-speckle scales can be performed with unprecedented size, speed, and fidelity.

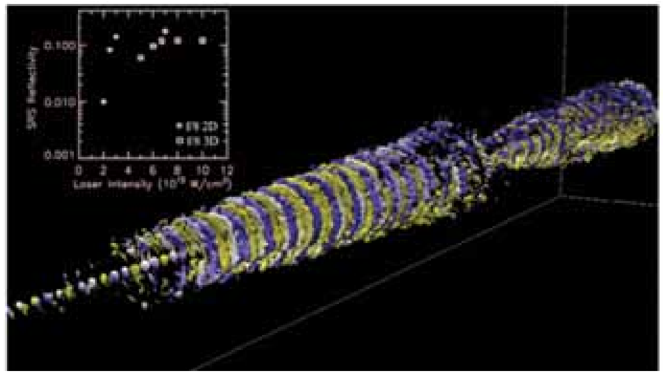


Figure 7. This figure shows VPIC simulations of plasma during two bursts of SRS growth. In the inset, VPIC simulations of SRS development reveal instability and saturation resulting from laser intensity.

New Cielo Supercomputer Arrives at Los Alamos

cielo

Cray Inc. has delivered a new supercomputing platform to support all three NNSA national laboratories: Los Alamos, Sandia, and Lawrence Livermore. Named Cielo (Spanish for "sky"), this petascale (more than one quadrillion floating point operations per second) supercomputer will help NNSA ensure the safety, security, and effectiveness of the nuclear stockpile while maintaining the moratorium on testing.

The first phase of Cielo installation at Los Alamos is complete. The 2010 installation consists of 72 cabinets, 6,704 compute nodes, 107,264 compute cores, and 221.5 terabytes of memory.

The total hardware will take up approximately 1,500 feet and use less than 4 megawatts of memory. The 2011 phase-two upgrade will expand the system to 96 cabinets with nearly 9,000 compute nodes, and approximately 300 terabytes of memory.

Cielo is the next-generation capability-class platform for the Advanced Simulation and Computing Program. Cielo will have more than 10 times the computing power of NNSA's current computing platform, the Purple supercomputer (about to be retired) at Lawrence Livermore. This additional increase in speed in Cielo will enable scientists to increase their understanding of complex physics, as well as improve confidence in the predictive capability for stockpile stewardship.

The supercomputer is housed at the Nicholas C. Metropolis Center for Modeling and Simulation, where both Los Alamos and Sandia will share day-to-day operations. In its primary role, Cielo will run the largest and most demanding workloads involving modeling and simulation. Cielo will be primarily utilized to perform milestone weapons calculations.

THE RAPIDLY CHANGING LANDSCAPE FOR MaRIE

JOHNSARRAO MARYHOCKADAY

Much has changed in the year since we last discussed Matter-Radiation Interactions in Extremes (MaRIE), LANL's proposed signature-facility concept. In this point of view, we provide a brief glimpse into these exciting times.

President Obama and his administration have made clear their commitment to ensure a nuclear deterrent that is safe, secure, reliable, and as small as possible. Active efforts include ratifying a New Strategic Arms Reduction Treaty (START) and Comprehensive Nuclear Test Ban Treaty. There is also growing consensus that effectively stewarding a shrinking stockpile will require investing in a sustained science and technology capability. Personnel involved with current budget deliberations are making strides in funding this vision, with Los Alamos playing a key role.

We have made significant technical strides. For example, we successfully executed the first hydrotests at the Dual-Axis Radiographic Hydrodynamic Test facility and participated in many experiments helping the National Ignition Campaign work towards its goal of attempting fusion in a laboratory setting—proposed to occur later this year.

In addition, our capabilities in proton radiography continue to deepen our understanding in areas such as high-explosive burn, and we are now defining a set of first experiments that will be fielded at the Advanced Photon Source for the proposed Dynamic Compression-Collaborative Access Team beamline. To gain process-aware understanding, we are (1) designing and conducting experiments that test material properties (such as strength) under dynamic-loading conditions and (2) evaluating how such processed materials respond within the context of microstructural changes.

LANL's MaRIE Project Program Director John Sarrao and Mary Hockaday, Weapons Directorate deputy, overlook the neutron science center.

Roadrunner's petascale-computing speed provides previously unimaginable resolution—and achieving exascale computation is actively underway. Recognized by the broader scientific community, the leadership of both NNSA and Los Alamos in experimentally validated simulation science plays a central role in defining exascale codesign centers and advances the frontiers of computational materials design.

As an example of the type of capability necessary for Los Alamos to retain this leadership, MaRIE stands to revolutionize materials in extremes, a challenge that spans a variety of DOE missions. For example, MaRIE will play a role in our energy and weapons programs by providing unprecedented in situ, transient measurements of real materials under relevant extremes, particularly dynamic loading and irradiation. Following is how MaRIE will address specific weapons needs:

- **Sustaining the current stockpile** by developing much better predictive capabilities for materials lifetimes and failures.
- **Weapons System rebuild and life extension** by providing materials "by design" to overcome costly "relearning" of old processes and myriad attempts to duplicate old materials.
- **Validating weapon performance** by better understanding the relationship between material microstructure (through material performance) and nuclear performance.

To meet these weapons needs, MaRIE will consist of a high-energy, low-average intensity source of x-ray photons (preconceptually a 50- to 100-keV x-ray free-electron laser) coupled to an existing high-intensity proton linear accelerator at the Los Alamos Neutron Science Center (LANSCE). There will be three measurement facilities: the Multi-Probe Diagnostic Hall; the Fission-Fusion Materials Facility; and the Making, Measuring, and Modeling Materials Facility. MaRIE will leverage existing DOE investments at LANSCE, the Laboratory's materials infrastructure, and the Office of Basic Energy Sciences national user facilities. MaRIE will also leverage current and planned investments, such as NNSA's LANSCE Linac Risk Mitigation Effort and the Materials Test Station.

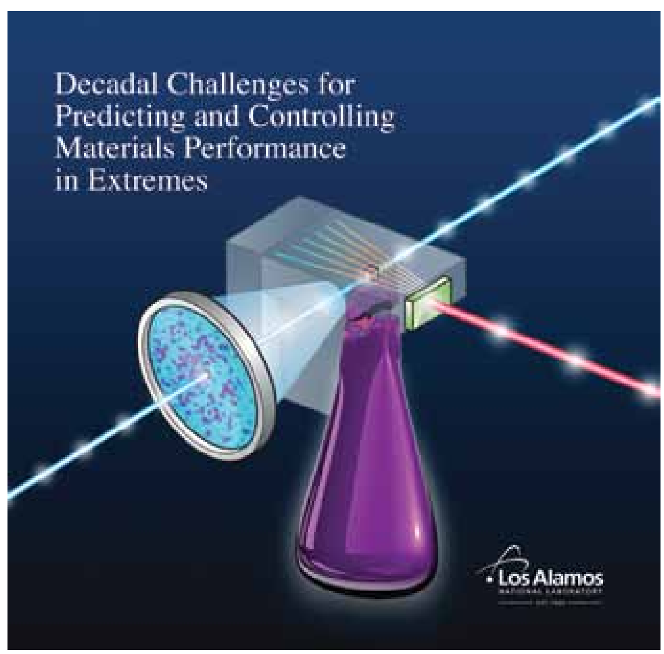
Recently, DOE Under Secretaries Thomas D'Agostino, Kristina Johnson, and Steven Koonin acknowledged the importance of LANSCE's role in stockpile stewardship over the next decade. The Under Secretaries requested that the Laboratory Director provide a plan for the full suite of issues that must be addressed to sustain LANSCE's current level of operations through the next decade. They also asked the Laboratory to address the longer-term need for high-quality experimental science capabilities, as well as suggested materials-in-extreme conditions as a possible focus area. As part of LANL's response, Director Anastasio asserted, "MaRIE…is the appropriate signature experimental facility for LANL," and "we believe that a mission need for a materials-in-extreme facility focused on in situ transient measurements exists."

Director Anastasio made these assertions based in part on a series of five workshops sponsored by LANL in 2009, culminating with the December 2009 workshop, entitled "Decadal Challenges for Predicting and Controlling Materials Performance in Extremes." At these workshops, more than 225 scientists from 80 institutions worked to identify scientific challenges and research directions to achieve predictive materials performance in extreme environments, focusing specifically on needed capabilities and tools. Workshop reports are available at http://www.lanl.gov/source/projects/marie/workshops.shtml.

Recently, MaRIE's External Advisory Board concluded that "outreach and engagement with the scientific community couldn't be better. It is particularly noteworthy that these workshops were not LANL-centric; i.e., were not focused on the use of MaRIE as a tool but rather were focused on defining technical challenges in broad areas of research, identifying needs."

Many scientific challenges are directly relevant to our mission, such as understanding the mechanisms of failure under dynamic-loading conditions. To better understand such mechanisms, Los Alamos scientists will use MaRIE's proposed x-ray free-electron laser and proton radiography simultaneously to probe well-characterized samples that are shock- or ramp-loaded. We also will use dynamic x-ray diffraction or ankylography to track defect generation and annihilation, with the resultant data used to validate atomistic to mesoscale models of dynamic response.

This past year, we experienced much activity focused on science and technology capabilities necessary for stockpile stewardship. Accelerating these activities holds great promise for sustaining important LANL capabilities. We can only hope that the upcoming year is as exciting as the last.



LANL Teams Receive **NNSA Awards**

The National Nuclear Security Administration (NNSA) honored hundreds of Los Alamos colleagues from thirteen teams with Defense Programs Awards of Excellence for exceptional performance in meeting national security challenges. New NNSA Deputy Administrator for Defense Programs, Don Cook, spoke at the awards ceremony and directorate all-hands meeting—hosted by Charles McMillan, Principal Associate Director for Weapons Programs—on August 30 at LANL. Cook also presented Pollution Prevention Awards.

Cook, a physicist who oversees the nuclear weapons program for NNSA, spoke about how nuclear deterrence and nonproliferation treaties and policies recently implemented make this an, "exceptional time" adding, "I have never seen a time like this." Cook proclaimed that Los Alamos continues to play a vital role in a national-security duality that involves modernizing the U.S. nuclear deterrent and ensuring effective arms control. He noted that as the size of the stockpile is reduced, the weapons must be modernized. Cook said LANL's unique combination of skills garnered the nation's trust for this work.

Defense Programs Awards of Excellence Recipients

Individual Award

Karin Hendrickson

This computional-physics staff member enabled Atomic Weapons Establishment personnel based in the United Kingdom to collaborate with the United States on the survivability engineering campaign during a three-month visit, resulting in a lengthy technical document supporting the international program.

Team Awards

Scott Runnels and the Lagrangian Hydrodynamics Integrated Product Team

This team's work has been the model for multidisciplinary software verification and was essential for solving stockpile Lagrangian hydrodynamics performance problems. Their work also increased project funding.

Francisco J. Souto and Anil K. Prinja

This two-member Theoretical Design Division nuclear safety team was nominated for their reevaluation of the Bell-Longmire-Mercer theory.

Robert A. Gore Verification and Validation Milestone Team

The team made significant achievements in weapons assessment. Gore's team performed a broad and in-depth evaluation of an Advanced Simulation and Computing Program code's performance-modeling capability, resulting in a monumental advance in the predictive capability. They achieved substantially higher quality matches to a wide set of experimental data, enabling better performance.

Bruce E. Takala and the LANSCE Operations Team

This team was extraordinarily committed to providing user beam time for the Los Alamos Neutron Science Center. A record number of beam hours were delivered to the Proton Radiography Facility, with a reliability factor approaching a remarkable 92 percent.

Donald L. Cook and Karin Hendrickson

Blake Wood and the W76-1 Alternate Material Certification Team

The certification team pursued a multi-pronged technical approach to support timely completion of the W76-1 Life Extension Program (LEP): detailed physics modeling, small-scale experimental analysis, and comparison to near-neighbor underground nuclear tests. This team's work provided data for future LEP's use of alternate materials, established a prototype for future component reuse design certification, and could reduce costs by millions of dollars.

Dave Funk and the First Dual-Axis Hydrotest Team

The team executed the first dual-axis hydrotest in support of our stewardship mission, successfully obtaining five dynamic images in 2009 (with three more successful test shots in 2010). The team completed multiple complex assessments while introducing administrative and engineered controls to establish confidence in the operation of DARHT—while simultaneously performing a DARHT firing point cleanup.

Steve McCready and the ABAQUS-MCNP Unstructured Mesh Team

This team created and tested a new unstructured mesh capability that has saved several man-years worth of effort, improved accuracy of stockpile stewardship simulations, and created and tested the next generation of code interconnectivity between neutron transport and thermo-mechanical codes. New capabilities will be useful towards stockpile work, medical physics, radiation shielding, space satellites, and other applications.

Mark Chadwick and the Fission Basis Team

Multidisciplinary teams from Los Alamos and Lawrence Livermore collaborated to resolve an outstanding 35-year issue: fundamental nuclear data associated with fission-product production from fission-spectrum neutron bombardment of plutonium. Results from the work significantly impact the FY10 joint level one milestone, all of the underground test suite modeling efforts, as well as the annual assessment review from the laboratory directors.

Christopher Fugard and the Weapon Analysis Team

The Weapon Analysis Team has designed and conducted experiments and evaluations to gain a better understanding of various aspects of protecting unauthorized access to assets and ensuring positive control and protection of those assets. The team has maintained high-level computing, simulation, and data and document storage capabilities.

Becky Olinger and LANL Homemade Explosives Training Team

This team created a training program to help U.S. military personnel combat a variety of explosives they might encounter while deployed. Military personnel attend an intensive three-day course to learn how to detect and identify homemade explosive's production sites, plus characterize a wide variety of improvised-explosive compounds, their ingredients or precursors, and possible chemical or mixing equipment. One of the key tools used overseas is the LANL-developed Emergency Response Explosives Field Guide that catalogs the spectrum of energetic materials and compounds, and is in use by the Department of Defense and in-theater customers.

Robert E. Chrien and the Primary Setup Suite Team

In 2009, a group of technical staff from the Simulation Analysis and Code Development X-3, together with collaborators from X-2, X-4, T-3 and HPC-1, assembled a collection of simulations known as the Primary Setup Suite. This team's efforts resulted in the first modern setups of several events with archived simulation results, improved reliability, increased designer productivity, and enhanced the quality of simulation models.

Laura Smilowitz and the High Explosive Violent Response (HEVR) Team

In 2005, this team demonstrated the first radiographic observation of the plastic-bonded explosive PBX 9501's density evolution during a thermal ignition resulting in HEVR, enabled by a unique laser synchronization technique developed at Los Alamos. 2009 brought record accomplishments: the laser synchronization technique was considerably extended by the first application of laser synchronization to a long aspect ratio experiment in a nonsymmetric configuration.

Sven C. Vogel Fundamental Materials Science of PZT Voltage Bars in Neutron Generators

Vogel's team discovered important new physics in lead-zirconium-titanate (PZT) ceramic voltage bars that scientifically underpins reliable operation of neutron generators. The increased body of knowledge they established through clever neutron-scattering experiments substantially decreases synthesis risks. The team's discoveries also support neutron generator operations and production.

Senatorial Delegation
Visits Los Alamos

On July 30, a delegation of senators paid a visit to Los Alamos to review capabilities associated with maintaining a reliable stockpile. The senators were gathering information related to ongoing deliberations for the New START arms-control treaty with Russia.

The following senators made up the delegation: Jon Kyl (Arizona), Bob Corker (Tennessee), John Thune (South Dakota), and James Risch (Idaho), and New Mexico's Jeff Bingaman and Tom Udall

The purpose of the New START treaty is to reduce the number of strategic nuclear warheads deployed by the United States and Russia.

Senators Jon Kyl, Tom Udall, and John Thune, with Michael Anastasio

Five Los Alamos researchers receive 2010 LANL Fellows Prizes

Five Los Alamos researchers were awarded 2010 Fellows Prizes in October for exemplary scientific research and leadership. The LANL Fellows organization awarded two Fellows Prizes for Outstanding Research in Science or Engineering to Sergei Tretiak and Geoffrey S. Waldo, two Fellows Prizes for Outstanding Leadership in Science or Engineering to Kerry Habiger and Clifford Unkefer, and a Fellows Prize for Special Achievement to Tammy P. Taylor.

The Fellows Prize selection committee selected Tretiak in part for his development of organic light-emitting diodes for flexible displays, organic lasers, light-harvesting energy devices, and other important technologies. Waldo's work has been integral to securing more than $50 million in research grants at the Laboratory.

The selection committee chose Habiger for being key to creating the SUMMIT program—a rapid-response engineering organization serving the United States intelligence community. Unkefer is leader of the newly formed Bioenergy and Environmental Science Group at the Laboratory and also serves as director of the National Stable Isotope Resource funded by the National Institutes of Health. Taylor led the Nuclear Defense Research and Development Subcommittee of the National Science and Technology Council and helped create a "Roadmap"—used by the U.S. Department of Homeland Security to prioritize tasks in nuclear materials detection, forensics, and response and recovery.

Los Alamos Serves as Lead Lab at this Year's NNSA LDRD Symposium

On June 9, NNSA hosted the 2010 NNSA Laboratory-Directed Research and Development (LDRD) Symposium in Washington, DC. This year's theme was "Reducing the Global Danger of Weapons of Mass Destruction."

More than 200 researchers from the national laboratories, including Los Alamos, participated in the event, which also attracted government officials, military personnel, and members from private industry.

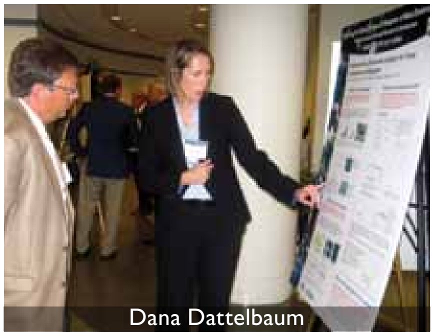

Dana Dattelbaum

PHOTO BY ROBERT SEVERI

Symposium topics covered nuclear counterterrorism, arms control and treaty monitoring, and countering biological and chemical threats. A panel of officials from NNSA and the Defense Threat Reduction Agency discussed current and future technical R&D challenges facing the nation's security from weapons of mass destruction. The symposium also included presentations and a poster session.

Los Alamos National Laboratory Principal Associate Director for Global Security William S. Reese, Jr., presented a talk about reducing global threats through innovative science and technology. Reese described the historic strengths of Los Alamos; how weapons of mass destruction cut across many areas, such as national and international infrastructure, cyber systems, space systems, intelligence, and terrorism; and the possible future missions of global security.

Also making a presentation at the symposium was Mike Rabin of LANL's International, Space and Response Division. Rabin's talk focused on the emerging science behind nuclear detection. He covered many of the sensing and analysis instrumentation under development at Los Alamos, as well as major science-driven challenges expected as instrumentation and threats continue to evolve.

The symposium's poster presentation covered many facets of global dangers. For example, Los Alamos scientist Bette Korber displayed a poster that discussed tracking the emergence of drug resistance to HIV and tuberculosis, both of which in 2008 alone caused two million deaths. Korber discussed how her Los Alamos team is working to develop innovations to track, treat, and better understand these two global killers.

Also on hand was Los Alamos scientist Marianne P. Wilkerson, whose poster addressed the molecular forensic science of nuclear materials. This Los Alamos team is working on developing analytical tools that can exploit chemistry and molecular speciation to identify the origin, intended use, and history of nuclear materials.

Los Alamos Honored with Five R&D 100 Awards

Los Alamos scientists won five of *R&D Magazine's* R&D 100 Awards, which honor the top 100 proven technological advances of the past year. Winning technologies are Movies Of eXtreme Imaging Experiments (MOXIE), DAAFox, Ultraconductus, Solution Deposition Planarization, and Ultrasonic Algal Biofuel Harvester.

"The scientific innovation and creativity at Los Alamos is exemplified by yet another set of five R&D 100 awards," said Laboratory Director Michael Anastasio. "My congratulations go out not only to this year's winners but to all eight teams chosen to submit entries, each one an example of the talent and determination of our excellent technical staff to produce game-changing science and technology in the national interest."

Developed by a team led by Scott Watson, MOXIE is the world's fastest camera that enables researchers to "see" into the unseen by imaging transient events from start to finish. The principal application for MOXIE is to create x-ray movies of mock detonations used to verify computer models, an essential component of nuclear weapon certification without nuclear testing. Other applications include studying the physical properties of materials and performing ballistic studies.

DAAFox is a new way to make an ideal secondary explosive (diaminoazoxyfurazan), one that can be used as an explosive booster for applications that require both insensitivity and enhanced performance. DAAFox is powerful (requires less explosive to achieve the same yield as other explosives), insensitive (resists accidental ignition), environmentally green (yields only salty water as a waste product), and easy to produce and scalable (one-step process produces a batch in only four hours). A Los Alamos team led by Elizabeth Francois developed DAAFox, which also won a Pollution Prevention Award from the National Nuclear Security Administration in 2009.

Ultraconductus, developed by a team headed up by James Maxwell, is a new nanotechnology designed to manufacture high-tech wires and cables that conduct electricity more easily than any other metal alloy.

Solution Deposition Planarization is an environmentally green way to produce superconducting wires that enable long-length energy transmission with zero energy loss. A team led by Vladimir Matias developed this breakthrough technology.

DAAFox

MOXIE

The Ultrasonic Algal Biofuel Harvester, developed by a team led by Greg Goddard, uses high-frequency sound to extract oils and proteins from algae in one integrated step. The harvester's end products are algal biofuels, protein (which can be used as animal feed), and easily recycled water.

Since 1978, Los Alamos has won 117 R&D 100 awards. The prestigious awards are chosen from industry, academia, and government-sponsored research.

Distinguished Performance Awards

LANL Director Michael Anastasio and the Lab's principal associate directors honored five individuals and seven teams who received LANL's 2009 Distinguished Performance Awards at multiple ceremonies in October for outstanding contributions.

Individual Recipients:

Christopher S. Fugard (IAT-3) added significantly to NNSA's understanding of the technical issues regarding potential nuclear threats; his work had an impact on NNSA's Defense Programs and Nuclear Counterterrorism efforts.

Lorenzo Gonzales (STBPO-EPDO), a Master Teacher in the Northern New Mexico Math and Science Academy—the Laboratory's community education outreach program for K-12 teachers—implemented many new teaching programs at the K-12 and collegiate levels in New Mexico.

Jagdish C. (J.C.) Laul (SB-TS), a principal safety engineer, developed the technical bases that justified establishing lower hazard designations for six nuclear and nonnuclear Laboratory sites.

Howard J. Patton (EES-17) developed and published a theory that explains the unusual surface wave energy found in the 2006 and 2009 North Korean nuclear weapons tests.

John E. Valencia (ISR-1) is a driving force behind space programs supporting the nation's nuclear nonproliferation treaty monitoring capabilities. His outstanding efforts on the GPS-III sensors ensure that the Space Nuclear Detonation Detection program is well positioned for global coverage of nuclear threats during the next 20 years.

Small Team Recipients:

B83 Peer Review Team

Biodefense Informatics Team

Fission Basis Team

Multiscale, Multiphysics Modeling and Simulations for Nuclear Fuels Team

ORCAS Hyperspectral Imager Team (proliferation detection)

Large Team Recipients:

Algal Biofuels Consortium Development Team

Fall Classic Project Team (nuclear diagnostics and validation)

H1N1 Analysis Team

MATLS-PE-09 Proficiency Test Team (nuclear forensics)

NCam Airborne Deployment Team (nonproliferation data collection)

NISC SCIF Expansion Project Team (national and global security)

Small Sample Plutonium Machining Team

Cisco Bailon and Michael Anastasio

NIF: On the Road to Ignition

The National Ignition Facility (NIF)—conceived as one of the cornerstones of stockpile stewardship—began operations in the summer of 2009. The NIF is able to heat and compress matter to temperatures and densities unattainable anywhere else on earth. The world's largest laser, NIF can deliver up to 1.8 MJ (megajoules, or one million joules) of laser light precisely into a small (≈3 mm) target. This target converts the laser energy into soft x-rays that then drive very strong shocks into the physics package within the target.

Los Alamos National Laboratory and its collaborators at the NIF are about to attempt inertial confinement fusion and create—very importantly—energy gain. The same fusion energy process that powers the sun could be our answer to power our planet. Will we unlock the stored energy of atomic nuclei and produce ten to 100 times the amount of energy required to start the fusion burn? If we can create—and therefore understand—stars, we can get answers to a plethora of questions about astrophysics (black holes, supernovas), materials science, and nuclear physics in a controlled setting. The NIF will also provide an excellent platform for understanding the physical phenomena that occur at extreme density and temperature. The NIF will not be used to generate electricity, but experiments could make fusion energy a viable source for vast amounts of energy.

In its first mission, NIF will be used to achieve thermonuclear ignition and burn in the laboratory by using those x-rays to compress deuterium and tritium fuel contained within a spherical capsule. This experimental campaign has so far addressed the energy balance within the target and determined how the capsule can be symmetrically compressed for maximum efficiency. In the next set of experiments, the timing of the several shocks that compress the capsule will be optimized and the final dimensions of the capsule and target will be tuned for optimum performance.

Using the extensive set of nuclear and non-nuclear diagnostics being commissioned, a large number of high-energy-density physics experiments in radiation flow, thermonuclear burn, mix, equation of state, and opacity, among other areas, are enabled. Los Alamos National Laboratory will commence experiments in many of these areas as the NIF becomes available.

Early this year, NIF's first experiments resulted in highly symmetrical compression of simulated fuel capsules—a requirement for NIF to achieve its goal of fusion ignition and energy gain when ignition experiments begin later this year. The test shots proved NIF's ability to deliver sufficient energy to the hohlraum to reach the radiation temperatures—more than 3 million degrees Centigrade—needed to create the intense bath of X-rays that compress the fuel capsule.

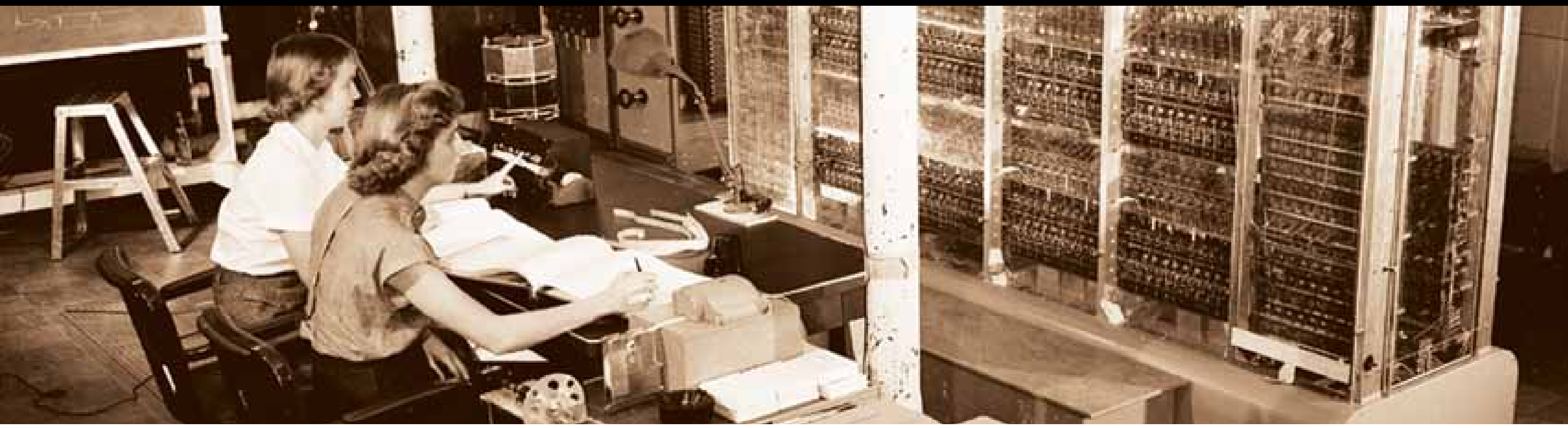
In October, the NIF completed its first integrated ignition experiment. In the test, the 192-beam laser system fired 1 megajoule of laser energy into its first cryogenically layered capsule, raising the drive energy by a factor of thirty over experiments previously conducted at the Omega laser at the University of Rochester. With the completion of this test, NIF is beginning its next phase of the campaign to culminate in fusion ignition tests.

This fall, the Project Management Institute lauded NIF with its 2010 Project of the Year award. Four NIF technologies also captured renowned R&D1 00 awards from *R&D Magazine* this year.

The NIF fusion ignition experiments are part of the National Ignition Campaign, a partnership among the National Nuclear Security Administration, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, the Laboratory for Laser Energetics, General Atomics, and Sandia National Laboratories and other national laboratories and universities.

Octavio Ramos Jr. and Kirsten Fox contributed to these news briefs.

NUCLEAR WEAPONS and the DAWN OF SUPERCOMPUTING



Today, our fastest supercomputers can perform at speeds greater than a petaFLOPS—that's one million billion operations per second. In fact, Los Alamos National Laboratory's Roadrunner was the world's first supercomputer to break the petaFLOPS barrier, as a result enabling researchers to achieve significant scientific breakthroughs.

The road toward achieving petaFLOPS performance is a very long one that started during the darkest days of World War II. In the spring of 1943, scientists from around the world gathered at Los Alamos during the Manhattan Project to design the world's first nuclear weapons. Such weapons required mathematical calculations on an unprecedented scale, so scientists turned to machines for assistance.

During the 1940s, the mechanical workhorses of the Laboratory were Marchant desk calculators and IBM accounting machines. The Marchants and IBMs successfully performed calculations pertaining to the physical properties of bomb materials, the hydrodynamics of implosion, and the potential yields of the completed devices. These calculations played an integral role in the success of the Manhattan Project.

During the war, Los Alamos staff pushed existing computing technology to its calculating limits. Scientists pondered building a full-scale computer capable of advanced calculations. A team under the direction of physicist Nicholas Metropolis built the first Los Alamos computer in 1952—the mathematical analyzer, numerical integrator, and computer (MANIAC).

Subsequent versions of the MANIAC featured enhanced speeds and employed floating-point arithmetic. Since then, the Laboratory has partnered with private industry to produce some of the world's most innovative machines. Separate partnerships with Control Data Corporation, Cray Research, Thinking Machines, and IBM have produced computers that have been recognized as the fastest in the world.

Current supercomputers at Los Alamos are used primarily to ensure the safety and reliability of the nation's nuclear deterrent. Scientists at the Laboratory also use the supercomputers for a variety of scientific applications, such as conducting medical research, modeling pandemics, assisting the nation during natural disasters, simulating astronomical phenomena, predicting global climate change, and redesigning the U.S. energy grid.

The continued need for fast, efficient, and reliable computers in the Los Alamos weapons program has largely driven the evolution of supercomputers, prompting Metropolis and Laboratory physicist Frank Harlow to write, "It is a stunning tribute to Los Alamos…that many of the most powerful procedures for taming computers to the myriad tasks of modern science and technology were developed right here…."

–Alan Carr

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July 1, 2010—Secretary of Defense Robert Gates came to the Laboratory for briefings from Director Michael Anastasio and others on LANL's warfighter program and stockpile stewardship efforts.

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