Lawrence Livermore National Laboratory

August 2021

Science & Technology REVIEW

PLANETARY RESEARCH

EXPLORING OUR PAST AND FUTURE

Also in this issue:

Laboratory Operations in a Pandemic

Energetic Materials Center Anniversary

Disruptive Research Results

About the Cover

As described in the multi-part feature beginning on p. 4, Lawrence Livermore National Laboratory's research expertise in astrophysics, nuclear science, cosmochemistry, and data science is uniquely tuned to answer questions about the past and future of our solar system. This month's cover illustration represents planets, moons, and other heavenly bodies, on a large scale, which researchers explore on a much smaller scale, including examination of biomolecules sparked by asteroid bombardments and isotopic differences among extraterrestrial samples.

Cover design: Mark Gartland

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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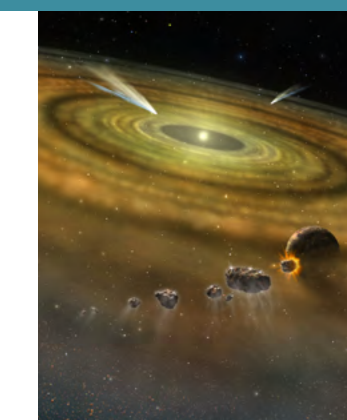


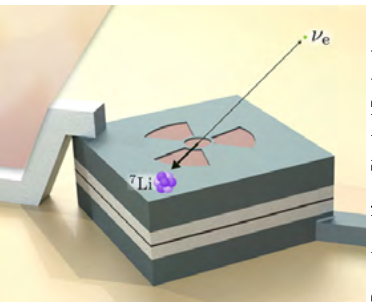
Research Highlights

Departments

Finding Sterile Neutrinos

The existence of theoretical particles called "sterile neutrinos" could offer a deeper understanding of dark matter, the strange material that permeates the universe and accounts for 85 percent of its total mass. Livermore scientist Stephan Friedrich led a team from Lawrence Livermore National Laboratory and the Colorado School of Mines in an experiment funded by the Laboratory Directed Research and Development (LDRD) Program demonstrating the power of using nuclear decay in high-rate quantum sensors in the search for sterile neutrinos. The findings are the first measurements of their kind and appeared in the January 13, 2021, issue of *Physical Review Letters.*

In the experiment, nicknamed the "BeEST" (Beryllium Electron-capture with Superconducting Tunnel junctions), researchers implanted radioactive beryllium-7 atoms into superconducting sensors developed at Livermore. A process called electron capture—in which an electron in an atom's inner shell is drawn into the nucleus and combines with a proton—decayed the beryllium-7, forming lithium-7 and a neutrino. The neutrino then escaped, making it undetectable, but the reduced recoil energy or byproduct of the lithium-7 produced a measurable signal of the neutrino mass.



Reproduced from *Physical Review Letters*

The team performed simulations on Laboratory supercomputers to gain confidence in the detection of sterile neutrinos and understand the materials effects in the detector. Friedrich says, "This research lays the groundwork for more intensive searches for these new particles using large arrays of sensors with new superconducting materials."

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Doubling Laser-Produced Antimatter

The ability to create numerous positrons in a laboratory setting opens new doors to antimatter research, including an understanding of the physics underlying astrophysical phenomena such as black-hole accretion and gamma-ray bursts. Livermore physicists used the high-intensity OMEGA Extended Performance (EP) laser at the University of Rochester's Laboratory for Laser Energetics to shoot through a gold target with microstructures, called a silicon microwire array, and produced high-energy electrons, generating electron–positron pairs. The research results appeared in the March 2, 2021, issue of *Applied Physics Letters*.

Prior to the physical experiment, particle-in-cell simulations optimized the spacing and length of the micro-structures added to the typical gold target. These highly ordered silicon microwire arrays faced the OMEGA EP laser pulse and guided the relativistic electron beam along a structured surface to facilitate a more direct laser acceleration. The laser irradiated the gold target's microstructures—much like assembled Legos, but only 1 millimeter in size. The laser–plasma interaction generated relativistic electrons and transported them through the material, making high-energy photons and spontaneously producing antimatter pairs in response to the laser energy transforming into mass.

Previous research, using flat, unstructured targets, produced around 100 billion particles of antimatter. These new experiments doubled the result, increasing antimatter production by 100 percent. "Adding front surface microstructures to the typical gold target constitutes a cost-effective approach to substantially increase the positron yield while keeping the same laser conditions, putting us one step closer toward using laser-generated positron sources for a variety of applications," says Sheng Jiang, the lead author of the paper.

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Clarifying Ignition Performance

In inertial confinement fusion experiments at Lawrence Livermore's National Ignition Facility (NIF), a spherical shell of deuterium–tritium fuel is imploded to reach the conditions needed for fusion, self-heating, and eventual ignition. Livermore researchers partnered with the University of Rochester's Laboratory for Laser Energetics and Los Alamos National Laboratory to develop a compression-scaling model benchmarked to 1D implosion simulations across relevant implosion designs. Ultimately, their results, featured in the April 13, 2021, issue of *Physics of Plasmas*, could lead to improved ignition efficacy.

The team developed an isobaric and isentropic compression scaling model incorporating sensitivity to key parameters involving pressure, implosion velocity, fuel aspect ratio, and mass ratio and compared the model to compressibility trends across NIF implosion data for three ablators—plastic, carbon, and beryllium. Researchers found the strength of the first shock is the dominant contributor setting maximum fuel convergence and observed additional sensitivities to successive shock strengths and fuel aspect ratios that improve the agreement between the expected and measured compression for carbon and beryllium designs.

The best compression levels followed the expectations of the model with the exception of high-energy-density carbon shells that exhibited a lower level of compression independent of the laser drive conditions. The paper's lead author, Livermore's Otto Landen, says, "Understanding compression trends as we varied laser and capsule parameters motivates further research in improving compression without necessarily demanding higher laser energy."

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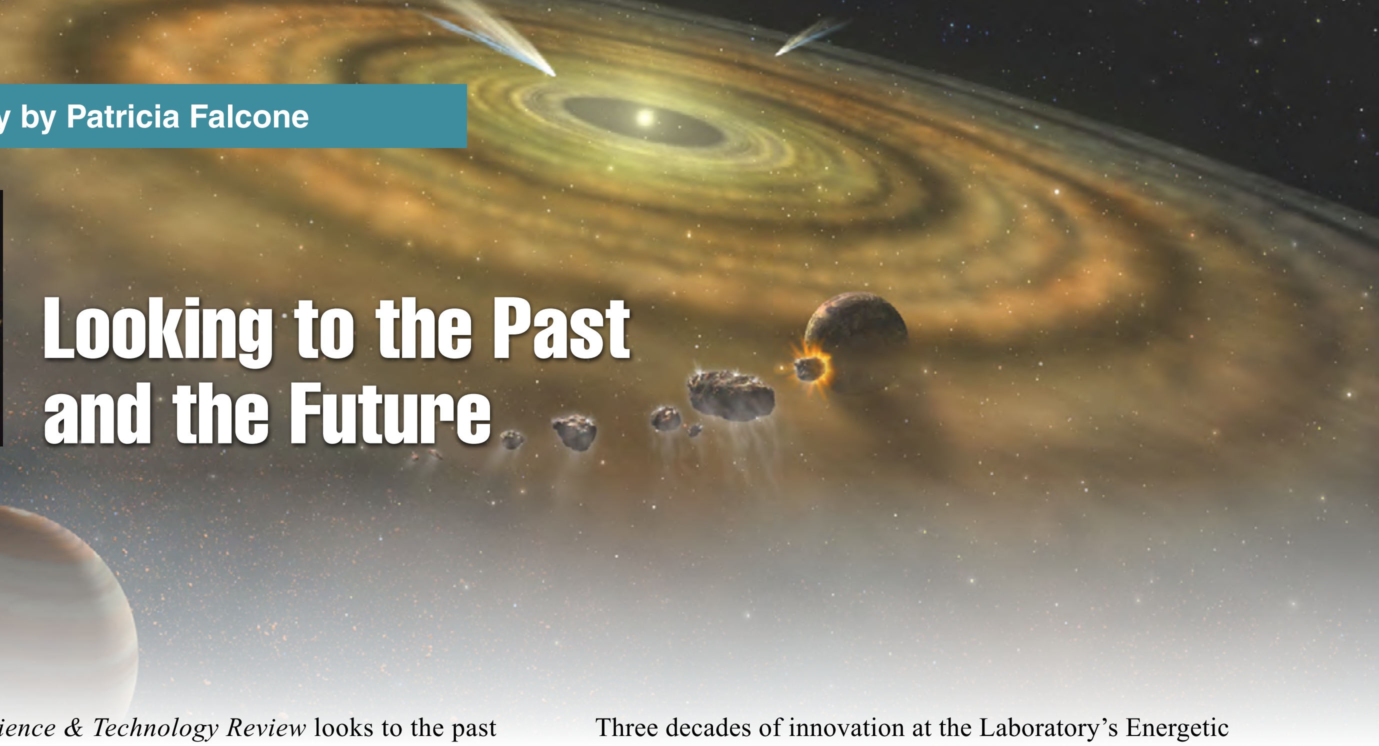


Looking to the Past and the Future

THIS issue of *Science & Technology Review* looks to the past and the future—in both our scientific discoveries and the Laboratory's extraordinary science and technology (S&T) research capabilities. By applying these capabilities, Laboratory scientists have made significant discoveries about the origins of the solar system and life on Earth; continue to advance nuclear weapons S&T in support of stockpile modernization; and strive for disruptive breakthroughs important to our national security missions.

The feature article, beginning on p. 4, is presented in four short pieces. It delves into facets of planetary and life sciences to reconstruct the past. Lawrence Livermore researchers are exploring an unexpected pathway to the organic precursors of early biomolecules and life—the bombardment of primordial Earth from comets and meteorites. They use Livermore's high-performance computers to simulate the chemistry that takes place in such collisions. Geochemists at the Laboratory are at the forefront of efforts to "discover" the evolution of our solar system and its planets, moons, and asteroids. By studying the isotopic signatures of radioactive isotopes in extraterrestrial rocky samples, they have reconstructed the sequence and timing of events in the solar system and dated the age of the Moon. Another team developed compact gamma-ray detectors that have orbited Mercury and will fly to the Psyche-16 asteroid to gain insights into the cores of the solar system's inner planets. In addition, a research team examined materials science issues that future space explorers will face.

These research efforts build on and enhance S&T expertise and tools that are vital to our national security missions. The high-performance computing capabilities required for exobiology simulations are the foundation of stockpile stewardship. Radiochemistry expertise is needed for assessing nuclear device performance and for nuclear incident response. Gamma-ray detectors are used to locate radioactive materials at shipping ports and border crossings and for nuclear safeguard applications. All mission areas at the Laboratory rely on materials science expertise.

Three decades of innovation at the Laboratory's Energetic Materials Center (EMC) are celebrated in the highlight beginning on p. 16. EMC scientists provide critical expertise and cutting-edge research in support of the nuclear deterrent and keeping the nation safe from emerging explosives and nuclear proliferation. As the country's leading repository of energetic-materials expertise, EMC has been responsible for many landmark S&T developments and faces significant future challenges supporting the nation's strategic modernization program. The Laboratory leads the charge to develop means to remanufacture an insensitive high explosive not in production since the early 1990s and has developed a novel new explosive for use in stockpile modernization.

We look to address future national needs and explore S&T possibilities through the Department of Energy's Laboratory Directed Research and Development (LDRD) Program. At the Laboratory, we created a Disruptive Research projects category within LDRD to support the pursuit of exceptionally innovative ideas with the potential to achieve mission-critical, transformational results. Three of the nine "out-of-the-box" initial projects are discussed in the highlight beginning on p. 20. A team of scientists has developed and tested a deep-learning algorithm to derive a small model—a mathematical equation—from larger models to make predictions. A second project aims to develop methods for performing complex nuclear calculations on a prototype quantum computer. Yet another team is striving to significantly increase laser power and intensity using plasma rather than solid optics as the amplifying medium.

All these remarkable projects are being carried out under COVID-19 pandemic conditions. A third highlight (p. 12) in this issue of *S&TR* discusses how we are enforcing a top priority, protecting employees' health, while pursuing "Science and Technology on a Mission" at Lawrence Livermore National Laboratory.

■ Patricia Falcone is deputy director for Science and Technology.

S&TR August 2021

PLANETARY RESEARCH EXPLORING OUR PAST AND FUTURE

How could life begin from a swirling chaos? How did Earth and its moon form? What can lunar rocks from the Apollo missions reveal? And what will scientists learn from exploration on distant moons? These questions are addressed in this four-part feature article on Lawrence Livermore's space science research.

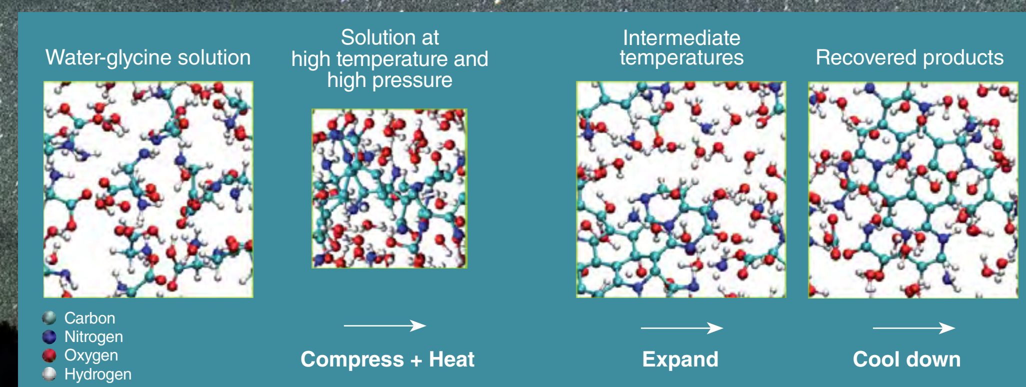
SHOCKING START TO LIFE

EARTH coalesced from a protoplanetary disk of gas, dust, and aggregations of particles about 4.5 billion years ago. Primordial Earth was a hostile place—volcanism, extreme heat, a turbulent atmosphere, intense ultraviolet radiation from a young, hot sun, and continual bombardment from comets and meteorites. How could such unwelcome conditions lead to a prebiotic chemistry that gave way to proteins, lipids, and other biomolecules between 3.5 and 4 billion years ago?

Researchers at Lawrence Livermore are exploring an unexpected pathway to the organic precursors of early biomolecules—precursors that originate with the impacts of astrophysical bodies on Earth. Comets, made mostly of water, ice, and dust, have been known since the 1970s to also contain a number of small molecules such as ammonia (NH_3) and methanol (CH_3OH). In 2009, the comet Wild II (pronounced "vilt 2") was found to contain glycine, the simplest protein-forming amino acid. The impact of comets provides abundant energy to drive chemical reactions that could produce a wide array of organic chemicals that are the building blocks of biomolecules.

Nir Goldman, a computational chemist and deputy group leader of the Non-Equilibrium Theory Group in the Laboratory's Materials Science Division, leads research that uses Livermore's high-performance computing (HPC) capabilities to simulate the chemistry that takes place when comets and other icy materials bearing organic chemicals collide with Earth. Goldman and his team build on an earlier study, funded by Livermore's Laboratory Directed Research and Development (LDRD) Program, of shock-compressed materials to determine whether prebiotic compounds such as amino acids might emerge under high temperatures and pressures.

"Experiments to recreate such conditions are extremely challenging due to the large number of interconnected variables at play," says Goldman. "Factors include the composition of the initial material to be studied and the peak conditions achieved during shock compression. Analyzing the products after the shock process is one of the biggest challenges. A plethora of reactions can take place, and contamination from biological sources—for example, a researcher's hands—is extremely easy."



In a simulation designed to show the effects of cometary impact, a water-glycine mix is compressed and heated, then expanded and cooled, yielding life-building hydrocarbons.

Simulating Shock

To help direct experimental shock compression efforts, Goldman and his colleagues performed quantum mechanical simulations of prebiotic shock synthesis to explore what happens chemically under impact conditions of a comet. After setting up initial conditions including pressure and temperature, initial mix of chemicals, strain rates, and other parameters, the simulations modeled comet impact conditions at the atomistic level while accurately describing the dynamic breaking and forming of chemical bonds. In this case, their simulations spanned more than 50 gigapascals (GPa)—nearly 500,000 times Earth's atmosphere—and temperatures up to 5,000 kelvin. "The real art of these simulations is the judicious choice of setting these boundary conditions to mimic the conditions you want," says staff scientist and computational chemist Matthew Kroonblawd, a member of Goldman's team.

To their surprise, simple mixtures containing water, small organic compounds, and ammonia yielded amino acids and a number of other potentially life-building compounds when subjected to these intense conditions. Later, confirming experiments were performed using a light gas-gun facility at the University of Kent. An aqueous mixture of similar composition was subjected to an impact shock of more than 50 GPa, and researchers identified a large variety of amino acids in the post-shock ice mixture.

A follow up study in 2019 by Kroonblawd, Goldman, and Livermore's Rebecca Lindsey reported the results of simulating a mix of glycine and water under impact scenarios including cooling and equilibrating to ambient conditions. In this case, carbon-rich structures condense under high pressures and temperatures and subsequently unfold into nitrogen-containing polycyclic aromatic hydrocarbons (NPAHs) during fracture and cooling. NPAHs are important prebiotic precursors for synthesizing molecules that are the basis of complex proteins such as RNA and DNA.

Path to Prebiotic Compounds

Research published in 2020 by Brad Steele, Goldman, I-Feng "Will" Kuo, and Kroonblawd simulated a rotational diamond anvil cell experiment. Rotating diamond anvils apply a compressive shearing force to a small chamber containing a glycine mixture. A modeled compressive shear stress of 10 GPa produced a complex chemistry of prebiotic compounds including polypeptides, such as chains of amino acids that form the building blocks of proteins. These studies indicate that simple molecules like glycine support richly varied chemistry under extreme conditions. Other simulation studies from Goldman's group have generated long-chain carbon molecules, formaldehyde, and hydrogen-nitrogen-carbon-oxygen compounds such as hydrogen cyanide, which are building blocks of biomolecules. "We've run hundreds of simulations on Livermore's HPC facility to get good statistics," says Goldman. "This work is only possible here and only because of the Laboratory's supercomputers."

Now funded by NASA's Exobiology program, Goldman's group is undertaking a study of a heterogenous system to determine the possible shock synthesis of organophosphates (compounds containing phosphate ions) that are key components of biomolecules such as DNA, RNA, and adenosine triphosphate. The team's studies will include aqueous mixtures of the iron-phosphorus mineral schreibersite, a common component of meteorites that may have contributed as much as 10 percent of the phosphorus thought to be present in the crust of early Earth. Schreibersite could have acted as both a source of elemental phosphorus and as a catalyst for lowering energetic barriers for organic chemical reactivity. Extreme thermodynamic conditions can act as a driving factor in creating more complicated chemical compounds with carbon-phosphorus bonds. This latest study will give Goldman and his team a unique opportunity to explore the catalysis of potentially life-building compounds in aqueous environments and answer long-standing questions in astrobiology.

Livermore's Nir Goldman (left) and Matthew Kroonblawd modeled cometary bombardment conditions to understand the chemical bonds broken and formed after impact. (Photo by Garry McLeod.)

—Allan Chen

Key Words: amino acids, comet, glycine, meteorite, organophosphates, prebiotic molecules, rotational diamond anvil cell, schreibersite.

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READING COSMIC ROCKS

WHO would have guessed that rocks could tell us so much—not just about Earth's geological history, but about the evolution of our solar system, and its planets, moons, and asteroids? Laboratory researchers Lars Borg and Greg Brennecka don't have to guess. They know.

In their roles as cosmochemists, Borg and Brennecka read the clues embedded in extraterrestrial samples gathered during targeted space missions as well as the random meteorites sourced mainly from the solar system's primary repository of history, the asteroid belt. Insights into the events that took place billions of years ago can be gleaned from isotopic signatures in general. The ticking clocks of radioactive isotopes embedded in these rocky samples are particularly helpful. Event ages can be determined by measuring specific elemental and isotopic ratios in a sample, and these ratios can reveal the age and origin of a sample, and importantly, the sequence and timing of events in the solar system. (See the box on p. 7.)

Investigations by the Livermore team cover a wide swath of time and space. Brennecka focuses on the earliest history of the solar system, the first 5 million or so years after the Sun ignited and the first solids formed. Borg, on the other hand, focuses on the evolution of satellites and planets such as the Moon, Mars, and Earth. Brennecka notes that their areas of interest overlap and reinforce each other. "As the Sun was gathering mass and igniting, the first solids in the solar system formed, followed by the accretion and differentiation of early protoplanets," he says. "These events determined the evolutionary course of our solar system and the planetary bodies within it."

Origin Stories

In 2010, the two researchers first teamed up to use Livermore-developed techniques to evaluate isotopic signatures in calcium aluminum–rich inclusions (CAIs) from the Allende meteorite that landed in Mexico in 1969. These CAIs were the earliest solids to form in our solar system, predating the terrestrial planets by more than a million years. The resultant isotopic signatures provided evidence indicating that the cloud of matter condensing to form the Sun and planets was showered with material produced by a nearby supernova explosion. (See *S&TR*, July/August 2014, pp. 12–14.)

Borg has turned a cosmochemist's eye upon the mystery of the Moon's origin as well. In one theory, the Moon formed at the same time as the Earth, accreting from a primordial cloud of gas and dust, making the Moon around 4.5 billion years old. Original isotopic analyses on samples gathered during the Apollo missions, which ran from 1969 to 1972, varied widely, suggesting the Moon could be between 4.32 billion to 4.56 billion years old. Beginning in the late 1990s, a team headed by Borg took another look at the samples using more modern techniques and equipment. It turned out that, no matter where the samples had been collected and what isotopic clocks were used, the rocks all told of a formation between 4.33 and 4.38 billion years ago, pointing to a much younger Moon. These Livermore analyses gave weight to the "Giant Impact" theory, in which a large body, approximately the size of Mars, smashed into early Earth. Superheated rock and dust hurtled into space, where, with the help of gravity, it eventually accreted, forming the Moon. (See *S&TR*, September 2017, pp. 12–15.)

Lars Borg (left) and Greg Brennecka prepare lunar samples for isotopic measurement to study the chronology of the Moon. (Photo by Garry McLeod.)

In more recent projects, including Borg's work with Livermore's Thomas Kruijer, Josh Wimpenny, and Corliss Sio, researchers have turned to isotopic analysis to pin down when Mars' "magma ocean" began to solidify into the planet's mantle. Thermal models predicted this solidification would have started less than 1 million years after the formation of the planet's core. To test this, the team applied the ^{53}Mn–^{53}Cr radiochronometer, a decay system where manganese-53 (half-life of approximately 3.7 million years) decays to chromium-53, to Martian meteorites. Results demonstrated this chronometer was not "alive" when Mars formed its mantle and crust, indicating that the magma ocean solidified at least 25 million years after the beginning of the solar system—at least 20 million years after the core is thought to have formed. One possible explanation, notes Borg, could be that early Mars sported a dense atmosphere that acted as an insulator keeping the magma ocean from solidifying.

Creating Timetables

The most exciting element of cosmochronology research, according to Brennecka, is learning how every facet links together. "Through examining a variety of samples, we can build a picture of not only how the planets form and evolve, but how the solar system came into being," he says. "The Laboratory enables this groundbreaking cosmochemistry work by having the best analytical capabilities and equipment to measure isotopic ratios. I can't think of any other place that has such an assortment of capabilities under one roof."

Work funded by Livermore's Laboratory Directed Research and Development (LDRD) Program united Brennecka and postdoc Jan Render to measure the isotopic signatures of neodymium and zirconium in samples of meteorites from the asteroid belt. Because many planets are not positioned where they originally formed, particularly the giant planets, these measurements of asteroid belt material determined where these samples initially formed, helping create a broad reconstruction of the primordial solar system.

Livermore's cosmochemists also serve with a team analyzing recently opened core samples gathered on the Moon in 1972, during the last Apollo mission. This work is focused on chronology of previously unexamined samples and serves to gather information on the behavior of volatile elements on the Moon and Earth.

Borg, who has been named to the National Academy of Science's Planetary Science and Astrobiology Decadal Survey steering committee, notes that this research effort positions the Laboratory for conducting forensic analyses of samples from future Moon missions. "Livermore has a seat at the table when the academy assesses key scientific questions in planetary science and astrobiology and identifies missions and initiatives for the decade 2023–2032," says Borg. Other sample-collection missions include the Mars Sample Return Campaign, scheduled to launch in 2026, and the OSIRIS-REx mission, set to return asteroid samples in 2023. In addition, large quantities of lunar samples from many new areas of the Moon are expected to be returned when NASA's ARTEMIS manned space flight program matures in the near future. "We have become a one-stop shop for extraterrestrial geochronological analysis and there are some fantastic sample analysis opportunities ahead," says Borg. "It's an exciting time to be in the field and at Lawrence Livermore."

—Ann Parker

Key Words: Allende meteorite, Apollo mission, asteroid, cosmochemistry, extraterrestrial geochronology, Giant Impact, isotope analysis, isotopic signature, Laboratory Directed Research and Development (LDRD) Program, Moon, Mars, meteorite, NASA, solar system.

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A Storied History of Isotopic Analysis

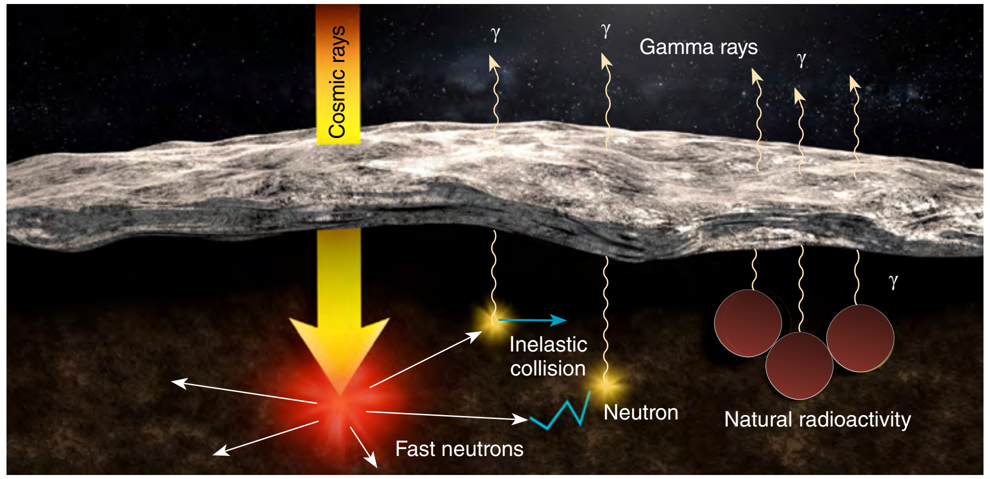
The Laboratory has long been in the business of studying isotopes. Early on, its radiochemists conducted isotopic analyses for atmospheric and underground nuclear tests; today, nuclear forensics plays a key role in the Laboratory's security missions. (See *S&TR*, April/May 2018, pp. 4–11 and *S&TR*, October/November 2014, pp. 12–18.) Livermore's Lars Borg sees only a short step from applying isotopic research to nuclear forensics to answering questions of cosmochemical importance. "Planetary materials undergo processes that are relevant to nuclear forensics, such as nuclear decay, neutron capture, and spallation," he says. "Additionally, the elements of interest to cosmochemistry have multiple isotopes of interest for forensic purposes. Finally, the analytical techniques are essentially identical for both applications." Noting important differences, Borg points out that the magnitude of isotopic effects can be much more muted in natural samples, requiring precision measurements to identify extremely small isotopic differences between samples of very little mass. In many cases, the procedures the Laboratory develops to answer a cosmochemical question, such as determining the nucleosynthetic sources for the elements in a meteorite sample, can also be used in nuclear forensics and other mission-critical work.

GAMMA RAY EYES ON DISTANT MOONS

GAMMA RAYS—high-energy electromagnetic waves produced by the decay of radioactive isotopes—are found in the depths of space and on the surface of planets, planetoids, and moons. In space, neutron stars, pulsars, and supernova explosions emit gamma rays. On planets, cosmic ray bombardment and the less dramatic process of radioactive decay produce gamma rays. Lightning and nuclear explosions on Earth yield them as well.

Since gamma–ray emission provides a unique fingerprint of a radioactive material's isotopic composition, the Laboratory has long been in the business of designing and fielding gamma-ray spectrometers. Used in national security, the devices locate radioactive materials at shipping ports and border crossings. As nuclear safeguards, they identify and quantify the isotopes in nuclear processing facilities.

Lawrence Livermore is also recognized for its development of germanium-based gamma-ray spectrometers for planetary exploration. The high-purity germanium crystals in these detectors provide excellent resolution at −180°C, a requirement that presents its own challenges when journeys take years and temperatures are extreme. Germanium-based gamma-ray detectors developed by Livermore's Morgan Burks, Geon-Bo Kim, and Nathan Hines will be part of deep-space missions to the asteroid Psyche-16 (launch date 2022), the two moons of Mars (2024), and Saturn's moon Titan (2027). The Livermore team collaborates with Johns Hopkins University Applied Physics Laboratory (APL) researchers, who integrate the gamma-ray detectors with other instrumentation and deliver the final systems to NASA.



When high-energy cosmic rays bombard an airless planetary surface, gamma rays are emitted through processes such as inelastic collision and neutron capture. Gamma rays can also be emitted from naturally occurring radioactive materials such as thorium, potassium, and uranium on the planetary surface. The GeMini-Plus will measure the energy of the gamma rays with high resolution, helping scientists to identify the asteroid's composition. (Rendering by Veronica Chen.)

An Established Collaboration

This effort isn't the "first rodeo" for the Livermore-APL collaboration. About 20 years ago, Livermore and APL developed a lightweight, germanium-based gamma-ray spectrometer for NASA's MESSENGER mission to Mercury (See *S&TR*, June 2005, p. 23–24.) The venture provided new insights, causing researchers to reconsider theories on Mercury's formation. That instrument led to the GeMini, a germanium (Ge)-based spectrometer with an ultraminiature electromechanical cooling system (Mini). Low power, low mass, low weight, and rugged, the R&D100 Award–winning GeMini was small enough to hold in the palm of one hand. (See *S&TR*, October/November 2009, pp. 8–9.)

The GeMini gave way to the versatile GeMini-Plus, which sports an improved, simplified, and more rugged design. The team recently delivered the GeMini-Plus for the mission to Psyche-16, located in the asteroid belt between Mars and Jupiter. Psyche is composed largely of iron, unlike most asteroids, which are mostly rock. "Psyche is thought to be a planetary core, a remnant of a collision during the early stages of the development of the solar system," says Burks. Data gathered by the GeMini-Plus on the elemental composition of Psyche's surface could provide insights into the cores of our solar system's "inner" planets—Earth, Mars, Mercury, and Venus—and into planetary evolution and formation. (See *S&TR*, May 2019, pp. 17–19.)

(From left to right) Livermore's Geon-Bo Kim, Nathan Hines, and Morgan Burks designed the GeMini-Plus, a high-resolution gamma-ray spectrometer that will be part of the NASA mission to the Psyche asteroid. The team is creating similar detectors for missions to the moons of Mars and to Saturn's moon, Titan. (Photo by Garry McLeod.)

Outfitting New Instrumentation

A modified GeMini-Plus will be incorporated into NASA's Mars-Moon Exploration with Gamma rays and Neutrons (MEGANE) instrument, which will use gamma-ray and neutron spectroscopy to measure the elemental composition of the two Mars moons, Phobos and Deimos. MEGANE is one of eleven instruments slated for the Japan Aerospace Exploration Agency's Martian Moons Explorer (MMX). "Our spectrometer may help answer some fundamental questions about how Mars's moons were formed," says Burks. "Are they captured asteroids? Remnants of a big impact on Mars? Or, accreted leftover material from Mars's formation? We hope to find out." After conducting remote-sensing measurements of both moons, the MMX will land on the surface of Phobos, grab a sample of its moon dust, and fly back to Earth. The round-trip mission is expected to take about five years.

While engineering the spectrometer for MEGANE/MMX, the team is also hard at work on the instrument for the Dragonfly mission. Part of NASA's New Frontiers program, Dragonfly will search for the building blocks of life on Saturn's largest moon, Titan. The eight-bladed rotorcraft will maneuver like a large drone, zooming about the icy moon's surface, landing to take samples, and taking off again. Livermore's gamma-ray detector will measure the elemental composition of the landing sites, helping with site characterization and sample selection. "Titan has a dense, nitrogen-based atmosphere along with methane clouds and rain," Burks notes. "The surface has liquids, ammonia ices, and complex organic molecules, which could be pre-cursor molecules to life."

In addition to preparing detectors for these missions, Burks and his team are also involved in a project funded by the Laboratory Directed Research and Development Program to develop a science capability that complements the Laboratory's space-based hardware competencies. Burks explains, "The Laboratory is now viewed as an expert in delivering gamma-ray spectroscopy instrumentation for space exploration. That expertise and our competencies in nuclear science put us in an excellent position to contribute to nuclear planetary science and aid in transferring the technology we've developed for space applications to the next-generation of terrestrial search instruments."

—Ann Parker

Key Words: asteroid belt, detector, Dragonfly, gamma-ray spectrometry, GeMini-Plus, germanium (Ge)-based spectrometer, Japan Aerospace Exploration Agency, Johns Hopkins University Applied Physics Laboratory (APL), Mars-Moon Exploration with Gamma rays and Neutrons (MEGANE), Martian Moons Explorer (MMX), MESSENGER, NASA, New Frontiers program, Phobos, Psyche-16, Saturn, Titan.

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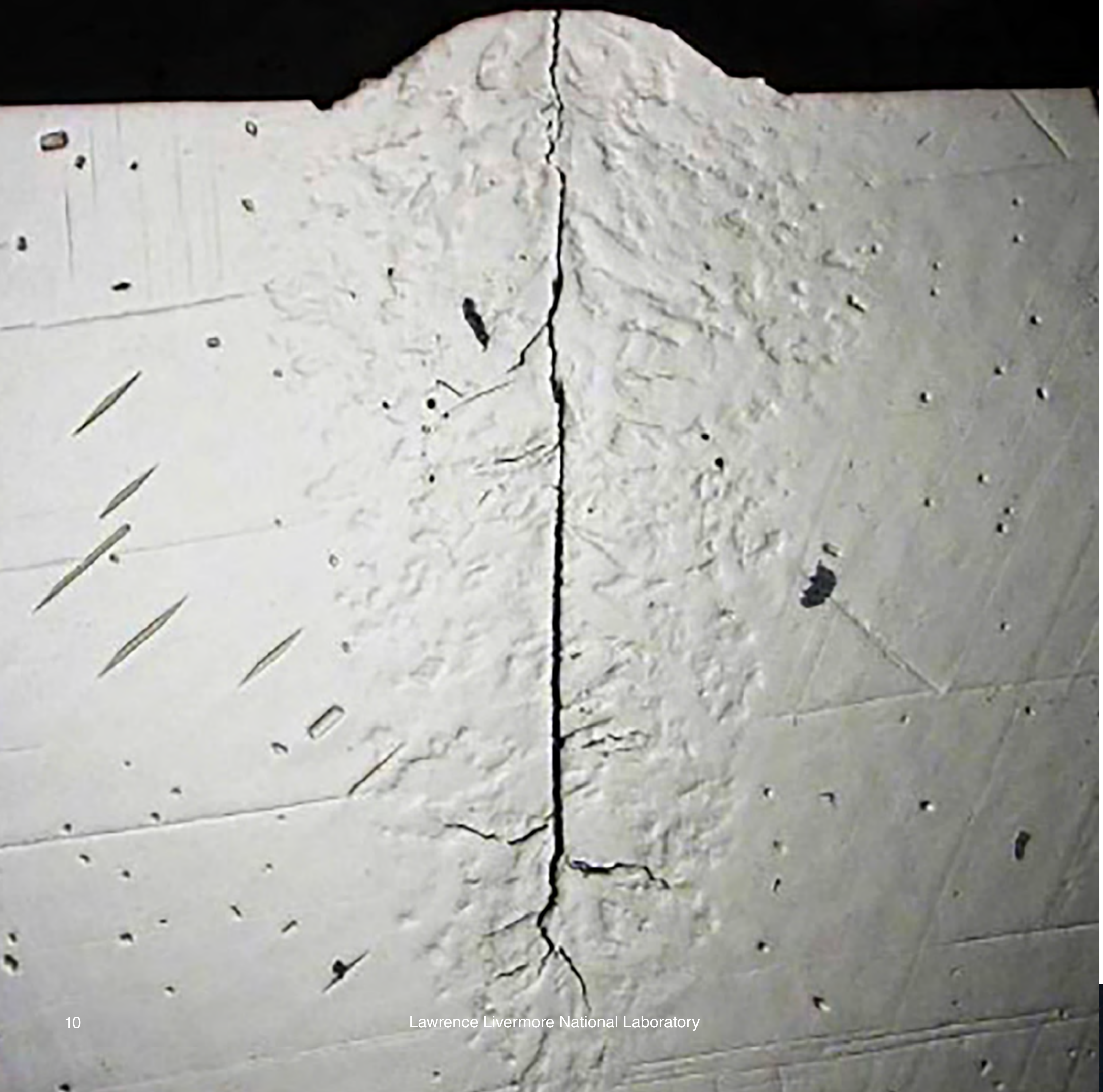
WELDING WITH ASTEROIDS?



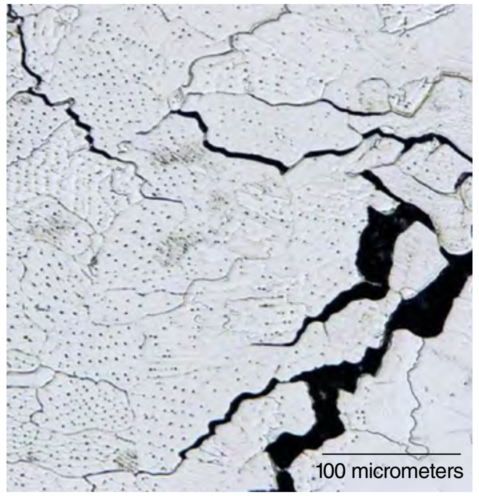
NEWS articles and media outlets regularly buzz with opinions and progress on the future of establishing colonies in space and on the Moon and Mars. Such possibilities, once the stuff of science fiction, are now on the way to becoming science fact. These endeavors will require building and maintaining structures for transportation and habitation.

For off-Earth structures, space adventurers will most likely need materials at hand for fabrication and repairs. Lawrence Livermore materials scientist John Elmer explains, "Transporting large amounts of traditional building materials such as aluminum, titanium, and stainless steel from Earth into space is expensive. Materials for space construction and repairs will most likely come from the Moon, asteroids, or meteorites." Asteroids—large "rocks" orbiting the Sun—and meteorites—asteroids that crash onto planets or moons—often have a high percentage of iron and nickel, two important elements of stainless steel and low expansion, Invar alloys. "People have suggested that perhaps these metal-rich objects could be used for extraterrestrial construction," says Elmer.

Key to construction is the capability to weld. In the 1970s, experiments on NASA's Skylab space station proved the feasibility of electron-beam welding steel in space, where conditions are ideal since the welding technique requires a vacuum to operate. However, the Skylab experiments used high-quality steel that had been refined on Earth to the proper chemistry for welding. Would the same technique work on extraterrestrial material that was rich in iron, the primary element of steel? Elmer decided to find out.

Meteorite Fragments Put to the Test

Elmer rounded up a team, including Livermore's Gordon Gibbs, Lenny Summers, Gil Gallegos, Cheryl Evans, and James Embree, and obtained a 722-gram specimen of the Canyon Diablo meteorite, which plunged to Earth about 50,000 years ago, shattering and forming the 1.3–kilometer-diameter Meteor Crater in Arizona. Nearly 30 tons of fragments of this iron-and-nickel-rich meteorite have been collected, making samples available for research.



(opposite) An electron-beam weld in the iron–nickel meteorite displays a large centerline crack. (above) A magnified image of the weld fusion zone shows where phosphorous compounds resulted in cracks at the grain boundaries.

Specimens were electron-beam welded at the Laboratory in a vacuum similar to the vacuum of space. The welds were several millimeters deep, typical of those needed to join parts. However, the small welds cooled much more rapidly than meteorites. "An asteroid in space can take a hundred million years to solidify and cool from its initial formation, a cooling rate that cannot be replicated here on Earth where solidification and cooling take place in less than a minute," Elmer explains. "I expected that the microstructures of our welds would be considerably different from that of the original meteorite, and they were." The vastly different cooling rates in the laboratory environment combined with the presence of phosphorous, sulfur, and carbon-rich particles scattered throughout the meteorite led to cracks in the welds and a weak joint. "Our experiments showed that welding meteoritic iron in its native state has significant challenges that won't be overcome by welding the same piece of metal over and over and hoping for the best," says Elmer. "However, the challenges are not insurmountable. We just need a different approach."

Refining Space Materials

One intriguing possibility, which Elmer described in a 2018 patent, would be to refine the asteroidal or meteoritical iron using existing elements known to be present on the Moon's regolithic surface. The first step would be identifying an asteroid or meteorite with a high percentage of iron, mining it, and then metallurgically refining the material to remove impurities harmful to steel making and welding. Once refined, the material could be atomized into powder, facilitated by the low-gravity and vacuum of space. "This powder could be used to additively manufacture steel parts using conventional electron-beam or laser-beam 3D printing methods—welding-related processes that also require high-quality metal," says Elmer. He adds that 3D printed parts could be welded together to create larger structures, as on Earth. In fact, the International Space Station and NASA demonstrated the feasibility of printing 3D parts in space in 2014.

Many challenges remain for doing this work using extraterrestrial iron. For instance, refining the metal requires significant amounts of energy, and electron-beam generation requires high voltage power supplies. "Still, it's an intriguing proposition that makes metallurgical sense," says Elmer. "With more innovative thought and experimentation, plus some creative, technical elbow grease, welding in space would become a reality."

—Ann Parker

Key Words: additive manufacturing, asteroid, electron-beam welding, iron, Mars, materials science, meteorite, Moon, space, steel.

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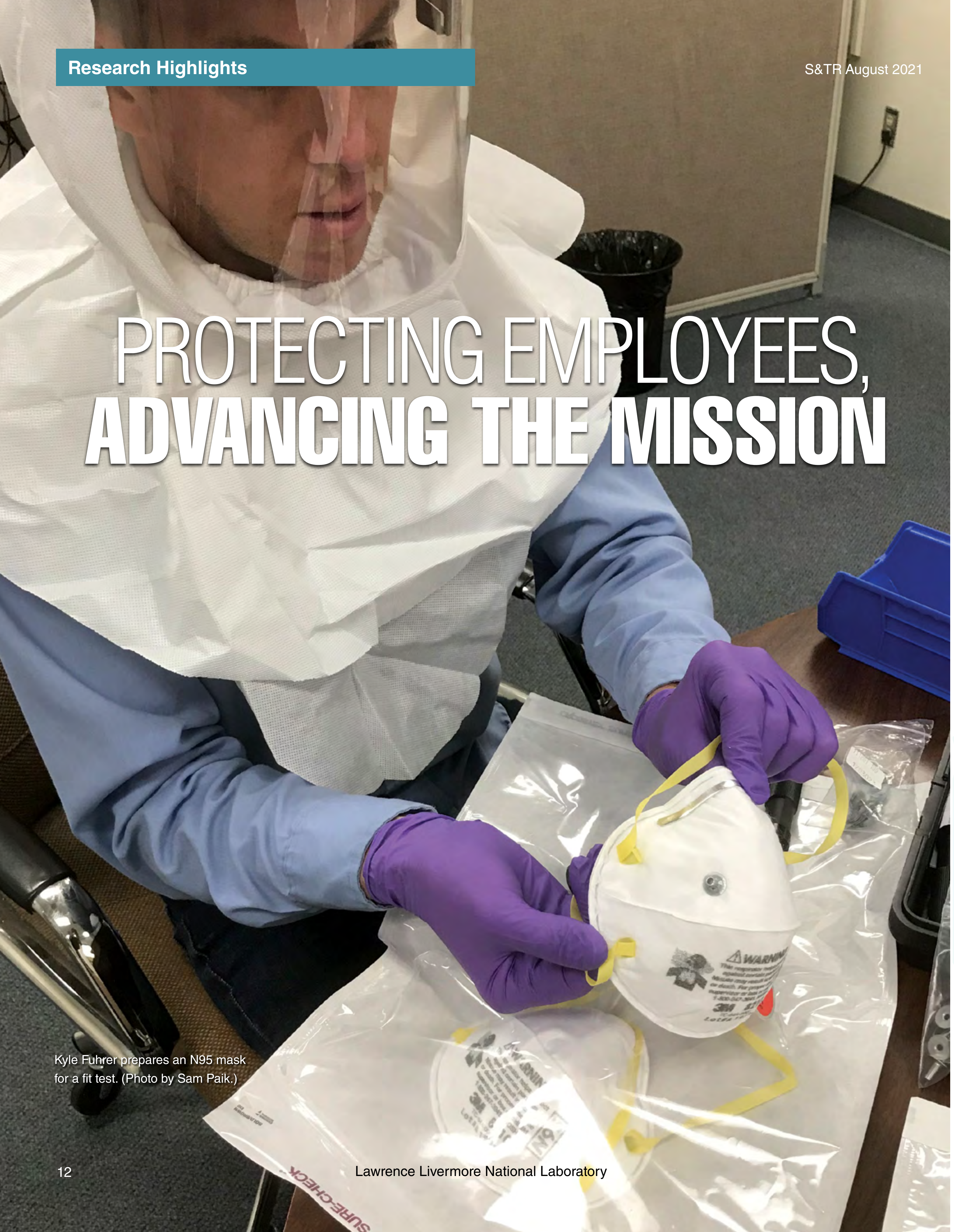

PROTECTING EMPLOYEES, ADVANCING THE MISSION

Kyle Fuhrer prepares an N95 mask for a fit test. (Photo by Sam Paik.)

AS the severe acute respiratory syndrome coronavirus 2 (SARS CoV-2, the virus that causes COVID-19) spread to the United States in early 2020, Livermore reacted rapidly, initiating a Pandemic Response Team (PRT) on February 3, 2020, to activate the Laboratory's pandemic plan. No one expected that the plan assembled in 2009 and updated every few years would be required for as long or have an operational impact as broad as the COVID-19 pandemic demanded. Since then, Livermore has worked diligently to keep employees safe while maintaining mission-critical operations to keep the nation safe.

Priority One: Safe Operations

Kathleen Noonan, a nurse practitioner with training in epidemiology and a shelf full of books about the 1918 Spanish Flu pandemic, stood ready to respond. As mission assurance manager for Livermore's Health Services Department (HSD), she was notified in January 2020 regarding an employee returning from China. "He was our first at-risk patient," says Noonan. "I met him at his Livermore home, asked him to quarantine, and provided him with a mask and cleaning supplies." From that point, HSD clinicians consulted a list of employees traveling outside the United States and isolated those returning from China and other at-risk areas.

On March 16, 2020, officials in Alameda County, California—which includes the city of Livermore—issued a shelter-in-place order to begin at midnight. The same day, then-Laboratory Director Bill Goldstein announced that Lawrence Livermore would move into minimum safe operations, reducing onsite staff to the minimal level required to operate the site and its facilities safely and securely, and to carry out a limited number of mission-critical activities. Overnight, the Laboratory's onsite population went from nearly 8,000 to just a few hundred. Employees who could telecommute were encouraged to do so, onsite visitors were limited, and business travel was restricted—all in an effort to prevent the virus from spreading.

Staff from the Operations and Business Principal Directorate addressed the formidable task of working through a checklist to ensure nonessential equipment and facilities were properly shutdown. The Security Organization implemented its standing plans to keep the Laboratory secure. Within a week, the shutdown was complete, leaving a skeleton crew of maintenance, facilities, and asset managers onsite to keep essential operations running.

Transition to Telecommuting

Shifting thousands of employees to telework placed new hardware and software demands on the Laboratory. While classified work must be conducted onsite, employees performing business functions and unclassified research working from home needed a virtual private network (VPN) to access the Laboratory's unclassified network. "Before the pandemic, about half of the Laboratory's population had VPN accounts," says chief information officer Doug East.

Signing up 3,000 people for a VPN account in one week is difficult. Prior to the shelter-in-place order, Livermore's Information and Technology (LivIT) Program had developed a simplified process to enable and create VPN accounts. LivIT dedicated many hours to add a second VPN service, more than doubling their capacity to meet the new demand. In addition, telecommuting employees required an at-home technology

A timeline illustrates the Laboratory's early response to the pandemic alongside national and local actions.




setup—laptop, monitor, and peripherals. Information technology organizations within each directorate and LivIT worked together to distribute computers as needed, and LivIT assisted with software and account setup.

The next challenge: addressing changes in the way telecommuting employees communicated with one another. In response, applications supporting video conferencing and collaboration such as WebEx, Microsoft Teams, and Jabber were expanded to serve all telecommuters. By late March, most Laboratory employees were teleworking effectively. “Everyone came together and, as a result of our efforts, telecommuting has proved to be a successful and viable form of work, opening the eyes of a lot of managers,” says East.

Other innovations included the implementation of cloud-based cyber protections for Laboratory email and networks and remote updates of software used at the National Ignition Facility (NIF). A secure, online platform to facilitate document review—replacing hard copy review—also came online quickly to keep projects running smoothly.

Planning for Onsite Returns

Just as quickly as the Laboratory moved into minimum safe operations, PRT and senior management began planning for a return to normal operations. Associate Deputy Director for Operations Sandra Brereton managed the Laboratory’s operational response to COVID-19. In that role, Brereton coordinated steps to safely restart mission-critical activities with the National Nuclear Security Administration. She partnered with HSD, the Biosafety Office, and the Environment Safety and Health Directorate to ensure safe onsite return.

Fully masked and maintaining social distancing, groups of managers and biosafety specialists, including Biosafety Office Leader Carolyn Hall, toured essential laboratory facilities to begin calculating how many people could work together in each setting given COVID-19 concerns, assuming everyone was properly masked. Next, the Laboratory adapted its facilities-planning software to determine the appropriate density of employees in shared spaces and to develop a customized plan for every work environment. With the help of the Laboratory’s Emergency Operations Center and the Procurement Department, each department was equipped with personal protective equipment, such as masks and hand sanitizer.

Hall led the effort to create a COVID-19 hotline running 24 hours a day, 7 days a week, which enables any employee exposed to COVID-19 or infected by the virus to call the Laboratory for help. “From the early days of the pandemic, our priority was keeping people safe,” says Brereton. “We were surrounded by uncertainty, asking ourselves ‘How can we ensure physical and mental well-being of the staff and help them navigate the pandemic’s challenges?’” HSD created a COVID-19 case-management team, providing counseling for employees with COVID-19 and implementing additional steps to prevent onsite coronavirus transmission. Employees confirmed to have COVID-19 (or unconfirmed but experiencing COVID-19 symptoms) were required to remain offsite until cleared by HSD to return to work, as were employees exposed to confirmed COVID-19 cases and those who had traveled or attended large social gatherings.

The COVID-19 team recruited and trained employee volunteers to handle contact tracing for employees who reported a positive diagnosis either while working at the Laboratory or within a short time after leaving the site. Livermore developed a database to track COVID-19 cases, providing data on positive cases among Laboratory employees and helpful resources on Laboratory procedures, telecommuting, and coping with COVID-19 at home. For cases confirmed among Laboratory employees, contact tracing suggested that less than a dozen cases may have been attributed to onsite transmission. For those incidences, the team reviewed steps to reduce the likelihood of similar conditions that could lead to reoccurrence.

Resuming Mission-Critical Work

A core group continued working onsite throughout Minimum Safe Operations to ensure essential nuclear facilities remained safe and operable and that activities essential to the nation’s security such as weapon modernization programs and the stockpile review process were uninterrupted. As early as March 2020, the Weapons and Complex Integration (WCI) Principal Directorate initiated planning for the return of other key personnel. Phil Pellette, WCI’s associate deputy director for operations, led the Directorate’s COVID-19 planning efforts. He joined HSD and Biosafety Office staff for walkthroughs of critical facilities, developing a checklist of procedures to bring staff back to each area. Pellette met with other directorate




leaders via WebEx to support their return-to-site planning. “One of the biggest challenges we faced was meshing together different restart procedures and operational methods, as every principal associate director and associate director has unique considerations when managing their facilities,” he says.

Cindy Atkins-Duffin, the principal deputy associate director for the Global Security Prinicpal Directorate, adds, “Balancing mission priority with safety under pandemic constraints was the biggest challenge at hand. Global Security maintains facilities required by the federal government to be available at all times, such as the National Atmospheric Release Advisory Center and the Forensic Science Center.” Lydia Camara, deputy principal associate director for operations in NIF and Photon Science Principal Directorate, adds, “One of our biggest operational challenges was communication. We wanted to give everyone up-to-date and accurate information, and we had to learn to navigate virtual communication methods and outlets together.”

Between April and June 2020, most of the essential facilities returned to operational status. By mid-July 2020, the Laboratory entered “normal operations with maximum telecommuting,” and an average of 3,500 to 4,000 people worked onsite every week. While the Laboratory opened to more staff, HSD and Biosafety experts continued monitoring COVID-19 data. An emphasis on safety and public-health protocols, such as wearing masks and social distancing, kept the virus under control at the Laboratory.

Expanding Health Services

In April 2020, as the demand for COVID-19 testing increased and community testing options remained backlogged, Biosciences and Biotechnology Division’s Thomas Bunt began exploring onsite testing options. Rapid, onsite testing capabilities would enable HSD case managers to make faster, more informed decisions about safeguarding employees. Bunt’s team acquired the equipment and reagents to perform real-time polymerase chain reaction (RT-PCR) SARS-CoV-2 tests, which had been authorized by the Food and Drug Administration during the pandemic. To meet the state of California’s legal requirements for administering the SARS-CoV-2 tests, the team applied for a Clinical and Public Health Laboratory License, registered as a Clinical Laboratory Improvement Amendments (CLIA) “high complexity testing” laboratory, and hired clinical laboratory scientists and a qualified CLIA laboratory director. After receiving the California Department of Public Health certification, Bunt and others worked with HSD to establish and pilot an end-to-end process of patient scheduling, testing, laboratory analysis, and data reporting.

On December 3, 2020, the Laboratory began onsite testing up to 20 tests a day, usually with same-day results. Over the following months the team ramped up to 100 tests per day. In January 2021, the Laboratory received authorization to provide onsite COVID-19 vaccinations to employees (federal employees and federal contractors) when vaccine supplies became available. As of the end of August 2021, HSD had dispensed well over 4,000 shots of the Pfizer vaccine. Vaccinations ramped up again in fall 2021 as the Laboratory supported its remaining unvaccinated employees in advance of a mandate requiring vaccination of federal employees and contractors.

The Laboratory’s Site Occupational Medical Director for the Laboratory, Patrick Keller, points to expanded services addressing unique needs during the pandemic. For example, HSD’s WorkingWell program titled “Health Talks” engages employees in virtual seminars and information sessions, providing updated information and findings on the virus, transition, and treatments. In time, the Laboratory reinitiated health-related activities that had been deferred in the earlier days of the pandemic such as hearing tests, in-person clinical visits, random drug testing, and assurance-testing protocols, among other services.

The Laboratory continues to maintain its COVID-19 operations and carry out its national security missions while maintaining maximum telecommuting where possible. Leaders credit the unified, laboratory-wide effort for such an effective response. “Livermore has exemplified an incredible amount of teamwork,” says Atkins-Duffin. “The entire Laboratory has come together and persevered through all the uncertainty and changes that COVID-19 brought about.”

—Allan Chen

Key Words: COVID-19, Health Services Department (HSD), Livermore’s Information and Technology (LivIT) Program, minimum safe operations, pandemic, Pandemic Response Team (PRT), severe acute respiratory syndrome coronavirus 2 (SARS CoV-2), telecommuting, virtual private network (VPN).

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THREE DECADES OF EXPLOSIVE INNOVATION

SINCE Lawrence Livermore's inception in 1952, Laboratory researchers have been among the nation's leaders in understanding, synthesizing, formulating, testing, assessing, and modeling the initiation systems and energetic materials (EM) that play an integral role in the U.S. nuclear deterrent, conventional munitions, and homeland security. The Laboratory's Energetic Materials Center (EMC), founded in 1991, continues to build upon that critical expertise, enabling scientific investigation in support of the nuclear deterrent and keeping the nation safe from emerging explosives and nuclear proliferation.

EMs—explosives, propellants, and pyrotechnics—store energy and release it precisely as needed, making them foundational to many Laboratory programs. This family of substances can morph from solid to gas nearly instantly, reaching temperatures of thousands of degrees Celsius, and move matter several miles per second. EMC has been the focal point for EM research and development at the Laboratory, launching many of the innovations that have strengthened the national security enterprise and national security efforts around Lawrence Livermore. After 30 years, the center's work is more important than ever as the nation faces increasingly complex nuclear and nonnuclear threats. EMC scientists apply their expertise to develop solutions for Department of Defense (DOD) conventional weapons, explore new ways to detect and defeat homemade explosives for the Department of Homeland Security, and develop strategies to counter the threat of improvised explosive devices for nuclear counterterrorism and counterproliferation.

Vital Expertise

EMC came to life at the end of the Cold War. Former EMC Director Randy Simpson recalls, "The Laboratory had contributed enormously to deterring the Soviets, and we were now shaken by their collapse." At the same time, an anticipated transition away from nuclear testing required weapons scientists and engineers to develop and use more advanced experimental, modeling, and computational capabilities to better understand not only how EMs perform in today's stockpile, but also how the materials' aging processes might affect weapons performance in the future. "People at the Laboratory and nationwide worked to reimagine the nuclear-weapons complex. At Livermore, we strategized how to build upon our best-in-class capabilities to replace underground testing," says Simpson.

Recognizing that expertise in high explosives (HEs)—a type of EM used, among other applications, to trigger nuclear devices—would remain vital to national security, the Laboratory proposed an organization in which chemists, engineers, and physicists would apply broad and deep wells of expertise and resources. The core disciplines of energetic materials maturation would combine with experimentation at world-class facilities, such as the High Explosives Applications Facility (HEAF) and the more remote Site 300, and high-fidelity modeling and simulation to provide the basis for scientific advances in EMs. Thus EMC was established to sustain ongoing HE research and serve four strategic goals: maintenance of needed capabilities for the nuclear-weapons program; development of strategic partnership programs with DOD; the transition of technology to industry from Department of Energy national laboratories; and the advancement of EM science in partnership with universities.

Home to EM "Firsts"

Over the decades, the center has transitioned from a component of stockpile sustainment to an essential player in modernizing the U.S. nuclear, conventional, missile-defense, industrial-capability, and other deterrents. As former director Ron Atkins put it, EMC has become "the country's most important repository of energetic materials expertise." The defense, oil-exploration, mining, and explosives-detection industries benefit as well, using EMC science and technology to optimize materials efficiency for applications as varied as warheads and oil well stimulation, improve operational safety, capitalize on novel materials, and improve radiographic and chemical detection.

New experimental platforms, advanced diagnostics, utilization of next-generation light sources, and techniques for enhanced in situ chemical and physical characterization of HE materials are also being developed. Advanced manufacturing methods aid material discovery to reduce development cycles for scale-up of feedstock materials and improve the responsiveness of manufacturing HE components. The proposed Energetic Materials Development Enclave at Site 300—a partnership between Lawrence Livermore and the Pantex Plant—will drive a new approach to accelerate the adoption of new explosive materials and production capability within the nuclear security enterprise. By working directly with Livermore's production agency partners, the enclave will enable concurrent design and production development and move from concept to production-ready materials seamlessly.

Energetic Materials Center (EMC) team members Albert Nichols, Randy Simpson, Ron Atkins, Ron Lee, Jon Maienschein, Lawrence Fried, and Phil Pagoria show off the precision cylinder experiment from the High Explosives Applications Facility 1-kilogram north firing tank, circa 1998.

Facing New Challenges

Since the mid-2010s, EMC has embarked on its greatest challenge yet with the launch of nuclear modernization efforts at Lawrence Livermore, beginning with the arrival of the W80-4 Life Extension Program (LEP) in 2014, and more recently with the W87-1 Modification Program in 2019. With the W80-4 LEP, the Laboratory leads the charge to develop means to remanufacture PBX 9502, an insensitive high explosive not in production at scale since the early 1990s.

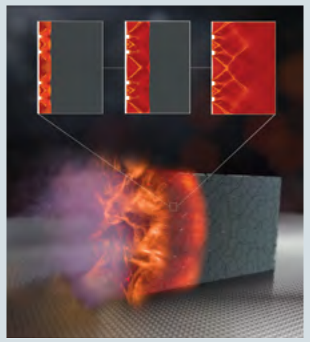
EMC researchers also shepherded development of the novel explosive LX-21, the first new explosive to be introduced into a nuclear warhead without full-scale underground testing. From explosives development and scale-up to production, Laboratory scientists have diligently moved forward. In the last decade, the Lawrence Livermore HE enterprise has earned the HE R&D Center of Excellence distinction, and EMC researchers play a critical role in maintaining the peak level of performance.

"You could say we've been waiting for this moment in time," remarks Lara Leininger, current director of the EMC. "The center has responded to address the magnitude of the

Energetic Materials Landmarks

High-Explosives (HE) Modeling

Lawrence Livermore created the thermochemical modeling codes Ruby, Tiger, CHEQ, and Cheetah. Cheetah is the first, and only, code that is widely distributed, used, and validated both as a stand–alone capability and coupled with a hydrodynamic code. Cheetah simulates detonations, predicting the effects of different chemical



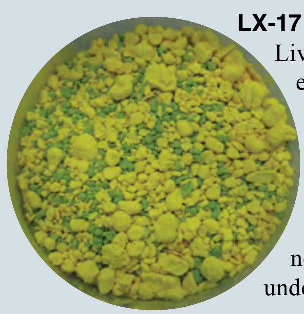
reactants; tracking reactions at the molecular level to obtain velocity and energy; and, using this data, designing optimized explosives with custom characteristics. In 2021, the Cheetah team enabled the code to operate on graphics processing unit–based exascale supercomputers.

The Reaction Sorption and Transport (ReSorT) model, which started as a Laboratory Directed Research and Development (LDRD) initiative and was recently implemented in Livermore's DIABLO simulation platform, was developed by scientists at the Energetic Materials Center (EMC) to assess long-term aging and compatibility of systems including those with energetic materials. The Laboratory's High Explosive Response to Mechanical Stimulus (HERMES), developed in Livermore's ALE3D simulation platform, is the first model to predict a range of post-ignition responses, as pictured above.

New Materials

LX-14

Livermore holds the patent for free-form shaped-charge design and has continued to lead in shaped-charge development including the material LX-14 (left), used in most Department of Defense (DOD) charges, designer wave-shaping, free-form applications, and an emergency severance tool to prevent environmental damage.



LX-17 and LX-21

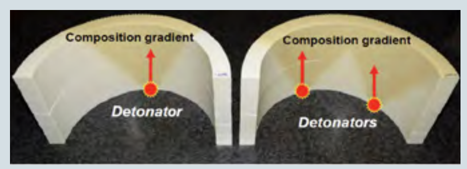
Livermore introduced insensitive high explosive (IHE) LX-17, based on triaminotrinitrobenzene (TATB), into a reentry system with ultrafine-TATB as the booster material. LX-21 (left) is based on the promising IHE candidate Lawrence Livermore Molecule–105 and will be the first new explosive to enter the stockpile without underground testing.

Safe Detonators

The Laboratory invented and implemented the Mechanical Safe Arming Device (MSAD) and the Slapper detonator (below), which prevents accidental or unintended detonation of a nuclear warhead in National Nuclear Security Administration and DOD custody, as demonstrated in cut-back experiments with LX-21 (above). MSAD is a discriminator stronglink—a critical component for nuclear safety requirements—that protects the nuclear weapon by preventing any potential activation from outside sources.

Advanced Manufacturing

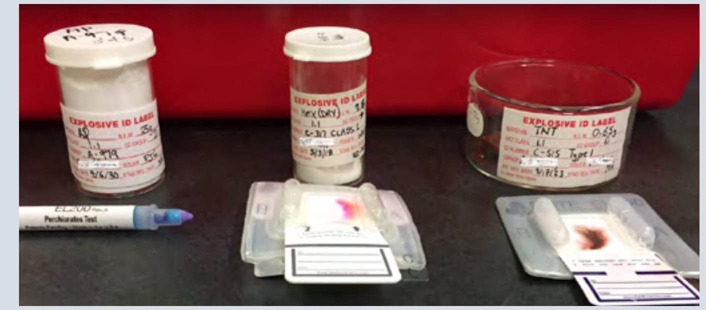
Livermore has always been an early-adopter of advanced manufacturing techniques including injection-molding for high-



power, high-precision applications, and the first-ever use of microreactor synthesis in the demonstration of continuous synthesis processes. The Laboratory has pioneered the use of direct-ink writing (DIW) for complex, multimaterial, explosive components and recently printed the first-ever kilogram-scale additively manufactured explosive and detonated it in the High Explosives Applications Facility. The resulting additively manufactured explosive test articles (above) were part of a proof-of-concept study. The image shows the test articles, with either one or two triangular regions of a "fast" detonation velocity explosive (white regions) printed with a "slow" explosive (mustard-colored regions). These composite charges were detonated on one edge (one detonator on the left and two detonators on the right), and the detonation propagated along the longitudinal direction of the hemicylinders as indicated.

Experimentation

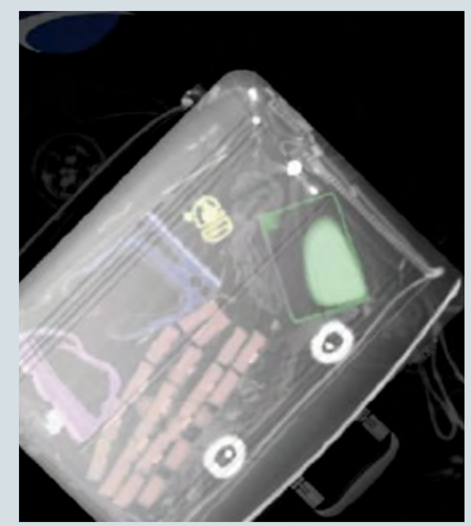
Two LDRD initiatives led to the development, design, and implementation of the first-ever explosives experiments at Argonne National Laboratory's Advanced Photon Source Dynamic Compression Section, the OMEGA Laser Facility at the University of Rochester, and the National Ignition Facility. Performance and safety data on detonators and explosives were captured for the first time, improving the understanding of the materials' performance and aging. An artist's rendition depicts the experiment in which a laser impacts a thin HE material target (shown in yellow) and the chemical reaction results in solid-carbon products (black shapes).



Diagnostics

Livermore developed handheld explosive detection protocols, some of which have been commercialized. Improvements are ongoing with two patents granted since 2018. Pictured above, the pocket-sized E.L.I.T.E.™ (Easy Livermore Inspection Test for Explosives) kit—a 2006 R&D100 Award winner and Federal Lab Consortium Award winner—uses chemical reactions to quickly detect explosives.

The Livermore Explosives Detection Program provides end-to-end characterization of explosives and other threats including algorithm development to enable the Department of Homeland



Security and the Transportation Security Administration to identify suspicious items in checked bags and differentiate explosives from harmless items. At left are samples of computerized tomography data from samples prepared and characterized by EMC and Non-destructive Characterization Institute scientists at HEAF.

Publications

EMC's *High Explosives Reference Guide*, following on from the first HE Handbook developed at EMC, is the standard for the documentation and distribution of critical explosives manufacturing, performance, and safety data and serves more than 1,300 users from the National Security Enterprise, DOD, and other government agencies. EMC also coedits *Propellants, Explosives, Pyrotechnics*, the largest scientific journal in the field.

Today's EMC team includes a blend of early career and veteran scientists.

challenges faced today. Our collaboration with colleagues in both the Weapons and Complex Integration and Global Security Principal Directorates has been excellent."

Looking toward the 2030s and beyond, the center aims to enable the study of a reacting material at nanosecond resolution and micrometer-length scales not previously possible. Future advances require scrutiny of predictive codes, taking advantage of graphics processing unit architectures and applying machine learning and data science. Other priorities include diagnostics to measure the temperature and product set of chemical reactions in situ at these shorter time and length scales; accelerated materials development through responsive and agile manufacturing and data science techniques; and development of new HE molecules by leveraging high-performance computing, computational chemistry, and scalable manufacturing processes.

Aggressive schedules have called for increased testing at a pace not seen for decades, and EMC plans to remain the first place the National Nuclear Security Administration, DOD, and other government agencies think of when they need energetics expertise. Says Leininger, "After 30 years, the Energetic Materials Center is ready and agile for whatever comes next."

— Margaret Davis and Ben Kennedy

Key Words: Department of Defense (DOD), Department of Energy, Department of Homeland Security, Energetic Materials (EM), Energetic Materials Center (EMC), Energetic Materials Development Enclave, High Explosives Applications Facility (HEAF), LX-21, National Nuclear Security Administration, nuclear test ban, PBX 9502, stockpile stewardship.

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EMBRACING RISK FOR TRANSFORMATIONAL RESULTS

A target assembly for plasma amplifier experiments combines beams inside a plasma created within each of two gas-filled bags situated at the center of shields to block stray light. The combined beams impact the tantalum disks in the center, and the resulting x-ray emission is used to measure beam intensity.

THE Department of Energy's Laboratory Directed Research and Development (LDRD) Program has been an engine of discovery for almost 30 years, investing in research that strengthens and advances Livermore's core competencies, develops future scientific leaders, and grows Livermore's intellectual property catalog. In 2018, the Laboratory initiated a pilot program for Disruptive Research (DR) projects to support the pursuit of exceptionally innovative ideas with the potential to open new research directions.

"All LDRD projects are high-risk, high-reward," says LDRD Program Director Doug Rotman. "In designing the DR pilot, we sought even more unconventional ideas, motivating the entire Laboratory to embrace scientific and technical risk to achieve mission-critical, transformational results." An interdisciplinary committee developed the pilot and crafted a call for proposals focused on disruptive ideas and high-risk tolerance. DR proposals identify the largest barrier to project goals and a strategy to surmount that barrier as early as possible, while also charting go–no-go decision points along with way.

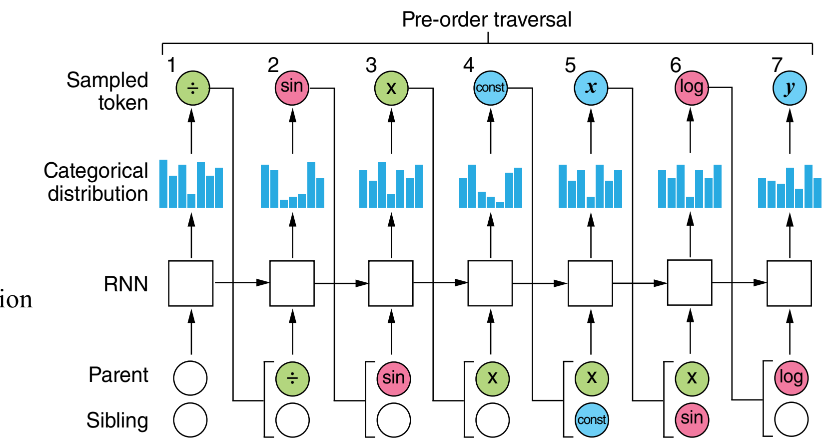
After down-selecting from the more than 80 white papers received, the committee selected nine proposals for the initial round of DR funding—between $400,000 and $2 million per year for up to three years. Project mentors meet with each team quarterly to discuss ideas, challenges, solutions, and exit strategies. "As scientists, we're trained to look for risk-mitigation strategies," says Materials Engineering Division Leader Chris Spadaccini, DR committee chair. "When designing the DR program, however, we took a different approach to managing risk. We hoped to inspire culture change at the Laboratory by investing in high-risk ideas and, if appropriate, accepting that researchers move on when results point in a different direction." The following projects, now in their third year of funding, represent the breadth and creativity of Livermore researchers selected for the pilot program.

Outside the Black Box

Historically, physicists have described fundamental knowledge using equations from which they derived follow-on discoveries. "From a simple physics equation like 'force equals mass times acceleration ($F = ma$),' you can, by inspection, glean insights and understanding about the underlying physical process," says computer scientist Brenden Petersen, who leads one of the DR projects. Artificial intelligence (AI), however, generates data without providing any interpretation. Deriving a mathematical expression to fit a data set—a problem known as "symbolic regression"—presents a challenging task for AI.

Models used in deep learning, a branch of machine learning that relies on neural networks to perform complicated functions such as image recognition, are considered black boxes. Researchers cannot easily interpret a neural network or explain its decision making. Petersen asks, "Can we use neural networks, these large models, to derive a small model—a mathematical equation—that makes predictions about the data?" The answer turns deep learning on its head. His team developed algorithms that use large neural network models to generate simple equations—not large, opaque models—and discard the neural network in the end. This disruptive concept leverages the power of deep learning while bypassing the need to interpret a neural network.

Petersen's team has developed and tested an algorithm that uses a recurrent neural network (RNN) to randomly generate mathematical expressions as sequences then train the model to generate better-fitting expressions. Each item in the sequence—whether a variable or a mathematical operator such as cosine—is drawn from a library of tokens. The algorithm samples expressions and trains the model using fitness to the data set as



In this potentially disruptive approach to generating simple equations that describe highly complex data sets using a recurrent neural network (RNN), each term in an equation such as a variable or mathematical operator is represented as a token (shown as circles, above). RNN emits a distribution over tokens, a token is sampled, and the parent and sibling of the next token are used as the next input. Subsequent tokens are sampled until the tree representing the mathematical expression is complete.

a learning signal. A paper describing the team's work ranked fifth out of nearly 3,000 submissions to the 2021 International Conference on Learning Representations.

The algorithm has broad applications such as learning interpretable strategies for optimal control or designing antibodies to bind to a particular pathogen. In this application, different amino acids take the place of operators like sine and cosine, and the algorithm uses binding affinity as a learning signal. In the project's final year, the team will test their framework for other discrete optimization problems.

Quantum Computing Leap

The collisions of atomic nuclei, and their constituent neutrons and protons (collectively called nucleons), power the evolution of stars and other astrophysical phenomena, create most of the universe's elements, and inform nuclear weapons stockpile stewardship. However, even with today's most powerful high-performance computing (HPC) machines, nuclear dynamics simulations add a high degree of difficulty as one additional particle can increase the number of equations exponentially. Livermore researcher Sofia Quaglioni leads a DR project to develop methods for performing complex nuclear calculations on a prototype quantum computer.

Livermore's Sierra computer, one of the world's fastest systems at 125 petaflops (125 quadrillion floating-point operations per second), represents a giant step over the Laboratory's first supercomputer, the Univac, installed in 1953.

> “Our simulation achieved more than 99 percent fidelity and a one-hundred-fold improvement in simulation time—500 timesteps versus less than six—compared to previous simulations on digital quantum computing platforms.”

The jump from classical to quantum computers could be as great a leap in computing power. Quantum computers use quantum states known as qubits to encode and process an exponentially larger amount of information than classical computers using bits, making them ideal to simulate nuclear dynamics. “However, quantum computers are still very experimental and, like the vacuum tube circuits of the 1950s, prone to error,” says Quaglioni.

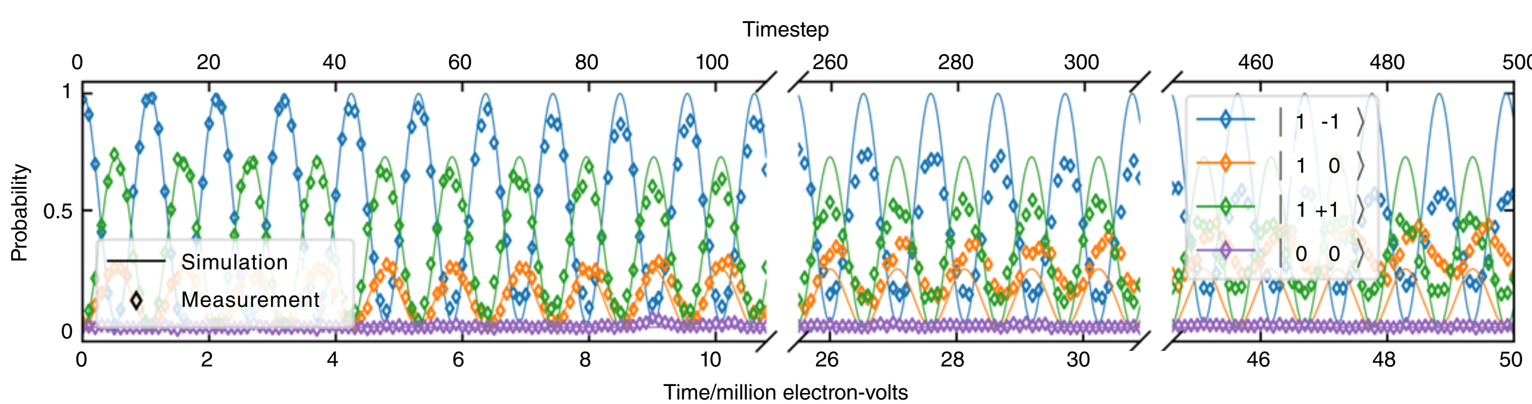
Sources of noise from uncontrollable physical processes in the equipment and in the environment around the quantum processor perturb and disrupt the operational fidelity of the qubits. Quaglioni’s DR project set out to establish an unconventional protocol resilient to the quantum noise and then demonstrate nuclear dynamics simulations on Livermore’s quantum computing test bed. The protocol employs a minimal number of continuous gates—discrete, preset quantum-logical operations—customized to realize the desired nuclear dynamic interaction rather than long sequences of gates typical in quantum computing. The team has tested its approach, demonstrating the evolution, with time, of two interacting neutrons. “Our simulation achieved more than 99 percent fidelity and a one-hundred-fold improvement in simulation time—500 timesteps versus less than six—compared to previous simulations on digital quantum computing platforms,” says Quaglioni.

The relatively simple two-particle simulation benchmarks the method’s performance. The protocol developed will increase quantum simulation capabilities by multiple orders of magnitude, enabling near-term quantum computing platforms to address a broad class of problems. “Quantum computers offer the promise of a unified approach to nuclear dynamics simulations from 5 to 250 nucleons,” says Kyle Wendt, a staff scientist working with Quaglioni. “The same simulations would require hundreds of millions of hours of computer time on a classical, digital HPC system.”

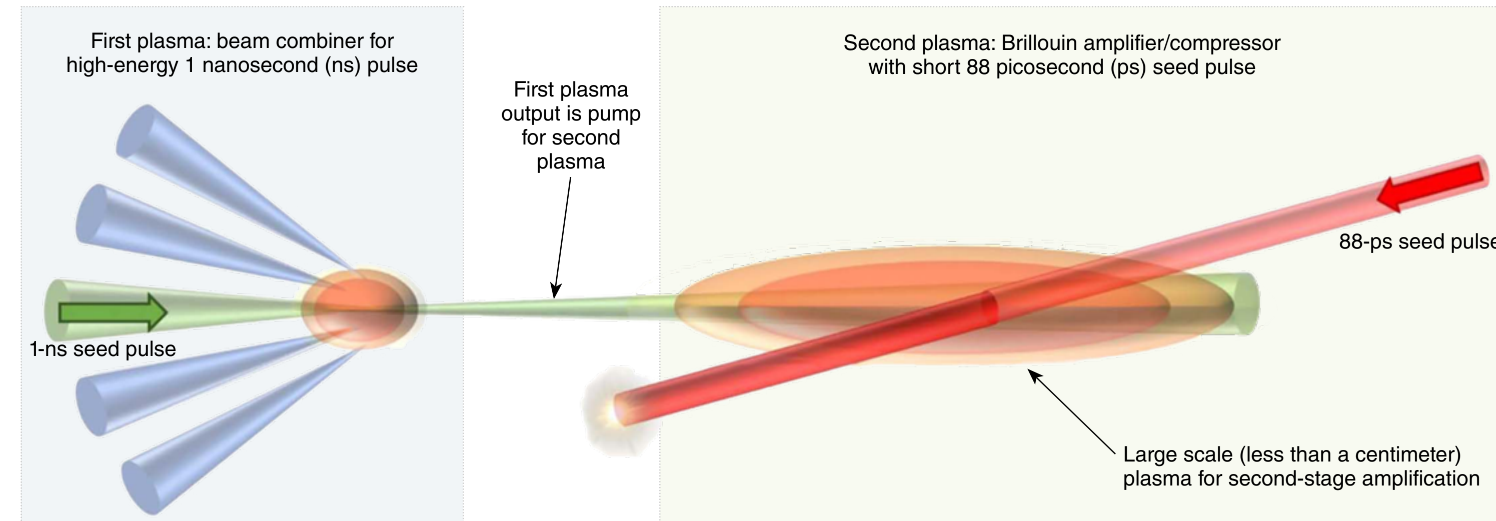
Plasma Optics for Brighter Lasers

The first lasers used crystals to generate beams of coherent light, earning a Nobel Prize for the inventors. By the late 1960s, lasers reached intensities of 10^{15} watts per square centimeter (W/cm^2). With the invention of chirped pulse amplification, ultrashort laser pulses can be amplified up to 10^{23} W/cm^2. (Donna Strickland, who worked at Livermore, shared the Nobel Prize for this development.) Further intensity increases have stalled because forcing more energy through solid laser optics damages the optics material or causes it to shatter. A DR project led by Patrick Poole aims to significantly increase laser power and intensity using plasma as the amplifying medium.

Plasma optics can be generated and manipulated, replacing conventional solid optics that have reached damage thresholds.



The output of a quantum simulation of two-neutron dynamics run on the Livermore quantum computing test bed shows the probability of finding the two neutrons' spins in a particular quantum state as a function of time. Colored symbols depict the output probability as a function of the simulation timestep. Solid lines represent the corresponding exact probabilities obtained using a classical computer.



Following the success of experiments to combine laser beams without damaging plasma optics, Laboratory researchers plan to use the original beam combiner (left) to produce a 1-nanosecond (ns) seed pulse that will feed into a second plasma amplifier to produce a shorter, more intense pulse of 88 picoseconds (ps) and further expand experimental applications.

Poole’s work takes a new approach to optics that builds on recent research at Livermore’s National Ignition Facility (NIF). A team of investigators combined several laser beams within a plasma (a high-temperature gas of ions and electrons) to create a single beam of 10 times higher energy than the original seed beam. Plasma optics advanced the power and intensity of lasers, boosting their ability to probe the physics of matter and energy.

Poole’s team has developed a plasma optic using a 10-millimeter plastic balloon filled with C_5H_{12} (pentane) gas, irradiating it with a cluster of laser beams in a prescribed sequence, heating the gas to a plasma, generating a high electron density, and then producing the output beam. In experiments at NIF, the researchers combined 21 laser beams into one with almost three times the intensity a single NIF beam could produce without damaging its solid optics. The team has demonstrated that the combined beam maintains its focusing properties after amplification, meaning it can be used for high-energy, single-beam applications, such as those where the target is too small to allow many beams inside.

With project milestones already reached—to create a higher energy beam with the high focus required for experimental use—the researchers will model and execute an experiment that produces a second plasma optic to reduce pulse time to below 88 picoseconds and use more plasma to boost the shorter pulse to even higher power. By focusing this amplified light at about 10^{24} W/cm^2, the research team hopes to demonstrate the possibility that beams can exceed the thresholds anticipated for next-generation, high-intensity laser facilities. “A number of applications at NIF could use a beam of this intensity to unlock new physics,” says Poole.

More Results on the Horizon

Beyond the potentially high-impact results of the LDRD Program’s inaugural DR projects, the researchers’ work has attracted follow-on research at Livermore. Project teams have also gained important information from the experimental paths that do not go as planned.

“Disruptive research involves risk, and we understand that some projects will not attain their original goals,” says Rotman. “Our message to investigators, and everyone at the Laboratory, is that pushing the envelope is great, and we should applaud efforts to spark transformative change. The teams leading our first group of DR projects have embraced these values to achieve truly disruptive research and results.”

—Allan Chen

Key Words: chirped pulse amplification, deep learning, disruptive research (DR), Laboratory Directed Research and Development (LDRD) Program, laser, machine learning, National Ignition Facility (NIF), neural networks, nuclear dynamics, nucleon, plasma amplifier, quantum computer, qubit, recurrent neural network (RNN), Sierra, Univac.

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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- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (https://www.uspto.gov).

Patents

Compounds for Reactivation of Acetylcholinesterase and Related Compositions, Methods, and Systems
Carlos Valdez, Nicholas Be, Brian Bennion, Tim Carpenter, Heather Enright, Felice Lightstone, Mike Malfatti, Margaret McNerney, Tuan Nguyen
10,590,498 B2
March 17, 2020

Engineered Microcompartment Protein and Related Methods and Systems of Engineering Bacterial Systems for Non-Native Protein Expression and Purification
Mimi Cho Yung, Timothy Carpenter, Tek Hyung Lee, David Savage
10,738,090 B2
August 11, 2020

Method and System for Compact Efficient Laser Architecture
Andrew James Bayramian, Kenneth Manes, Robert Deri, Al Erlandson, John Caird, Mary Spaeth
10,777,964 B2
September 15, 2020

Tool for Shared Engineering Mesh-Run Integration with Version Evolution Tracking
William Elmer
10,930,067 B2
February 23, 2021

Electrochemical Flow-Cell for Hydrogen Production and Nicotinamide Dependent Target Reduction and Related Methods and Systems
Paul Hoeprich, Jr., Sangil Kim
10,934,628 B2
March 2, 2021

Object Discrimination Based On a Swarm of Agents
Reginald Beer, David Chambers, Hema Chandrasekaran
10,935,635 B2
March 2, 2021

Integrated Telescope for Imaging Applications
Brian Bauman, Alexander Pertica
10,935,780 B2
March 2, 2021

Imaging System and Method for Enhanced Visualization of Near Surface Vascular Structures
Stavros Demos
10,939,869 B2
March 9, 2021

Microporous Membrane for Stereolithography Resin Delivery
Joshua Deotte
10,946,580 B2
March 16, 2021

Genetically Engineered Foot and Mouth Disease Virus and Related Proteins, Polynucleotides, Compositions, Methods, and Systems
Aida Reider, Teresa De Los Santos, Luis Rodriguez, Devendra Rai, Fayna Diaz-San Segundo, Paul Hoeprich
10,953,085 B2
March 23, 2021

Non-Destructive, In-Situ Evaluation of Water Presence Using Thermal Contrast and Cooled Detector
Mihail Bora
10,962,417 B2
March 30, 2021

Click-Chemistry Compatible Structures, Click-Chemistry Functionalized Structures, and Materials and Methods for Making the Same
Patrick Campbell, Eric Duoss, James Oakdale
10,962,879 B2
March 30, 2021

Preparation of Large Ultrathin Free-Standing Polymer Films
Michael Stadermann, Salmaan Baxamusa, William Floyd III, Phillip Miller, Tayyab Suratwala, Anatolios Tambazidis, Kelly Youngblood, Chantel Aracne-Ruddle, Art Nelson, Maverick Chea, Shuali Li
10,968,325 B2
April 6, 2021

System and Method for Focal-Plane Illuminator/Detector (FASID) Design for Improved Graded Index Lenses
Jeffrey Bude, Eyal Feigenbaum
10,969,300 B2
April 6, 2021

Awards

Bronis R. de Supinski, chief technology officer for Livermore Computing (LC), was named one of ***HPCwire's* People to Watch**, a list of top influencers in the high-performance computing industry for 2021. The magazine recognized de Supinski, a two-time Gorden Bell Prize winner, for his work in devising and executing Livermore's large-scale high-performance computing strategy including the upcoming exascale-class system, El Capitan, and his selection as general chair for the 2021 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC21).

Three Lawrence Livermore postdoctoral appointees—**Oluwatomi (Tomi) Akindele, Matthew Edwards and Wei Jia Ong**—were **selected to attend the 70th annual Lindau Nobel Laureate meeting**, an international forum in which students and postdocs meet with 30 to 40 Nobel laureates to foster an exchange among scientists of different generations, cultures, and disciplines. Akindele researches the use of antineutrinos to detect the operational status of a nuclear reactor at a distance. Edwards studies light and plasma applied to building next-generation lasers and accelerators. Ong applies an interdisciplinary approach to investigate the origins of heavy elements in the cosmos.

Abstract

Planetary Research: Exploring our Past and Future

As represented by the work of four Lawrence Livermore research teams, the Laboratory's foundational research in astrophysics, nuclear science, cosmochemistry, and data science and its state-of-the-art facilities yield a fascinating range of discoveries that inform the origins of space and generate tools for new breakthroughs. A computational chemist leads research to simulate past extraterrestrial events, such as cometary impact, that sparked the organic precursors of early biomolecules, and, ultimately, the building blocks of proteins. In other work, cosmochemists use nuclear forensics to study meteorites and Moon rock samples from the Apollo missions to understand the sequence and timing of the solar system's evolution. A collaborative team from Livermore and Johns Hopkins University Applied Physics Laboratory develops gamma-ray spectrometers small enough to hold in one hand yet rugged enough to operate onboard vehicles exploring the moons of Mars and Saturn. Finally, Laboratory materials scientists study meteorite specimens to propose welding technologies for building colonies in space and on other planets. As these, and similar, research projects progress, the nation and the world will gain more answers to questions about our past and our future in space.

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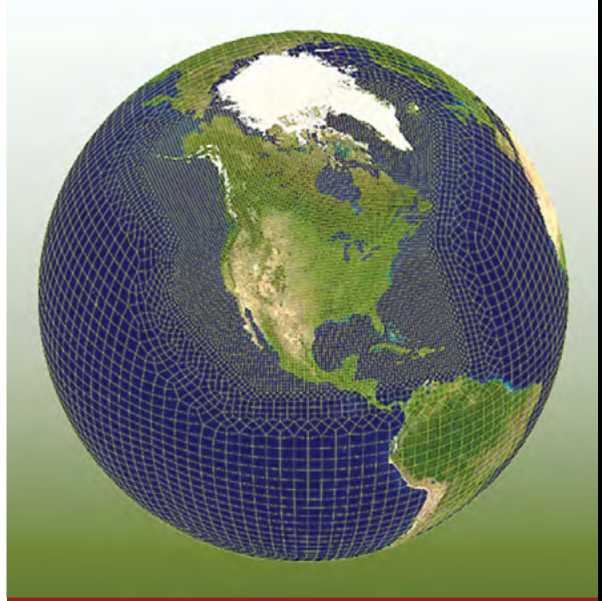
A Clearer Picture of Climate Change



Advanced computer models, simulations, and analysis capabilities help scientists zoom in on earth-system processes and improve climate research.

Also in the next issue:

- *Tools to support data processing workflow reveal the multifaceted nature of traumatic brain injury.*
- *Lawrence Livermore's Distinguished Member of Technical Staff Program awards leaders on the scientific career path.*
- *Nanosatellites take thousands of images of space and Earth thanks to a Laboratory–industry partnership.*

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