Lawrence Livermore National Laboratory

Science & Technology Review

October/November 2018

NEW LIFE FOR A LEGACY WARHEAD

Also in this issue:

Improving Earthquake Preparedness

Science-Based Emergency Planning

More Efficient Data Analysis

About the Cover

In 2014, the National Nuclear Security Administration (NNSA) selected Lawrence Livermore as the lead nuclear design agency for refurbishing the W80-1 nuclear explosives package as the W80-4 life-extension program (LEP). As the article beginning on p. 4 describes, Livermore is using its full suite of computational, experimental, and manufacturing capabilities for the LEP effort, which aims to provide the warhead with another 30 years of service life. On the cover are Livermore senior mechanical technicians (from left) Greg Sherman and Roger Bopp.

Cover design: Mark Gartland; Cover photo: Randy Wong

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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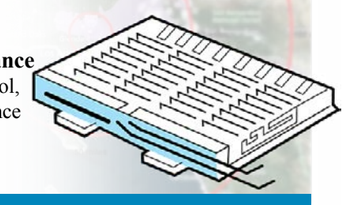

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Scientists Shed New Light on Supernovae

Livermore scientists at the National Ignition Facility (NIF) have gained new insights into the after-effects of a supernova explosion. The results of their research, which were published in the April 19, 2018, edition of *Nature Communications*, could play a role in how inertial confinement fusion and high-energy-density science experiments are conducted at the Laboratory.

When a supernova explodes, it creates an enormous shock wave with high energy flux (heat and radiation) that penetrates into the surrounding medium. When the shock reaches the end of the medium, it forms a reverse shock that runs back into the expanding ejecta material and piles up the ejecta in the high-density mass. This interface between the low-density, heated surrounding medium and the high-density mass, pressured by the shock wave, creates Rayleigh–Taylor (RT) hydrodynamic instabilities. RT instabilities play an important role in a supernova as they can change the dynamics of heavy-elements transfer from the supernova core to the surrounding medium. Similar phenomenon can occur during fusion experiments at NIF, where RT hydrodynamic instabilities can cause too much target capsule material to mix with the fuel, impeding the fusion reaction.

In the study, Laboratory physicists Hye-Sook Park and Channing Huntington, along with international researchers and colleagues at the University of Michigan, used NIF to generate high-energy radiation fluxes to determine whether the fluxes had an effect on growth of RT instabilities. The team ultimately found that the amount of heat generated by high-energy fluxes lessens mixing of the materials and therefore could reduce the growth of RT instabilities in supernova remnants. Based on their findings, Park and the research team are now ready to conduct further tests. "We can be creative about how we produce heat fluxes using the NIF laser to more closely mimic astrophysical conditions," says Park. "Many avenues of opportunity are open to explore."

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Experiments Probe Exoplanetary Cores

Using high-powered laser beams, scientists from Lawrence Livermore, Johns Hopkins University, Princeton University, and the University of Rochester have compressed iron–silicon alloys to unprecedented pressures—matching those found in the center of planets the size of three Earth masses. The measurements of the crystal structure and density of the compressed alloys have provided potential details about the interior makeup of other Earthlike planets. The research appeared in the April 25, 2018, edition of *Science Advances*.

The interior pressure of large exoplanets (ranging in size between Earth and Neptune) exceeds that at the center of the Earth by more than 10 times—beyond the range of conventional experimental techniques. Thus, the structure and composition of these planetary interiors remains largely unknown. Although scientists know that Earth's core is composed primarily of iron, research indicates that silicon is likely another major ingredient. "A pure iron core is not realistic, as the process of planetary formation will inevitably lead to the incorporation of significant amounts of lighter elements," says Raymond Smith, lead researcher from Lawrence Livermore. "Our study is the first to consider these more realistic core compositions."

The research team used the Omega laser, located at the University of Rochester's Laboratory for Laser Energetics, to compress iron–silicon alloys to ultrahigh pressures—more than 13 million atmospheres—and then direct a bright x-ray pulse into the test sample to create a diffraction pattern, which provides information on the density and crystal structure of the alloys in the sample. The pressures achieved in the experiments is more than three times the pressure at the center of the Earth and constitutes the highest x-ray diffraction measurements ever reported. Future research will be directed toward understanding how other candidate elements such as carbon or sulfur will affect the structure and density of iron at ultrahigh pressure conditions, as well as measuring other key physical properties of iron alloys needed to constrain plausible models of planetary interior structure and evolution.

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New Tool Enables Better Analysis of Chemical Bonding

Livermore scientists have developed a new open-source software application that can compute, analyze, and potentially predict the trajectories of atoms during the course of bond breaking and formation in dynamical simulations. Called TopoMS, the tool could enable breakthroughs in important research areas, such as battery storage and power. The scientists' research was detailed in the June 2018 issue of the *Journal of Computational Chemistry*.

In a multiyear initiative involving Lawrence Livermore, Lawrence Berkeley National Laboratory, and the University of Utah, scientists devised a new methodology for performing complex quantum molecular dynamics simulations on supercomputers by combining modern computational science with traditional chemistry and the quantum mechanical theory of atoms in molecules. "We combined highly accurate numerical algorithms with discrete representations that guarantee that the computational analysis is consistent with the theory of smooth functions," says Livermore computer scientist and lead code developer Harsh Bhatia.

According to Bhatia, TopoMS leverages cutting-edge methods and codes from computational topology to robustly and efficiently compute the Morse-Smale Complex, a mathematical construct used to analyze topology and characterize scalar fields. TopoMS can analyze tens of thousands of atoms at once, eliminating the need for assumptions and producing a much more robust and transferable analysis. In addition, TopoMS is so fast that it could potentially be used in tandem with actual simulations, allowing scientists to observe chemical bonding as it happens. Researchers say the next step is to integrate TopoMS with widely used simulation codes.

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Commentary by Charlie Verdon

Life-Extension Programs Require Outstanding Resources and Partnerships

ONE of the nation's most consistently challenging scientific and engineering endeavors is the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program. This science-based effort, now in its 24th year, is dedicated to ensuring the safety, security, and effectiveness of the nation's nuclear weapons. The program's record of outstanding success has resulted from the capabilities provided by high-performance computing (HPC), one-of-a-kind experimental research facilities, and the expertise of dedicated stockpile stewards at the NNSA national security laboratories and production organizations.

One of stockpile stewardship's most critical elements is the life-extension program (LEP), which extends the life of a warhead by 30 years through replacement or refurbishment of components essential to safety, security, or reliability. LEPs address issues that could lead to degradation of a weapon's performance. Such issues are discovered through routine surveillance and annual stockpile assessments and are often due to aging effects as weapons remain in the stockpile long after their originally designed lifetimes.

As the article beginning on p. 4 describes, Lawrence Livermore is actively engaged in an LEP for refurbishing the W80-1 warhead carried on the U.S. Air Force Air-Launched Cruise Missile (ALCM). The resulting W80-4 warhead will be deployed in the ALCM's replacement, the Long-Range Standoff (LRSO) missile. The W80-4 is the first U.S. warhead LEP for use with a new Department of Defense (DOD) carrier since nuclear testing ended in 1992. As a result, an important aspect of the LEP is adapting the refurbished warhead to the LRSO missile. An added complexity is that the missile is still being designed, requiring close cooperation between Lawrence Livermore and the Air Force, as well as the two contractors vying to build the LRSO. In that respect, success requires maintaining strong partnerships with the DOD, Sandia National Laboratories (our LEP partner), and NNSA.

The W80-4 LEP effort requires the full array of NNSA's computational, experimental, and manufacturing capabilities to meet all the prototyping, proof-of-concept testing, and certification requirements. The LEP takes advantage of Livermore's HPC resources to produce simulations that provide a computational surrogate for nuclear testing by modeling nuclear weapon systems with extraordinary temporal and spatial resolution.

Experiments at Livermore and other NNSA facilities play an essential role in providing the data needed to improve computational models used in LEPs. For example, National Ignition Facility (NIF) experiments offer valuable data for validating LEP design options prior to implementation. The largest and most energetic laser in the world, NIF is NNSA's preeminent high-energy-density stockpile stewardship experimental facility. Livermore's world-class experimental facilities also include the High Explosives Applications Facility (HEAF) as well as high explosives synthesis and testing facilities at our remote Site 300. Other resources at Site 300 that support LEP activities include the Contained Firing Facility, the largest indoor firing chamber in the nation.

Livermore materials scientists are mindful that some NNSA manufacturing processes are five decades old, and sustaining these legacy processes for producing LEP components presents an increasing challenge. Livermore scientists search for new processes to manufacture replacements that are less expensive, more environmentally friendly, simpler to certify, and can meet ambitious production schedules. We are working with NNSA production facilities such as the Kansas City National Security Campus to explore the potential of advanced manufacturing technologies to meet modern requirements.

While work continues on the W80-4 at a rapid pace, we anticipate resuming the W78 replacement program, which was paused five years ago to accelerate the W80-4 LEP. Clearly, Livermore stockpile stewards will be fully occupied for the next several years ensuring we meet the goals of both the W80-4 LEP and W78 replacement program. We look forward to working closely with Sandia, DOD, and the NNSA production organizations over the next decade as the W80-4 warhead and the W78 replacement warhead take shape.

■ At the time this commentary was written, Charlie Verdon served as Lawrence Livermore's principal associate director for Weapons and Complex Integration. He currently serves as deputy administrator for Defense Programs at the National Nuclear Security Administration.

S&TR October/November 2018

EXTENDING THE LIFE OF A WORKHORSE WARHEAD

Researchers are combining simulations, experiments, and manufacturing capabilities to confer another 30 years of life to the W80 warhead.

IN today's era of stockpile stewardship, no effort focuses the Laboratory's technical resources as much as a life-extension program (LEP) aimed at adding 30 years of service life to an aging nuclear warhead. In 2014, the National Nuclear Security Administration (NNSA) selected Lawrence Livermore as the lead nuclear design agency for refurbishing the W80-1 nuclear explosives package as the W80-4 LEP, setting in motion the most significant weapons development program at the Laboratory since the end of the Cold War.

The W80-1 warhead, originally developed by Los Alamos and Sandia national laboratories, is carried on the Air-Launched Cruise Missile (ACLM), which entered service in 1982. Thirty-six years later, both the missile and its warhead are well past their planned lives. The Long-Range Standoff (LRSO) missile, currently under design, will be the ALCM's replacement. LRSO, coupled with the W80-4, will be carried on the U.S. Air Force B-52 and B-21 aircraft.

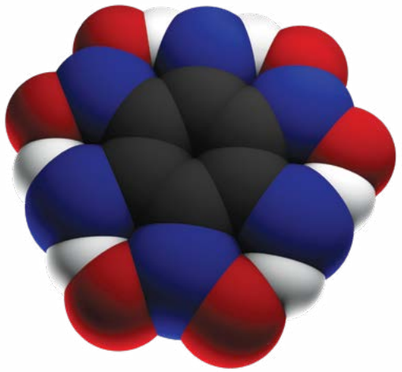
Six Decades of Experience

The full array of NNSA's computational, experimental, and manufacturing capabilities are needed for all prototyping, proof-of-concept design testing, certification, and surveillance activities required by an LEP. In particular, the program takes advantage of Livermore's high-performance computing (HPC) and experimental tools developed through the NNSA's science-based Stockpile Stewardship Program, which ensures the safety, security, and effectiveness of the nation's nuclear arsenal without resorting to nuclear explosive tests. Key capabilities also include the Contained Firing Facility (CFF), the largest

Livermore engineers (from left) Tom Horrillo, Bert Jorgensen, Veronica Harwood, and Travis Paladichuk pose with a model of the W80-4. (Photo by Randy Wong.)

indoor firing chamber in the United States; the National Ignition Facility (NIF), the world's largest and most energetic laser; and the High Explosives Applications Facility (HEAF), a Department of Energy–NNSA Center of Excellence for high explosives (HE) research and development.

Tom Horrillo is the Livermore program manager for the LEP effort and serves as the principal liaison with NNSA, other NNSA sites, and the Department of Defense. "We have a very good and close working relationship with Sandia National Laboratories, NNSA, and the U.S. Air Force," says Horrillo. He notes that other sites across the NNSA complex will participate in production of the W80-4 warhead. Livermore scientists and engineers are collaborating with Sandia, the lead (nonnuclear) engineering laboratory for the LEP, and the NNSA production plants to develop options for replacing aging components and materials, including new manufacturing methods that minimize costs, increase throughput, and reduce the use of environmentally sensitive materials and processes.



Triaminotrinitrobenzene (TATB) is an insensitive high explosive that will be used for the warhead's main charge. Livermore engineers and chemists are helping to restart the TATB production process after 30 years of dormancy. (Rendering by Adam Connell.)

Horrillo notes the refurbished warhead will not introduce any capabilities that do not already exist in the nuclear stockpile. However, the W80-4 warhead will incorporate modern electronics and safety features and use nonnuclear component technologies and designs developed for other LEPs to limit costs and risks. The effort also involves developing a booster that supports safety enhancements and restarting production of triaminotrinitrobenzene (TATB) for the warhead's main charge. "The W80-4 is projected to go out of service in the 2060s," says Horrillo. "Since some warhead parts will be in use for about 80 years, we will need to assess them every year to ensure they meet their original specifications."

Missile Interface Is Critical

The W80-4 is the first U.S. warhead designed for use with a new carrier since nuclear testing ended in 1992. As a result, an important aspect of the LEP effort is adapting the refurbished warhead to the LRSO missile. The complexities of designing a new missile in parallel with extending the life of the warhead demand close cooperation with the Air Force. Two U.S. contractors, Lockheed Martin and Raytheon, are competing for the contract to build the LRSO missile—the Air Force will decide the winner during the 2022 fiscal year (FY). Says Horrillo, "Lawrence Livermore and Sandia have the responsibility for defining and validating the interface between the warhead and missile." Livermore and Sandia engineers meet regularly with representatives from the Air Force and both contractors to review interface issues.

The W80-4 warhead (depicted in this artist's rendering) is being developed in partnership with the Department of Defense and will serve the nation into the second half of the century. (Rendering by Adam Connell.)

Anatomy of a Life-Extension Program

After nuclear testing ended in 1992, the United States began extending the life of existing warheads rather than developing new ones. The science-based Stockpile Stewardship Program, established in 1994, is based on advanced simulations and experiments conducted at the National Ignition Facility and elsewhere within the National Nuclear Security Administration complex to provide improved knowledge of the underlying physics and engineering of modern U.S. nuclear weapons in the stockpile.

A critical part of stockpile stewardship is the life-extension program (LEP), which aims to reuse, replace, or redesign aging components that are reaching the end of their service life and therefore require modernization to ensure they remain safe, secure, and effective. Reused components are requalified to go back into a weapon without change. Components determined to be past their original service lives are remanufactured to their original specifications, and if they cannot be remade to those specifications (because the materials are no longer available), they are redesigned using modern materials and manufacturing technologies. LEPs may also use advanced technologies to enhance safety and security characteristics.

Lawrence Livermore scientists and engineers are responsible for the nuclear explosives package for LEPs and must certify the life-extended warheads as they enter the stockpile. Certification of the life-extended warhead is accomplished by extensive component testing, warhead simulations that model the integration of the warhead into the missile, and high-fidelity flight tests. LEPs typically extend the operational lives of weapons by 20 to 30 years.

In the 1990s, Lawrence Livermore scientists, engineers, and technicians began the first LEP, which was undertaken for the W87 ballistic missile warhead. In addition to the current W80-4 LEP effort, Livermore has been assigned to the replacement program for the W78 warhead deployed on the Minuteman III ballistic missile. That effort will resume in the 2019 fiscal year following a five-year hiatus. As with the W80-4 LEP, the planned replacement program for the W78 represents an important opportunity to extend the warhead's service life and incorporate modern safety and security features.

At Site 300, several facilities subject prototype components to vibration, shock, impact, acceleration, and extreme temperatures. Shown here, an engineer prepares for a laser vibrometer to measure noncontact vibration of a W80-1 test component. (Photo by George Kitrinos.)

One aspect of the W80-4 LEP is a program management process that closely tracks costs and technical progress. The process is an outgrowth of findings from previous LEPs, recommendations of multiple NNSA reviews, and industry best practices. Called the Earned Value Management system, the process is designed to ensure more accurate cost estimation and timely delivery of LEP milestones through the "6.X" process, which includes design, development, systems integration, testing, production, and surveillance.

The LEP process begins with Phase 6.1 (concept assessment), which for the W80-4 program commenced in 2014. The following year, the team started Phase 6.2 (feasibility study and design options). In October 2017, the program transitioned to Phase 6.2A (design definition and cost study) to establish detailed cost estimates for all design options. This phase is scheduled to conclude during FY 2019, when program representatives present the team's final design recommendations to the Nuclear Weapons Council. During Phase 6.3 (design engineering),

Technicians know as "ramrods" set up an experiment inside the Contained Firing Facility (CFF), the nation's largest indoor firing chamber. Hydrodynamic experiments at CFF create extreme temperature and pressure conditions to assess the performance of nonnuclear weapon components for life-extension programs (LEPs). (Photo by George Kitrinos.)

scientists and engineers will ensure the warhead meets military requirements. Phases 6.4 (production engineering) and 6.5 (first production) will begin in FY 2022 and FY 2025, respectively, and Phase 6.6 (quantity production and stockpile) will begin in FY 2026.

Facility Modernization Is Key

The experimental campaign for the W80-4 requires robust part and material testing to meet manufacturing and inspection requirements. To support the timely execution of LEP activities, NNSA's Capabilities-Based Investment (CBI) Program has funded a wide range of programmatic equipment recapitalization worth about $75 million. In addition, NNSA's Office of Safety, Infrastructure, and Operations has funded an array of facility improvements worth more than $100 million over the last five years. These investments are aimed at modernizing both the equipment and buildings at Livermore's main site and its remote Site 300, which is located some 32 kilometers away. (Many Lawrence Livermore facilities are 50 years old—or older.) Travis Paladichuk, who leads a large group of engineers assigned to the LEP effort, says that the infrastructure supporting the W80-4 LEP is in high demand. He adds, "We do not have much capacity to spare. Our machine shops are extremely busy."

The LEP effort uses most of Site 300's testing and engineering facilities. The extensive range of tests conducted at the site provide confidence in the performance of W80-4 LEP design options. One type of test simulates the potential environmental conditions a weapon may experience. Prototype HEs, detonators, and other nonnuclear components are subjected to vibration, shock, impact, acceleration, and extreme heat and cold. Other investments in advanced diagnostics provide enhanced data from experiments. For example, CFF hydrodynamic tests combined with the high-energy diagnostic known as the Flash X Ray provide data to assess the science and operation of nonnuclear weapon components for LEPs. (See *S&TR*, July/August 2018, pp. 20–23.) These tests use surrogate metals in place of nuclear materials and create temperatures and pressures so great that solids behave similarly to liquids. Results of hydrodynamic tests help scientists refine computational models that simulate nuclear weapon performance.

At Livermore's main site, investments have been focused at HEAF—incorporating computed tomography and other advanced diagnostics—and at several key engineering facilities. In addition, a 31-ton, state-of-the-art hydraulic press, called a hydroform, was brought online in 2016 as part of the CBI Program. The hydroform is used to build nonnuclear parts for LEP-related experiments. The computer-controlled machine replaces a manually operated hydroform and offers higher part throughput and improved repeatability with reduced material waste.

Analysis of Aging Materials

The W80-4 must be effective for three decades, thus a critical task of the LEP is understanding how the warhead's constituent parts will age and assuring that those aging processes will not significantly degrade performance of a particular component or one located nearby. "We will be putting old and new parts together in the refurbished warhead," says lead materials scientist Pat Allen. "In particular, new materials, especially those produced with advanced manufacturing processes not available two decades ago, require careful accelerated aging and compatibility testing." Allen explains that a polymer, for example, may emit low levels of residual water over time as it ages. He says, "We need to know whether the water could affect other parts of the system, or if a very small amount of water proves harmless."

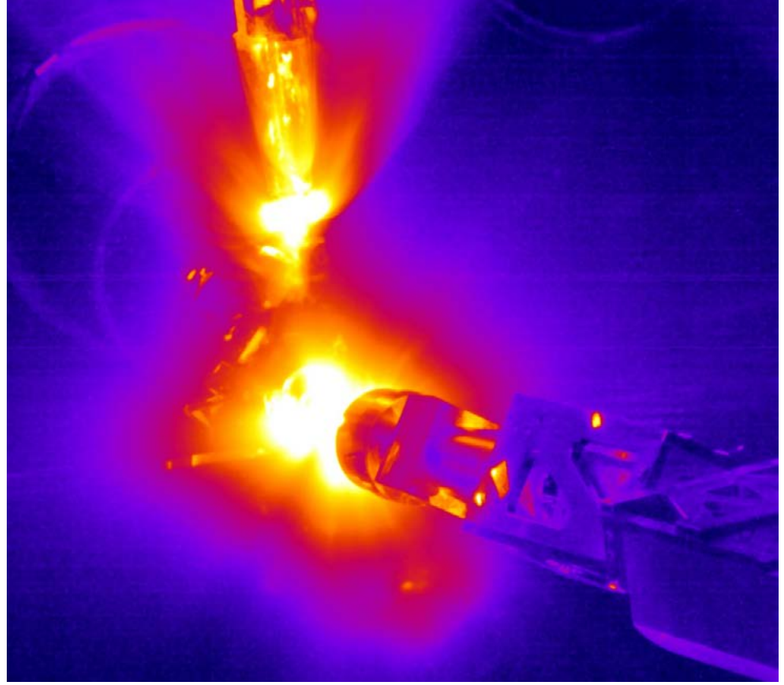
Researchers have at their disposal two types of controls for accelerated aging tests. The first is temperature, to accelerate chemical reactions by "cooking" materials at elevated levels. The second is radiation, for approximating the exposure effects to parts over their 30 years in close proximity to special nuclear materials. Allen notes that data gathered from accelerated aging tests are supplemented with computer models, which through the years have helped scientists predict the behavior of aging materials and mitigate potential aging issues.

Starting Up HE Production

For added safety, the W80-4 will use a modern initiation train to set off the HEs that ultimately lead to nuclear detonation. This system includes a detonator, booster, and the main HE charge, each of which uses different HE formulations (explosive molecule and inert binder). Veronica Harwood, lead HE engineer for the LEP, notes that once the W80-1 warheads are disassembled, the legacy HE cannot be reused.

The main charge uses PBX 9502, which consists of TATB and binder. TATB is an insensitive high explosive (IHE), which means it has greatly lessened the possibility of accidental initiation from heat, shock, bullet impact, electrostatic discharge, or other unplanned stimuli. Livermore engineers and chemists have been working to restart the TATB production process after 30 years of dormancy because not enough of the material exists in reserves for the forthcoming W80-4 warheads. The goal is to manufacture TATB with the same performance characteristics as the W80-1. Unfortunately, many of the production details from three decades ago have been lost.

Machinists Wes Scoggins (left) and Ron Cabeceiras examine a steel sheet before pressing it into a test part with a new hydroform, the key tool for building experimental parts for the W80-4 LEP. (Photo by Julie Russell.)



Experiments conducted at the National Ignition Facility (NIF) are uniquely capable of informing and validating three-dimensional weapons-simulation computer codes that support the W80-4 LEP effort. This NIF experiment was aimed at developing a high-pressure strength measurement capability for plutonium.

Livermore chemists have analyzed more than 50 pilot-scale batches of TATB to establish a reproducible set of manufacturing conditions. “We want to understand how the physics performance relates to synthesis parameters,” says Harwood. Conditions such as different stirring rates and the scaleup to 1,000-gallon production equipment can affect the size and morphology of TATB particles. Harwood notes that subsequent LEPs will also rely on PBX 9502 formulated using the newly produced process. As a result, the Livermore team has been diligently documenting how the newly synthesized TATB’s manufacturing details affect its performance.

Separately, a research team is preparing a new HE booster with improved safety performance. The LX-21 booster is an IHE “candidate” and consists of LLM-105, an energetic molecule developed at Livermore. In another effort, the detonator will use the explosive LX-16, a Livermore formulation. Paramount to the HE research and development program are HEAF and Site 300 facilities that support synthesis, formulation, processing, testing, and evaluation of newly manufactured HEs. A small plant for producing TATB and LLM-105 is planned for Site 300.

Simulating by the Nanosecond

As the nation’s weapons age long past the point at which the designers assumed they would be replaced, Livermore scientists must assess their performance with the highest possible level of confidence. Simulations conducted as part of NNSA’s Advanced Simulation and Computing Program offer a computational surrogate for informing judgment on weapons behavior, which was historically done via simulations combined with nuclear testing. Simulations model much of the complexities of nuclear weapon systems and provide a clearer understanding of the factors affecting weapons performance. Three-dimensional (3D), high-fidelity simulations allow physicists to more clearly observe phenomena at nanosecond-scale resolution.

Scientists combine extensive experimental data with computer simulations to understand and assess the safety and performance of refurbished and new components. For example, a family of increasingly accurate computer codes predicts the performance of new energetic material formulations, as validated with experiments. In addition, accurate simulations help reduce design iterations compared to building and testing prototypes. The large number of simulations is also driven by the requirement that the refurbished warhead be compatible with the LRSO missile.

In all, LEP-affiliated simulations consume about 40 percent of Livermore’s enormous classified supercomputer capacity. Sierra, the Laboratory’s next-generation supercomputer, with a peak speed of 125 floating-point operations per second, will play an important role in assessing W80-4 performance and LEP certification.

192 Beams of Light

NIF experiments strengthen the technical foundation of the W80-4 LEP and inform design and material options. The most extreme conditions that can be created in a laboratory are in the high-energy-density (HED) regime, where materials often behave in unexpected ways. NIF makes it possible to test materials in HED regimes formerly inaccessible to scientists.

Physicist Seran Gibbard conducts HED experiments at NIF that focus on determining materials’ equation of state (EOS)—that is, the relationship between pressure, temperature, and density. Data from these experiments help advance scientific understanding and refine supercomputer models. Gibbard notes that the LEP efforts involve replacing legacy materials with counterparts made using new processes. “With EOS experiments, we heat the material, run a shock wave through it, and see how the material responds. We test legacy and new materials simultaneously, so we can directly compare the two.”

Gibbard also conducts a second type of NIF experiment that studies the behavior of new materials exposed to radiation for determining whether the inevitable impurities found in every material could affect performance. In both EOS and radiation experiments, NIF laser beams typically strike the inside of a hollow gold-lined cylinder called a hohlraum and produce x rays. For EOS tests, the x rays heat the material and create a shock, and for radiation experiments, the x rays penetrate the materials under study.

Approximately a dozen NIF tests are conducted yearly that support the W80-4 LEP. Together, data generated from NIF experiments and accelerated aging tests help to inform and validate 3D weapons-simulation computer codes and facilitate a broader understanding of important weapons physics. Says Gibbard, “In the absence of nuclear testing, NIF is the only experimental facility that can produce the energy levels we require for capturing the necessary data.”

Where Art and Necessity Meet

The physicists and engineers working on the W80-4 LEP are presented with a formidable challenge. They must be able to confidently certify that the myriad parts of the life-extended warhead will have the desired performance. The key to addressing this difficult task is what Livermore design physicists call “the art of design.” Mike Dunning, acting principal associate director for Livermore’s Weapons and Complex Integration Principal Directorate, says, “The designer must fully grasp the objectives of the LEP effort and make them happen.”

Dunning explains that the art of design is knowing how to differentiate between needing to solve a problem directly and getting around it without compromising performance or safety. “Sometimes we have to understand the chemistry or physics in exquisite detail. Other times we can design around a particular challenge by avoiding areas we do not comprehend as well as we would like.” In addition, designers must also be mindful of what can be accomplished within the NNSA production complex.

> **“The W80-4 is projected to go out of service in the 2060s. Since some warhead parts will be in use for about 80 years, we will need to assess them every year to ensure they meet their original specification.”**

According to Dunning, experienced designers know how to navigate this complicated landscape. A particular necessity is training new people to be “navigation” experts, especially the hundreds of scientists and engineers hired in the past few years to help meet the Laboratory’s growing national security responsibilities. In this respect, the W80-4 LEP affords people an opportunity to exercise existing skills and learn new ones by conducting experiments at NIF and other one-of-a-kind facilities at the Laboratory.

Dunning observes that many members of the W80-4 team have been at Lawrence Livermore for less than a decade and are working alongside more experienced staff on the program. “Very few people at the Laboratory have LEP experience,” says Horrillo. “We are training a whole new generation.” Lead program engineer Paladichuk notes that almost all engineers working on the W80-4 are participating in their first LEP. “We have a lot of learning and training to do,” he says. Toward this end, the engineering team has been reviewing lessons learned from other stockpile stewardship efforts and previous LEP activities.

Lead HE engineer Harwood notes that when the LEP started three years ago, the Laboratory had to hire much more staff—from chemists to machinists—in support of the HE effort. She says, “These are truly stellar people,” who nevertheless must be trained in new skills and taught the technical knowledge that was not offered in academia. “We are exercising every aspect of our HE capabilities in training the next generation. We want to lay a strong foundation for the next LEP.”

From infrastructure investment to research and development and workforce management, the W80-4 is no small undertaking. Horrillo notes that the fiscal and staff resources required to support the LEP are significant. However, the payoffs are equally significant: ensuring the nation’s nuclear deterrent force remains safe, secure, and effective; enhancing scientific understanding of materials under extreme conditions; advancing new manufacturing processes; and ultimately ensuring the next generation of stockpile stewards is ready and waiting in service to the nation.

—Arnie Heller

Key Words: air-launched cruise missile (ALCM), Capabilities-Based Investment (CBI) Program, Contained Firing Facility (CFF), Earned Value Management system, High Explosives Applications Facility (HEAF), life-extension program (LEP), long-range standoff (LRSO) missile, National Ignition Facility (NIF), National Nuclear Security Administration (NNSA), Sierra, Site 300, Stockpile Stewardship Program, triaminotrinitrobenzene (TATB), W80-1, W80-4.

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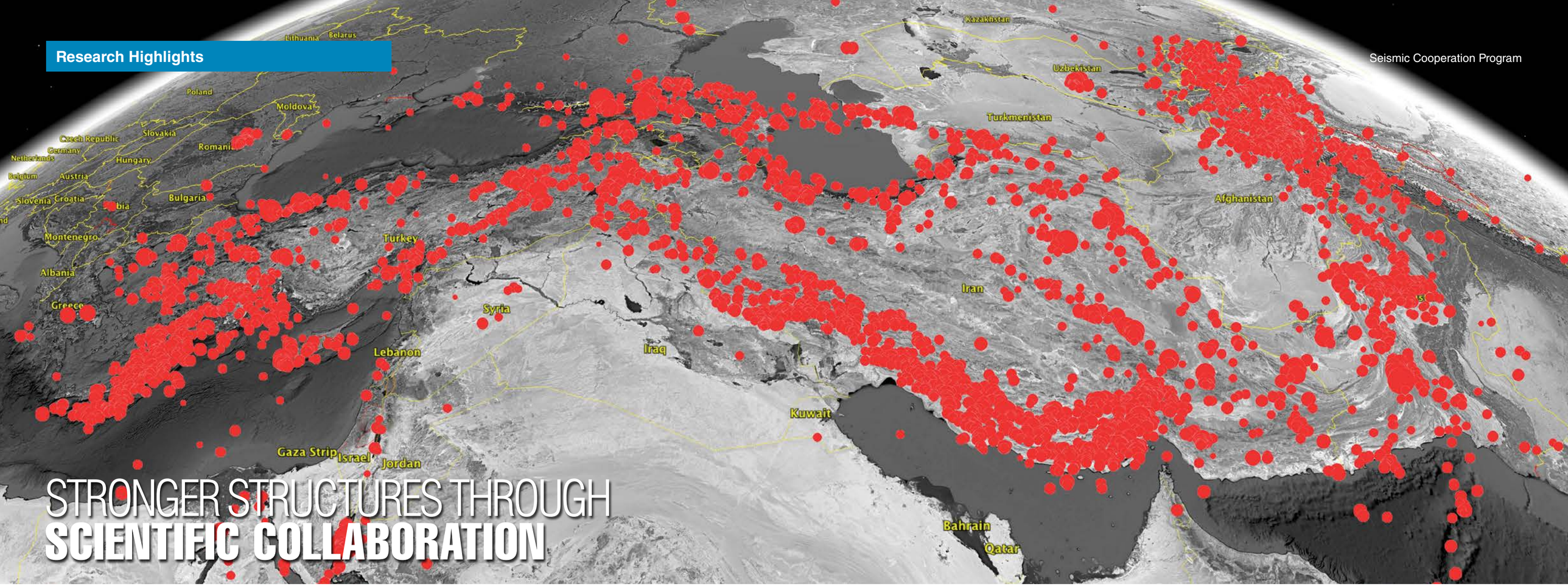


STRONGER STRUCTURES THROUGH SCIENTIFIC COLLABORATION

IN August 1999, Turkey experienced a 7.4-magnitude earthquake—one of the most devastating seismic events of the 20th century. The earthquake wreaked havoc on the major city of Izmit (located 104 kilometers from Istanbul), killing an estimated 17,000 people and leaving another 500,000 homeless. This disastrous event, along with a second 7.2 earthquake in November that same year, demonstrated to the country—and the world—the need for resilient infrastructure and adequate building codes.

To help at-risk countries improve earthquake monitoring capabilities, implement suitable seismic building codes, and plan disaster response, Lawrence Livermore established its Seismic Cooperation Program (SCP). Funded by the National Nuclear Security Administration and led by Laboratory seismologist Rengin Gok, the program gives countries an opportunity to limit the potential for catastrophic loss if an earthquake should occur.

Predicting the Unpredictable

Seismologists use various resources to forecast earthquakes and predict their possible strengths and repercussions. These resources include records indicating the locations of past earthquakes and active faults as well as analyses and models of ground motion characteristics. Most importantly, calculations of moment magnitudes, a measurement of the size of an earthquake based on its maximum wave amplitude, provide the most reliable measurement for an earthquake's size. Using this diverse information, seismologists can perform area-specific probabilistic seismic hazard assessments (PSHAs) that inform seismic provisions in building codes—mandatory requirements for ensuring a structure's integrity. "All buildings should be built according to these standards," says Gok. "Past earthquakes have shown that modern building codes significantly reduce injury, death, and economic loss to communities."

As part of SCP, Gok works with Livermore colleagues and a private sector collaborator, seismic hazard and risk consultant Dr. Tuna Onur, to conduct PSHAs and provide long-term support to local seismologists and engineers in target regions, including the Middle East, Caucasus, and Central Asia. PSHAs are conducted in two phases. First, researchers identify the tectonics and faults

(above) Target regions for probabilistic seismic hazard assessments (PSHAs) include Iraq, the Caucasus, and Central Asia. This image shows the locations of all earthquakes in the area that have had a magnitude greater than 5.0 since 1970. (Image courtesy of Google). (left) The 1999 Izmit earthquake in Turkey was one of the most devastating seismic events of the 20th century. As shown here, the violent shaking caused buildings to collapse, leading to the deaths of an estimated 17,000 people. (Photo courtesy of the U.S. Geological Survey.)

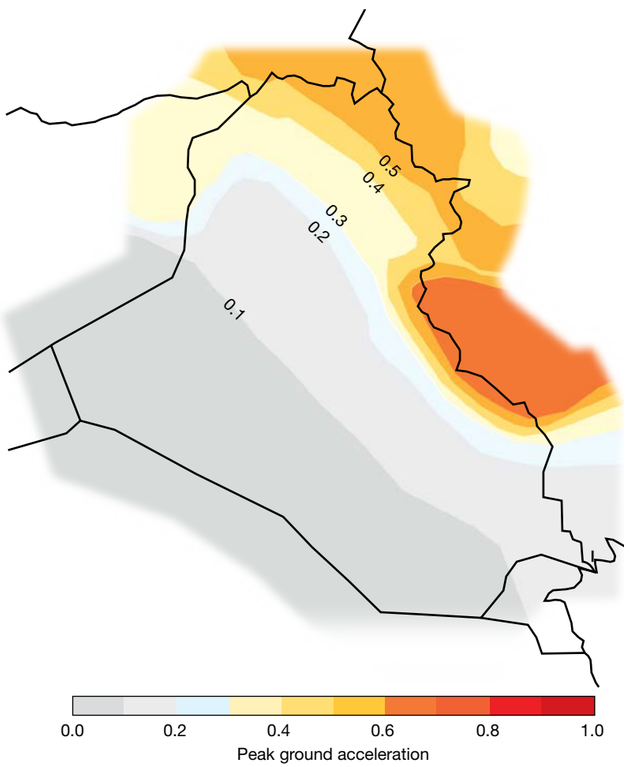
in a region and begin to compile an earthquake catalog, which documents the dates, locations, and times of past earthquakes. Second, seismic sensors, such as accelerometers, are implemented in the target region to monitor and analyze strong ground motions. Together, these data are used to help improve existing building codes to minimize the probability of structural collapse.

A Successful Case Study

A prime example of PSHA planning and implementation was work done by Gok and colleagues over the last few years in

Iraq. At the start of the project, the most updated version of the country's national building code dated back to 1997. The code was primarily based on general ground motion prediction equations (GMPEs) and an earthquake catalog that lacked the last 20 years of seismic activity.

To develop a more cohesive and accurate moment magnitude–based catalog, Gok and the team first looked at "pre-instumentation" earthquake data, such as historical written records, to help understand the country's seismic past. Says Gok, "Part of the PSHA effort is enabling countries to engage with historic information as a way of creating modern building codes." This information helps pinpoint potential source locations for future earthquakes. The team also looked at existing earthquake catalogs



A seismic hazard map for Iraq estimates peak ground acceleration (as a fraction of acceleration of gravity) with a 2 percent chance of exceedance in 50 years. Areas that are most vulnerable to shaking are marked by a darker gradient. This information will be used to modernize the country's building code to improve structural integrity.

that contained instrument-derived data over time, starting with the *Bulletin of the International Seismological Centre*.

For earthquakes occurring after 1989, the team applied the Coda Calibration Tool (CCT), created by Livermore developer Justin Barno, to calculate reliable moment magnitudes for small-to-moderate-sized events. In seismology, coda waves are the residual vibrations post-earthquake that decay slowly and uniformly with time. In coda calibration, scientists measure the wave amplitudes at multiple frequency bands to determine source spectra at each seismic station in a particular region. CCT improves existing catalog magnitudes for PSHAs and provides a rapid and robust estimate of these features for the operational needs of seismic centers worldwide. The combination of these data results in a well-rounded and streamlined seismic record.

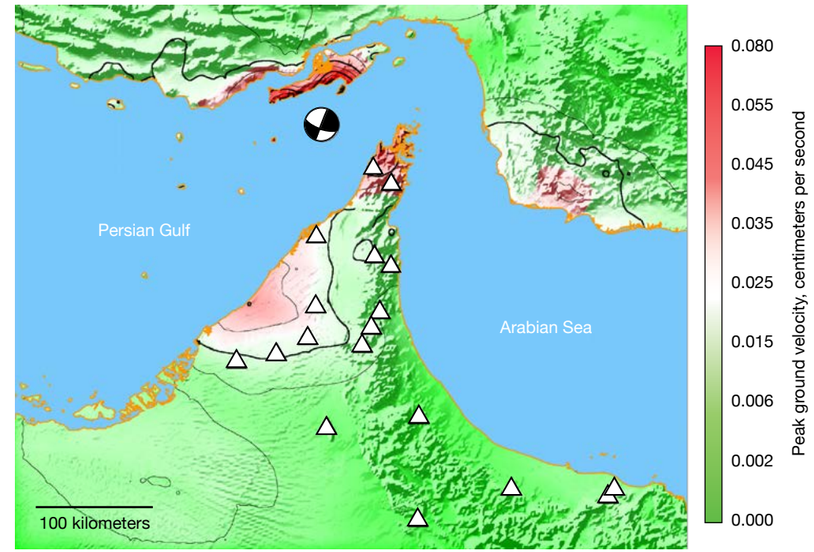
As part of the second phase of the PSHA effort in Iraq, Gok's team installed equipment to measure both strong and weak ground motions in the target regions. Pending data from the instruments, the team used globally derived GMPEs that factor in local attenuation characteristics (the gradual weakening of seismic waves as they move away from their source) with attenuation tomography for the assessment. Together, past records, new measurements, and improved data through instrumentation serve as the basis for Iraq's comprehensive earthquake catalog (published in 2017) and will factor into the seismic provisions of the country's updated building code.

All this information is incorporated into a probabilistic framework to perform a PSHA and prepare seismic hazard maps for the new building code. Engineers calculate the forces that the building should withstand using the mass of the building and the accelerations from the earthquake shaking. The probabilities are helpful to determine acceptable risk levels. For example, a "2 percent chance of exceedance in 50 years" means that in the lifespan of a building (assumed to be 50 years on average), the actual earthquake shaking that will occur has only a 2 percent chance of being higher than the load levels that the building was constructed to resist.

In addition to completing Iraq's PSHA, SCP held local training workshops and has continued to collaborate with seismologists and engineers in the area to help facilitate local adoption and document ownership and management of Iraq's seismic data. Says Gok, "If we have trained local seismologists, geologists, and engineers to perform the hazard analysis, produce new seismic hazard maps, and enable the country to formally incorporate these maps into building codes, then we can consider the process a success."

A Closer Look at Simulating Ground Motions

"In some cases, such as when large, three-dimensional topographical variations exist in a populated city, a PSHA is not enough to estimate earthquake ground motions and their effects," says Gok. "In such cases, we use high-performance computing (HPC) to produce records of strong ground motion



Seismologists simulated the long-period ground motions of a 5.9-magnitude earthquake on the island of Qeshm in the Persian Gulf. Triangles represent seismic stations while the circle reflects the direction of the pushing (black) and pulling (white) forces in the region.

that can be used to generate GMPEs." For example, the team used HPC systems to generate data for a 5.9-magnitude earthquake on Iran's largest island—Qeshm—in the Persian Gulf, which occurred on September 10, 2008. Using the Livermore-developed SW4 (seismic waves 4th order) computer code, SCP seismologist Arben Pitarka simulated long-period ground motions (5–20 seconds) for a broad region of the Persian Gulf affected by the event.

The SW4 code accurately models the surface topography of a region and the structural heterogeneity effects of an earthquake on elastic wave propagation—that is, the process by which particles are displaced by an external force and then restored to their original position by an equally proportional force. The seismic velocity (wave propagation speed) model used in the simulations covered a 700-square-kilometer area, including parts of both the Gulf and the nearby Zagros Mountains, producing waveforms that allowed scientists to create a map of the ground motions. The study revealed that an earthquake stemming from the Gulf could produce large ground motions at both the epicenter of the earthquake and along the eastern shore of the Arabian Peninsula because of the amplification caused by the area's subsurface topography.

Building Better Community Relations

Another important result of SCP's work has been facilitating multilateral, regional collaboration among countries. "Teamwork is important because many of these countries share fault lines," says Gok. "They have to work together to prepare for earthquakes." The results align well with Gok's goals for the project: improved earthquake disaster management through international partnerships, scientific data exchange, and promotion of science-based research. "You can change people's lives with science," she says.

Looking forward, Gok wants to conduct a PSHA in Central Asia after wrapping up work in the Caucasus region, for which a comprehensive earthquake catalog study is nearly complete. In Central Asia, the team has thus far conducted three PSHA workshops—in Kazakhstan, Kyrgyzstan, and Tajikistan—and received positive feedback from participants, including seismologists, geologists, and engineers. Paper records of instrumental seismicity in Central Asia go back to the 1950s, so Gok's team is working to make those records more accessible. Says Gok, "We are digitizing millions of data entries using web-based tools in collaboration with local experts. These entries will help identify active earthquake zones and prepare realistic hazard maps."

According to Gok, the work done by the PSHA team to aid countries in modernizing building codes and to better understand seismic risks in their regions is an important and necessary endeavor. She says, "People ask us why we bother conducting these assessments when we don't know when an earthquake will strike." For Gok, the answer is simple and sobering. "By determining the important seismic parameters generated through PSHA efforts, countries can better protect their infrastructure and their citizens. Earthquakes don't kill people, structures do."

—Lauren Casonhua

Key Words: building code, Coda Calibration Tool (CCT), earthquake, earthquake catalog, ground motions, moment magnitudes, probabilistic seismic hazard assessment (PSHA), Seismic Cooperation Program (SCP), seismology.

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A SCIENCE-BASED TOOL FOR EMERGENCY PLANNING

THE Scout motto "Be prepared" applies to many fields, including federal, state, and city emergency preparedness. For several decades, Lawrence Livermore researchers have helped federal emergency officials and their state and local counterparts gain a better understanding of the science behind natural and human-caused disasters. (See *S&TR*, April/May 2015, pp. 4–13.) As a part of that effort, Livermore engineer Maureen Alai and a team of Laboratory engineers, computer scientists, and health physicists have recently developed a planning resource that can assist local governments in determining the best actions to take following the detonation of an improvised nuclear device (IND).

The IND City Planner Resource (iCPR) grew out of an earlier request from the Federal Emergency Management Agency (FEMA) and other Department of Homeland Security (DHS) agencies to further the science-based understanding of what to expect from an IND detonation. Several years ago, DHS—which provides technical guidance for regional, state, and local authorities that prepare IND response plans—asked the Laboratory to develop a detailed assessment of how U.S. cities and regions could prepare for a hypothetical scenario in which a 10-kiloton (kt) IND detonates. Such a device would release energy equivalent to 10,000 metric tons of TNT. At the time, little science-based research existed on the likely effects and best mitigation strategies for a low-yield, ground-level IND detonation in a modern U.S. city.

Working with other national laboratories, technical organizations, and federal agencies, Lawrence Livermore demonstrated that local planning could save thousands of lives. The analyses, which originally focused on seven major U.S. cities, were well received and highly valued by the areas' emergency planners. The success of this work prompted other cities and regions to request their own evaluations. However, a detailed city-specific analysis took approximately one year to complete, making it difficult to meet the growing demand for "more." Born from this need, iCPR provides U.S. cities and regions a less costly, more efficient tool for developing response protocols.

Doing More for Less

The genesis of iCPR began when FEMA and DHS's Science and Technology National Urban Security Technology Laboratory (NUSTL) asked Livermore to explore ways of providing faster, more cost-efficient analyses for emergency planners. As part of the effort, Alai and the research team were tasked with developing a tool that provided in-depth analyses for 60 major cities under 2 IND scenarios—1-kt and 10-kt ground detonations. Alai, along with colleague and materials scientist Amy Waters, proposed a standardized modeling and post-processing approach to develop a web-based tool for providing city-specific, scientifically based IND effects information. The approach leveraged the Laboratory's computer science expertise and the modeling system at the National Atmospheric Release Advisory Center (NARAC). FEMA and NUSTL accepted their proposal, co-funding a three-year project to develop iCPR.

In the project's first phase, Alai and computer scientist Lisa Belk in Livermore's Computation Directorate defined the planning tool's requirements. Alai explains, "We talked with stakeholders to define their needs and evaluated available FEMA-developed information analysis briefs (IAB), which are used to develop emergency plans and operational strategies." Alai and Belk also defined model, software, scenario, and product requirements. For instance, users wanted animations showing fallout effects evolving over time. They also wanted data on the protection provided by buildings at various locations to better plan evacuation strategies.

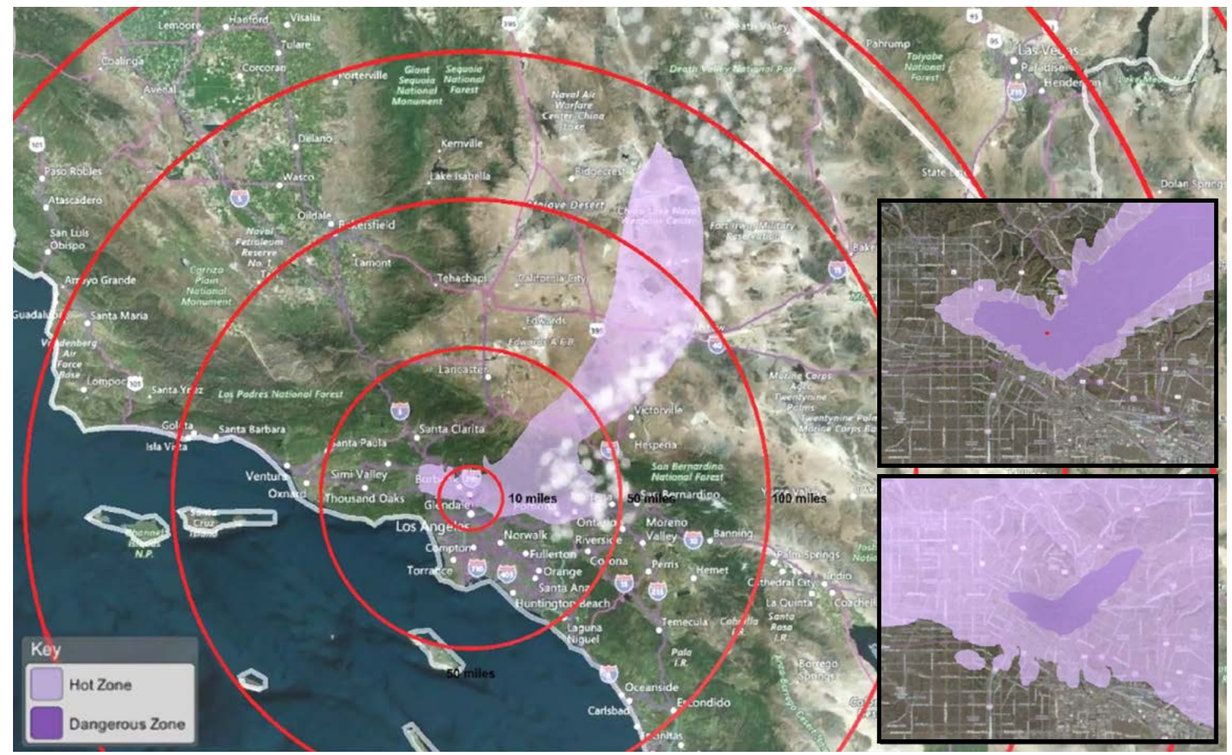
Livermore's Brooke Buddemeier, a certified health physicist, was the architect of the earlier city planning assessment strategy. The resulting documents from that effort provided key planning factors to

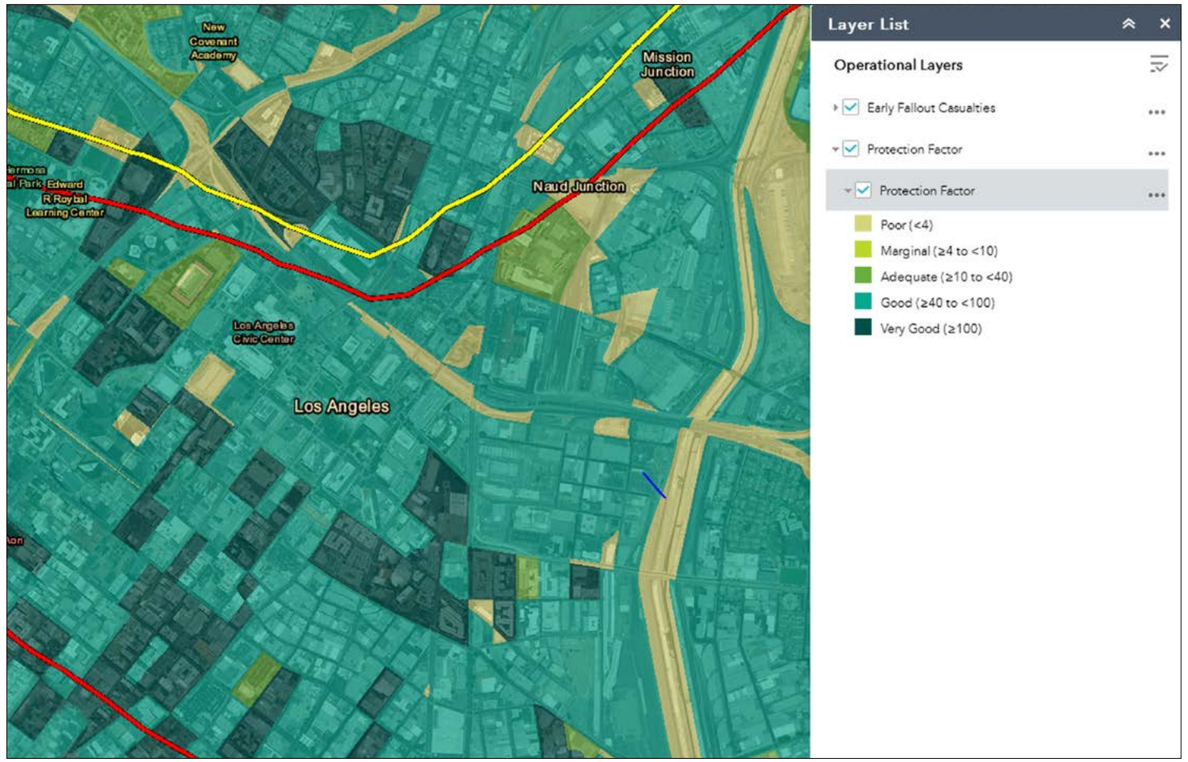
substantially aid the response and recovery process by accelerating the speed of execution, improving public health and safety, and addressing major resource limitations and critical decisions before an incident. The technical foundation for iCPR stemmed from this previous work. Ultimately, a successful iCPR tool needed to provide users with several key features: an IND's prompt and delayed effects (to guide evacuation planning); potential impacts to critical infrastructure and key resources, such as power grids and hospitals (to determine the availability of resources); building protection factors (to show how sheltering in structures could affect radiation doses from fallout); and injury and casualty information (to help ascertain the medical needs of victims).

Alai, computational engineer Stephanie Neuscamman, and statistician Kristin Lennox also identified two "uncertainty drivers" for the scenarios—terrain and weather. Alai explains, "Since the fallout cloud forms into the atmosphere's upper levels, we initially speculated terrain might be unimportant in how fallout patterns evolve. Models and simulations showed differently. Based on this information, we set aside a simpler dispersion model in favor of a more complex one." As expected, weather was a key driver for correctly modeling the IND fallout effects. The team tested and applied a statistical technique to 10 years of vertical weather data, obtaining the cities' predominant weather patterns for each of the 4 seasons and over a 12-month period.

The project's second phase involved incorporating the weather patterns into fallout and nuclear blast models for the 60 iCPR cities using NARAC's modeling system. A federal facility located

To help cities prepare and plan for the potential detonation of an improvised nuclear device (IND), the IND City Planner Resource (iCPR) provides downloadable animations that show how fallout radiation's effect on an area evolves over time, from detonation out to one year. This hypothetical example illustrates plume projections (top right) 55 minutes and (bottom right) 11 hours after detonation.



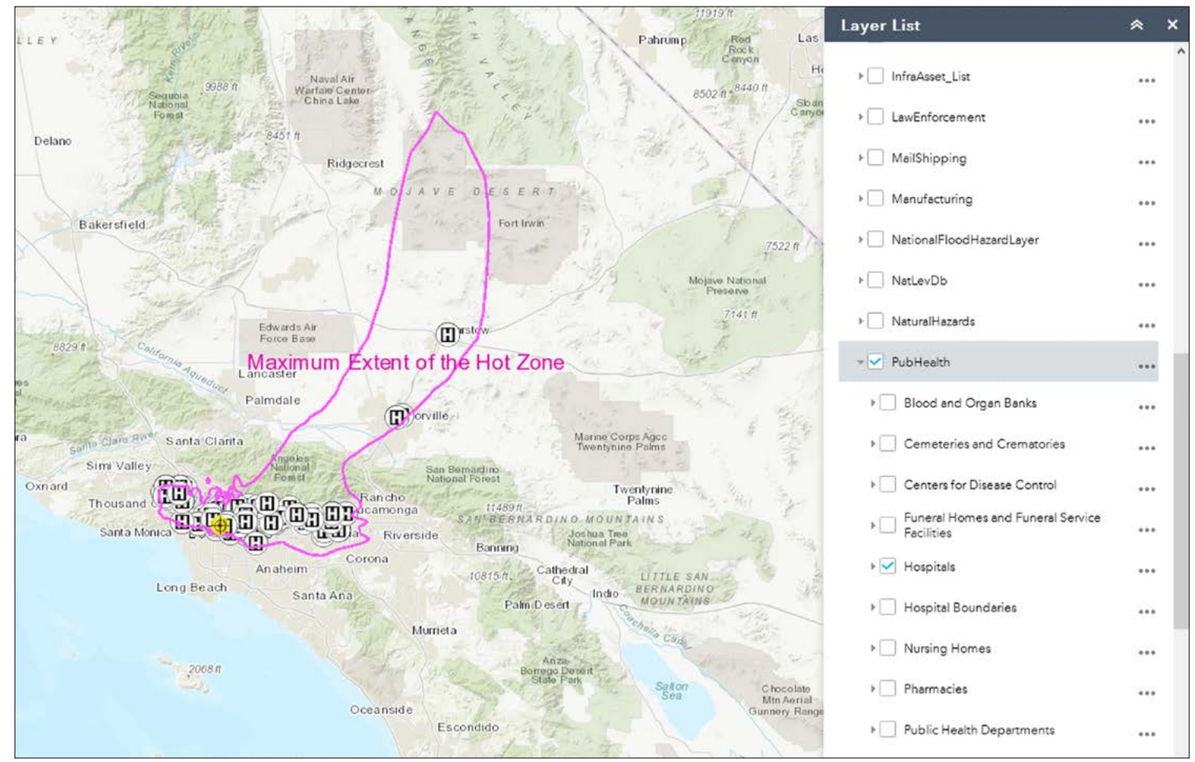


The interactive geographic information system (GIS) combines information from the Federal Emergency Management Agency's HAZUS database, which includes information on building types, along with protection factors developed by the National Atmospheric Release Advisory Center. Together, the resulting images show the estimated radiation protection provided by buildings at the census block level.

at Livermore, NARAC is the Department of Energy's (DOE's) plume-modeling center for real-time and predictive assessments of the effects of nuclear, radiological, chemical, biological, or natural emissions. The center's assessments are used to inform decisions on actions to protect the public and the environment.

With scenario results in hand, the team built standardized reports based on stakeholder feedback, IAB analyses, and data from the previous key response planning factor effort. Each city-specific report summarized prompt effects immediately after a detonation, shelter options, fallout effects over time, and how to apply federal guidance. To help planners and decision makers understand how an IND event unfolds, data visualization developer Ryan Chen developed hundreds of animations using NARAC simulation data. In addition, computer scientist JoAnne Levatin developed and implemented detailed injury and casualty analyses based on a methodology from a previous project by Buddemeier that provided essential estimates of health impacts for each scenario. Levatin also used FEMA's HAZUS database—which typically helps estimate and visualize potential losses from earthquakes, floods, hurricanes, and tsunamis—to obtain detailed information on building types for each area. Using HAZUS data and NARAC model–based building protection factors, Levatin developed map estimates illustrating the protection provided by buildings from fallout radiation down to the census block level. Such maps can inform planning strategies for sheltering in place and evacuation.

In addition, computer scientist Whitney Kirkendall developed an interactive geographic information system (GIS) component consisting of infrastructure and building protection modules. Using this capability, IND effects data can be overlain onto customizable maps. Alternatively, the DHS-supported Homeland Security Infrastructure Program Gold database, or Levatin's building protection data, can also be overlain onto GIS and queried for each of the iCPR scenarios. This GIS component helps planners see the specific effects of an IND on their community.



Emergency planners can use the interactive GIS at the heart of iCPR to display a fallout radiation zone on a map, change maps, and explore different critical infrastructure and key resources, such as hospitals (shown here).

Bringing Results to the Planners

The iCPR tool's documents, animations, GIS capability, and supplemental resources are hosted on NARAC's CMweb. In all, the hundreds of NARAC modeling runs for the iCPR effort resulted in 600 animations, 1,800 individualized reports, and the interactive GIS capability that integrates the data. Alai notes, "The results for each city or region include videos that track the fallout radiation for a year after the event. All the data is precalculated, and users can download the videos as well as scenario reports and GIS files, technical references, and federal guidance to help with their emergency planning processes."

The enthusiastic reception of iCPR led to FEMA requesting additional planning tools—chemCPR for chemical events and bioCPR for biological emergencies. FEMA, NUSTL, and DOE also requested that Livermore expand iCPR to include additional nuclear detonation yields for planning an expanded threat portfolio. The iCPR end user base has also been extended to include state, local, and tribal emergency planners.

Through their efforts to improve emergency preparedness, Lawrence Livermore researchers have taken on a leadership role in this important field. Buddemeier notes, "We are giving emergency planners the information they need to help save lives. For instance, hundreds of thousands of people may be saved through simple actions, such as sheltering in place for 24 hours." Alai adds, "We are proud that our efforts to provide scientifically informed analyses in ways that are useful to nontechnical end users have been so well received. Proper planning, supported by effective tools such as iCPR, is key to emergency preparedness."

—Ann Parker

Key Words: Department of Homeland Security (DHS), emergency preparedness, fallout, Federal Emergency Management Agency (FEMA), geographic information systems (GIS), improvised nuclear device (IND), IND City Planner Resource (iCPR), National Atmospheric Release Advisory Center (NARAC).

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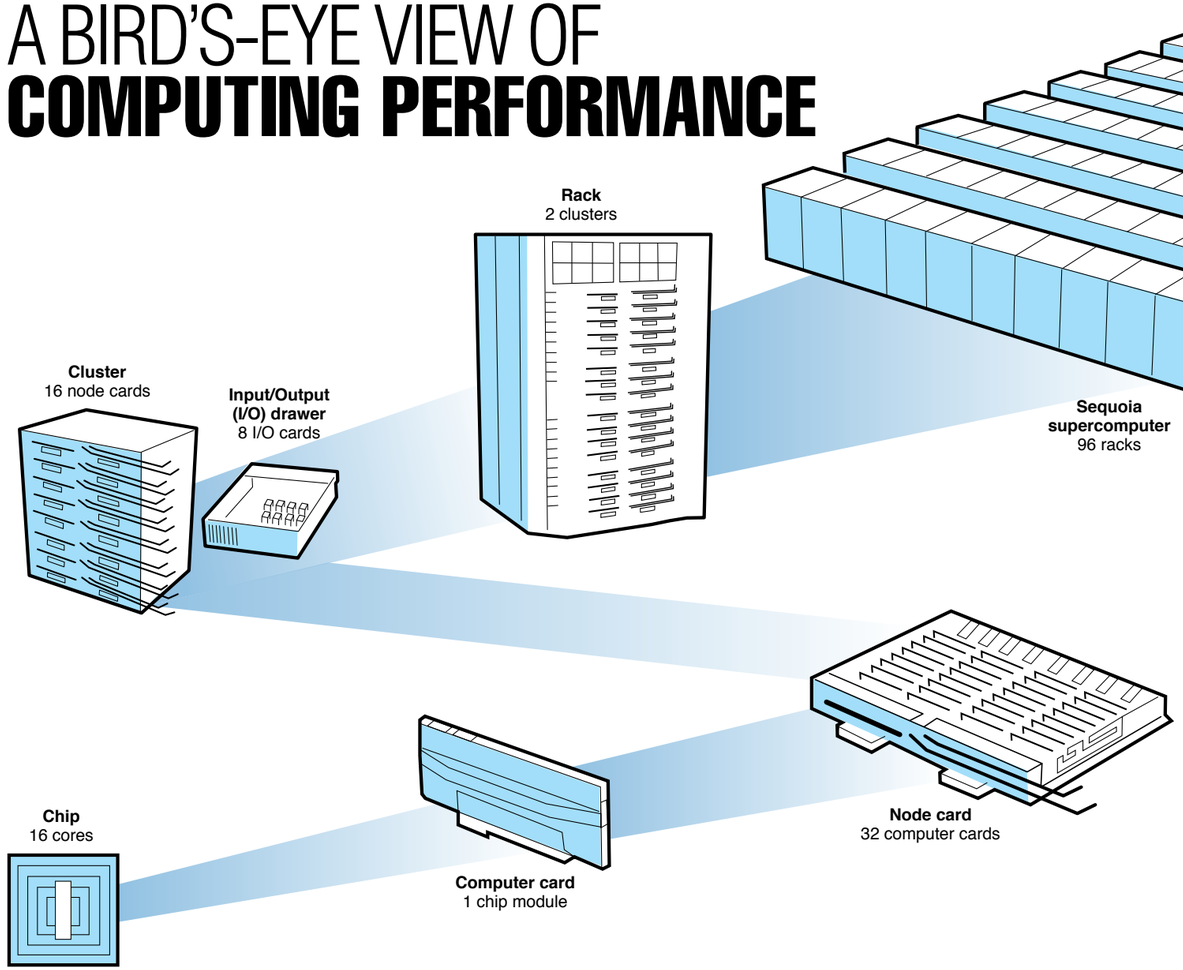
S&TR October/November 2018

A BIRD'S-EYE VIEW OF **COMPUTING PERFORMANCE**



The Sequoia supercomputer at Lawrence Livermore is shown here separated into its constituent parts—from the overall system to individual computer chips—to illustrate the scope of available performance data that are gathered at every level of this hardware hierarchy.

LAWRENCE Livermore's high-performance computing (HPC) center runs 24 hours a day, 7 days a week. Inside the facility, the noisy hum of supercomputers mixes with the air currents of the building's sophisticated cooling system, providing evidence of the otherwise unseen high-powered processing that is required for a wide range of scientific applications. While the machines are hard at work, performance analysts collect data about every component within the HPC center to ensure smooth and efficient operations. Computer scientist Alfredo Giménez says, "To evaluate our facility's performance, we must make sense of the substantial amount of data the HPC systems generate."

HPC performance data is collected from many different sources within the facility and includes metrics on network utilization, rack temperature and humidity, power consumption, application runtimes, and message routing. Such information is essential for understanding how efficiently the facility operates. For example, if analysts can determine which applications generate the most heat during processing, they can reconfigure job scheduling policies to prevent resources from overheating. The challenge is that performance data quickly accumulates, making it more difficult to interpret. "As we explored various analytical approaches, we discovered that every data science problem created a data integration problem," says Giménez. "Understanding data from many sources is more complex than one might initially imagine."

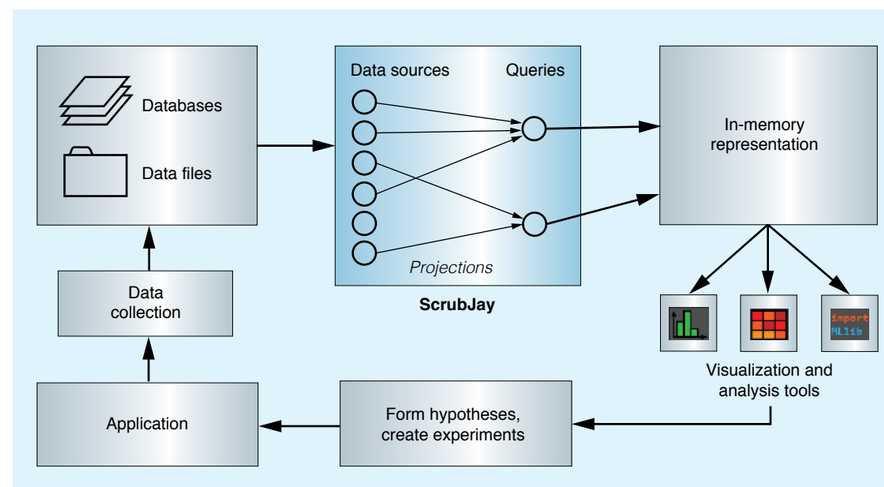
Giménez, along with colleagues in the Laboratory's Computation Directorate, investigates the information that can be extracted from data sources by defining the semantics (or meaning) of the data for better integration and analysis. Giménez incorporated this concept into an analysis tool called ScrubJay—named for the resourceful bird that memorizes scattered locations of food caches. ScrubJay automates and simplifies performance data analysis, helping analysts better understand interactions between applications and the complex systems within the HPC center.

Finding Common Ground

Although many open-source performance analysis tools exist, ScrubJay is unique in that it provides a way to integrate information from various data sources. For example, the batch system that runs parallel applications on Livermore's machines records which nodes ran an application, while the network monitoring system captures the amount of data written on each node. To optimize network utilization, ScrubJay can help analysts cross-reference these two data sets, and others, to determine how different applications affect network communication. Computer scientist Todd Gamblin states, "If we can identify the cause of performance problems, we can schedule jobs to avoid saturating the network or other resources."

Furthermore, analysts must contend with variations in formats, databases, and data types. One data collection tool may record comma-separated values in a plain-text file, and another may store facility information in a third-party database. In addition, time stamps may vary between data sets. ScrubJay eliminates the need for manual integration of such heterogeneous data by first annotating raw data sets with semantics that describe the types of information—for example, whether a table column contains time or temperature recordings. When analysts query ScrubJay, data sets are converted into common in-memory representations via parsing functions known as data wrappers.

ScrubJay's semantics are generalizable to many kinds of numerical and categorical data. Values in a data set can be defined as ordered or unordered, continuous or discrete, and so on. An analyst can also input customized semantics, such as



ScrubJay helps performance analysts evaluate how applications interact with complex high-performance computing systems and enables them to focus on high-level analysis queries rather than detailed data-processing operations.

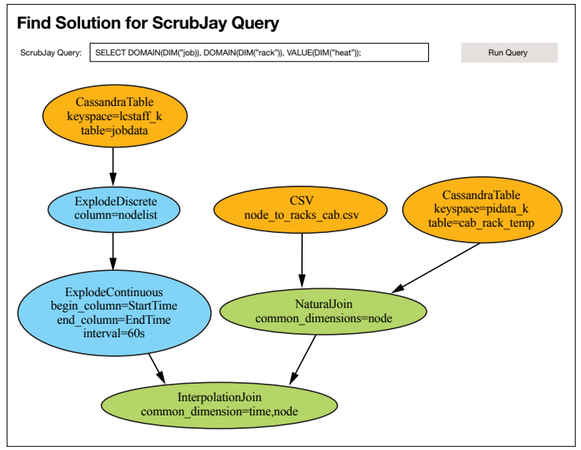
particle lookup functions in a particle-transport code. ScrubJay's "derivation engine," named after inference engines proposed for artificial intelligence in the 1980s, uses the semantics to determine which information can be obtained from one or more available data sets. For example, a new data set may arise from the conversion of units or when a range of values is separated into discrete values. Alternatively, two data sets may merge when their values are mapped to each other. In both cases, ScrubJay integrates the data points through a common semantic dictionary and in a shared format. In addition, ScrubJay contains logic for overlapping data. For one-to-many relationships, the derivation engine aggregates values with the same semantics. This process may result in averaged values, such as a single point in time mapped to multiple temperature readings.

A Collaborative Ecosystem

ScrubJay arose from a Livermore project called PAVE (Performance Analysis and Visualization at Exascale), which established a framework for analyzing the performance of parallel scientific codes. Giménez cites Boxfish, a Livermore-developed platform for performance data visualization, as another important influence in ScrubJay's development. He states, "Boxfish exposed many research problems identified by PAVE that we subsequently targeted in ScrubJay, such as how to relate different parts of the computing center to each other."

Now funded by multiple programs across the Laboratory, ScrubJay plays an important role in the larger HPC ecosystem. The HPC center's sheer volume of performance data—tens of gigabytes per day—is monitored, collected, stored, and processed by an infrastructure called Sonar. The system consists of a dedicated computing cluster, a distributed database, and monitoring tools that continuously and securely manage performance data without affecting computing operations. Gamblin, who manages Sonar, explains, "No single person has the knowledge of code experts, data analysts, and system administrators to pull together data from millions of processors. Sonar brings all of the information into one place where ScrubJay can integrate it."

Analysts access ScrubJay via a web-based dashboard. Instead of querying specific database tables, analysts enter the desired data sources and measurements. The tool automatically stores derivation sequences that can be re-run later or modified. "Analysts can examine a saved 'recipe' to see how ScrubJay derived the resulting data set. This reproducibility saves time for both analysts and the machines," says Giménez. The dashboard interface also allows analysts to create visualizations of the data.

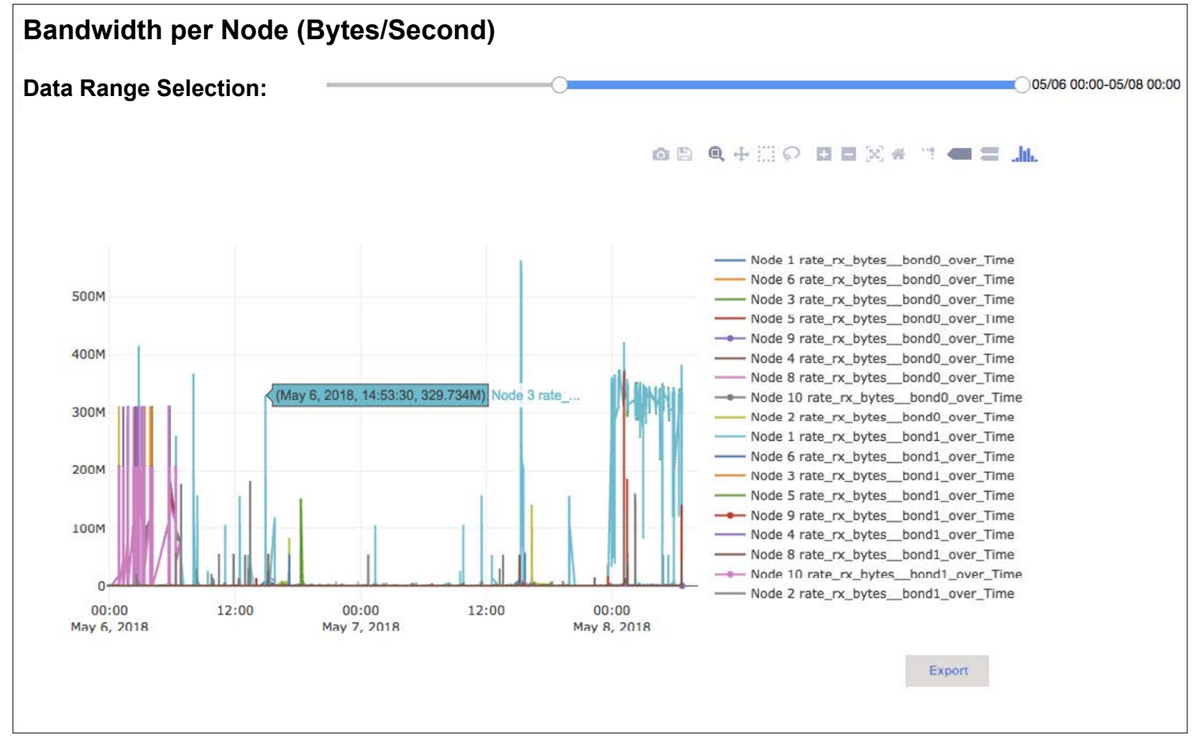


Analysts query ScrubJay through a dashboard that displays the derivation sequence and interactively renders the resulting data. In this case, the analyst requested a data set describing the heat generated from different jobs and their corresponding racks. ScrubJay produced a solution involving three original data sets (orange), two transformations (blue), and two combinations (green).

Proof Positive

The ScrubJay team presented two case studies at the international SC17 supercomputing conference to illustrate the tool's accuracy in integrating facility-wide information. In the first study, Giménez's team collected job queue logs; rack temperature, humidity, and power usage; and nodes-per-rack layout for one of Livermore's production clusters. "We wanted to analyze correlations between heterogenous workloads on the cluster, ultimately discerning which applications generated the most heat within the facility," states Giménez. The team incorporated the resulting data wrappers and semantics into ScrubJay's knowledge base for future analysis of the cluster's performance.

The second ScrubJay study added motherboard status, central processing unit (CPU) counters, and other performance variables to the query. The team sought to evaluate the effect of variable CPU frequency on node power consumption. The cluster's temperature readings were recorded every two minutes, while raw CPU, motherboard, and node data were collected at one- to three-second intervals. Manual analysis would have required tedious mapping of time stamps as well as raw data conversion to derive performance rates of different components on the motherboard. ScrubJay's automated transformations enabled the team to create visualizations of the derived information to answer their questions. Giménez notes, "This information is useful for understanding how architectural designs affect the way power is consumed from different computing resources."



An interactive plot of a ScrubJay-derived data set shows active bandwidth on different networking interfaces for each node in a cluster. The raw data set contains the number of bytes transferred over time, from which ScrubJay obtains bandwidth per node. This information helps analysts determine how much available bandwidth is being used over prolonged periods of time.

The team has also overcome efficiency challenges. ScrubJay is configured to search a large number of possible data derivations, then execute them on multiple large data sets. ScrubJay also distributes the data-processing operations over the entire Sonar cluster. Giménez explains, "We're improving ScrubJay's efficiency in a few ways, including caching intermediate results for reuse."

New Ideas Take Flight

HPC performance analysis must keep pace with evolving technology. As Livermore's Sierra supercomputer comes online with ever-faster processing speed, the Laboratory's HPC teams are adapting complex computing architectures to meet powerful performance requirements. (See *S&TR*, September 2016, pp. 4–11; and March 2017, pp. 4–11.) Optimized performance leads to better scalability, so monitoring and analysis tools such as ScrubJay are crucial for ensuring the Laboratory's HPC center functions at its best.

Giménez is working toward releasing ScrubJay as open-source software (https://github.com/LLNL/ScrubJay), and he looks forward to learning about external researchers' experiences with the tool at other HPC facilities. In the meantime, he plans to incorporate additional data transformations and apply machine learning to explore conditions that affect a code's efficiency. Giménez is also adapting ScrubJay for integration with other scientific and simulation data, including physical simulations from Livermore's National Ignition Facility. He states, "Data integration is a big challenge for all data scientists. We hope our solutions can help a variety of scientific fields."

—Holly Auten

Key Words: data analysis, data integration, data science, derivation engine, high-performance computing (HPC), ScrubJay, Sonar.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (http://www.uspto.gov).

Patents

Using Colloidal Silica as Isolator, Diverter and Blocking Agent for Subsurface Geological Applications
William L. Bourcier, Sarah K. Roberts, Jeffery J. Roberts, Souheil M. Ezzedine, Jonathan D. Hunt
U.S. Patent 9,909,052 B2
March 6, 2018

Isotachophoresis System Having Larger-Diameter Channels Flowing into Channels with Reduced Diameter and with Selectable Counter-Flow
Raymond P. Mariella, Jr.
U.S. Patent 9,910,011 B2
March 6, 2018

Porous Substrates Filled with Nanomaterials
Marcus A. Worsley, Theodore F. Baumann, Joe H. Satcher, Jr., Michael Stadermann
U.S. Patent RE46,771 E
April 3, 2018

Methods and Compositions for Rapid Thermal Cycling
Neil Reginald Beer, William J. Benett, James M. Frank, Joshua R. Deotte, Christopher Spadaccini
U.S. Patent 9,939,170 B2
April 10, 2018

High Performance, Rapid Thermal/UV Curing Epoxy Resin for Additive Manufacturing of Short and Continuous Carbon Fiber Epoxy Composites
James Lewicki
U.S. Patent 9,944,016 B2
April 17, 2018

Ultralow-Dose, Feedback Imaging with Laser-Compton X-ray and Laser-Compton Gamma Ray Sources
Christopher P. J. Barty
U.S. Patent 9,983,151 B2
May 29, 2018

Awards

Four teams of Laboratory researchers and one individual were honored with **National Nuclear Security Administration Defense Programs Awards of Excellence** for work performed in 2016. The Exceptional Achievement Award was awarded to **Bruno Van Wonterghem** for his tireless dedication to ensuring the National Ignition Facility (NIF) delivers high-quality experiments for all its users in support of the Stockpile Stewardship Program (SSP).

The **NIF High-Z Raleigh–Taylor Strength Team** executed the first plutonium (Pu) strength experiment at NIF in support of the SSP mission. The team fielded the first high-pressure Pu strength experiment at NIF using a Rayleigh–Taylor instability growth platform that has been developed and matured over the past decade at NIF and the Omega Laser Facility using tantalum samples. This first experiment ushered in a new era in high-energy-density experimentation for SSP. This achievement required developing new polymer materials and low-density foams, fabricating a complex target with submicrometer tolerances, building unique x ray–hardened diagnostics, the high-purity winning of Pu at the 100-millligram scale, the development of new x-ray backlighter technology, and the physics design and execution of a complex experiment to obtain strength data on Pu at the highest pressures of any platform to date.

The **Anti-Reflective Grating Debris Shield (AR-GDS) Team** developed the AR-GDS for NIF, which greatly enhanced the facility's ability to operate at high laser energies while decreasing costs. The AR-GDS reduces the laser damage rate by an incredible factor of more than 50 over the previous grating debris shield (GDS) process. The AR-GDS is being used on all of NIF's 192 beamlines, putting NIF on a path to reducing GDS operating cost by a factor of at least six over its predecessor. More importantly, this breakthrough increases shots for users at NIF's full energy, making more rapid progress in the Inertial Confinement Fusion (ICF) Program possible. This breakthrough has also made it possible to explore higher energy operation at NIF.

The **Fill-Tube Science Team** improved diagnosis and understanding of fill-tube effects in ICF implosions. The team studied the effect of the capsule fill-tube on ICF implosions and found the perturbation from the fill-tube was bigger than expected. Their careful and thorough approach ensured that the data was unambiguous, and thus motivated quick action to explore how the fill-tube perturbation could be mitigated. The success of this complex endeavor resulted from excellent teamwork and a careful and thorough scientific approach of dividing the integrated experiment into a series of component experiments. This approach led to the discovery of effects not initially modeled or predicted, coupled with the use of new diagnostics and target fabrication innovations, to arrive at better modeling, understanding, and performance.

The **Broadband Laser Ranging (BLR) Analysis and Software Development Team** supported development of an optical method of providing surface position as a function of time. According to National Security Technologies, Inc., in Nevada, the BLR technique is a vast improvement over the pins used in the past where each one only gave a signal for one location at a single point in time. In combination with photonic doppler velocimetry, BLR can provide much more detailed characterization of an implosion, thus providing more constraining data for validating simulations and improving predictive capability. The BLR diagnostic removes the time-intensive steps associated with a previous technique, saving significant time and money.

Abstract

Extending the Life of a Workhorse Warhead

In 2014, the National Nuclear Security Administration (NNSA) selected Lawrence Livermore as the lead nuclear design agency for refurbishing the W80-1 nuclear explosives package as the W80-4 life-extension program (LEP). The W80-1 warhead is carried on the Air-Launched Cruise Missile (ALCM), and both the missile and its warhead are well past their planned lives. The ALCM's replacement is the Long-Range Standoff missile, currently under design. Aimed at providing 30 years of service life to an aging nuclear warhead, LEPs use NNSA's computational, experimental, and manufacturing capabilities for the required prototyping, proof-of-concept design testing, certification, and surveillance activities. The W80-4 LEP takes advantage of Livermore's high-performance computing and experimental tools developed through the NNSA's science-based Stockpile Stewardship Program, which ensures the safety, security, and effectiveness of the nation's nuclear arsenal without resorting to additional nuclear explosive tests. Key tools include the Contained Firing Facility (the largest indoor firing chamber in the nation), the National Ignition Facility (the world's largest laser); and the High Explosives Applications Facility, a Department of Energy–NNSA Center of Excellence.
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