Lawrence Livermore National Laboratory

Science & Technology Review

March 2021

SIMULATING BIG ENERGY

Also in this issue:

Hydrogen Vehicles

Plutonium Detection

Extreme Blood Tests

About the Cover

Scientists at Lawrence Livermore National Laboratory have always thrived on collaboration and innovation. Research into inertial confinement fusion (ICF) is paying dividends toward the Laboratory's most important mission: keeping the nation's nuclear deterrent safe and reliable. The feature article beginning on page 4 outlines the ways in which stockpile stewardship benefits from ICF and what the path forward looks like for both. On the cover are Livermore scientists (from left) Daniel Casey and Annie Kritcher.

Cover design: Alii Diaz, Photo by 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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Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 422-1266. Our e-mail address is str-mail@llnl.gov. S&TR is available on the Web at str.llnl.gov.

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S&TR Staff

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***S&TR* Online**
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Print Coordinator
Chris Brown

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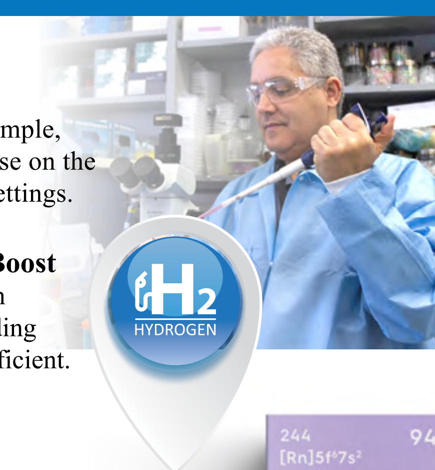
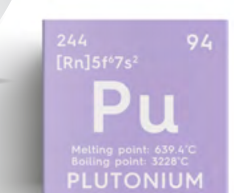




Departments

Learning about the products of supernovae

When a supernova explodes, streams of its plasma flow together and through one another, producing filament-like structures that create their own magnetic and electric fields via the Weibel instability. These fields produce even more filaments, until they become so strong that the filaments stop flowing and a collisionless shock is produced. The concentration of particles produced by these explosions is very low; some particles might travel light-years without colliding. In a paper recently published by *Physical Review Letters*, a team of researchers including scientists from Lawrence Livermore National Laboratory details the first quantitative measurements of the magnetic field structure of plasma filamentation driven by the Weibel instability.

The powerful magnetic fields associated with the shock have another effect: their turbulent motion in the plasma accelerates charged particles to high energy, producing cosmic rays that can be observed on Earth.

Using the OMEGA facility at the University of Rochester's Laboratory for Laser Energetics, the team heated pairs of 1-millimeter-diameter beryllium disks using 1-nanosecond laser pulses. The heated surfaces expanded, producing plasma flows with peak speeds of 3.3 million miles per hour. The researchers collided the flows and studied the behavior of the plasma at the collision center using the optical Thomson scattering diagnostic, which measures the temperature, density, and velocity of the plasma streams. This process enabled direct observation of the formation of plasma filaments due to the Weibel instability and measurement of the current and magnetic field associated with those filaments.

Contact: George Swadling (925) 423-8289 (swadling1@llnl.gov)

Fighting COVID-19 with machine learning

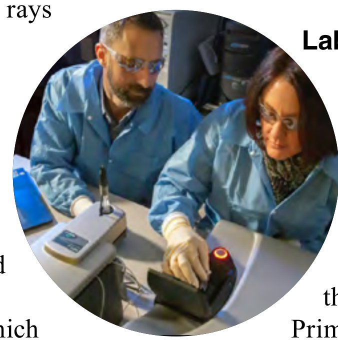
A team of Livermore materials and computer scientists are applying sophisticated machine-learning tools to the fight against COVID-19. Using state-of-the-art natural language processing, image analysis, computer vision, and visualization techniques, machine-learning tools are scanning nanomaterials literature to determine if information can be extracted and help accelerate COVID-19 research. The paper appears in the May 13 *Journal for Chemical Information and Modeling.*

Nanomaterials are widely used at the Laboratory. Their shape, size, and composition can impart unique optical, electrical, mechanical, or catalytic properties needed for a particular application. However, synthesizing an individual nanomaterial and scaling up its production is often challenging because a small change in the process or the addition of a specific chemical can have a dramatic effect on the product. These effects have historically only been discovered by time-consuming trial-and-error experimentation and by reading the scientific literature.

The new machine-learning tools have enabled the creation of a personalized knowledge base for nanomaterials synthesis that can be mined to help inform further development. Starting with approximately 35,000 nanomaterials-related articles, the team developed models to classify articles according to the nanomaterial's composition and morphology, extract synthesis protocols from within the article text, and extract, normalize, and categorize chemical terms within synthesis protocols.

In addition to processing articles' text, microscopy images of nanomaterials within the articles are automatically identified and analyzed to determine the nanomaterials' morphologies and size distributions. To enable users to easily explore the database, a complementary browser-based visualization tool was developed that provides flexibility in comparing subsets of articles of interest.

Contact: Anna Hiszpanski (925) 422-8987 (hiszpanski2@llnl.gov)



LLNL researchers Nick Fischer and Amy Rasley are characterizing nanolipoprotein particle vaccine formulations using a dynamic light-scattering instrument. Detailed characterization of the nanoparticles provides an important quality-control metric for vaccine development. Photo by Julie Russell/LLNL

Laboratory team helps develop tularemia vaccine

Two Lawrence Livermore researchers who have worked to develop a tularemia vaccine are part of a three-institution team that has been funded to make their vaccine candidate ready for use.

The two biomedical scientists, Nick Fischer and Amy Rasley, have worked for eight years on this research and will collaborate with scientists from the University of New Mexico and the Tulane National Primate Research Center under a five-year, $7.5 million grant from the Defense Threat Reduction Agency.

Using the candidate vaccine, the LLNL scientists have demonstrated the ability of a subunit vaccine, incorporating different antigens from the *Francisella tularensis* bacteria into a single particle, to protect against high doses of this bacteria when aerosolized. *F. tularensis* is the bacteria that causes the disease tularemia, more commonly known as rabbit fever.

The scientists will build on a nanotechnology—called nanolipoprotein particles (NLPs)—that was developed at the Laboratory for delivering vaccines and drugs inside the human body. Using the NLPs as a delivery platform, the *F. tularensis* antigens can be co-delivered with another molecule, which stimulates the immune response against the antigens. Lab researchers see NLPs as flexible tools that can broadly be applied to developing vaccines for different pathogens.

F. tularensis is classified as a class-A, high-priority pathogen and select agent by the Centers for Disease Control and Prevention. It is considered a potential biothreat agent based on its extremely low infectious dose. Disease manifestations vary depending on the route of exposure. It is an infectious disease that can cause fever, skin ulcers, enlarged lymph nodes, pneumonia, and throat infection with inhalational disease (pulmonary tularemia) being most severe.

Contact: Amy Rasley (925) 423-1284 (rasley2@llnl.gov)

Pursuing Ignition for National Security

WHEN the United States ended underground nuclear testing in 1992, Livermore was faced with a grand challenge: developing a range of proficiencies that would ensure the safety, security, and effectiveness of the nation's nuclear stockpile without further explosive nuclear testing. Having a strong nuclear deterrent sends a signal to our country's adversaries that—whatever capabilities they bring forward—we, as a nation, are ready and able to respond.

The Stockpile Stewardship Program (SSP) was created in 1995 with the goal of improving the science and technology for assessing the aging nuclear weapons stockpile without requiring additional nuclear testing. The competencies brought to bear on this challenge include advanced computing and predictive modeling, sophisticated experimental facilities, and a cadre of technical experts that is second to none. Livermore has consistently pioneered the use of large, high-speed computers to run the sophisticated simulation codes essential to the SSP. Such codes are incredible tools, but they can only know what we know. So, it is critically important that we test these tools against very complex experiments, such as those we conduct at the National Ignition Facility (NIF). At NIF, we explore realms of extreme temperatures and pressures where our understanding of the physics is not complete. One such realm is that of thermonuclear burn or fusion "ignition," in which the energy output from a controlled fusion reaction is greater than the energy required to sustain the reaction. From the very beginning, the SSP's goal has been to develop a method to study ignition, the gateway to enabling direct access to weapon conditions, in the laboratory.

The pursuit of ignition also provides an important function for the weapons design community. The Laboratory is responsible for recruiting, training, retaining, and, perhaps most importantly, challenging current and future stockpile stewards. The quest for ignition allows them to practice the "art of design" and test their technical judgment against real data on both ignition and other weapons-related experiments at NIF. Ultimately, it is the technical judgments of these stockpile experts that provides the foundation of confidence in the nation's nuclear deterrent.

Over the time of NIF's operation, we have made amazing progress and have learned much about ignition, about weapons modeling and simulation, and about the NIF system and its diagnostics. The journey to date has brought us unprecedented insights, and we now understand the key impediments to achieving ignition and how to approach solving them.

Still, achieving ignition is not a "sure thing." It is truly a technical grand challenge of our era. We will need to push the laser, our precision target fabrication capabilities, and our diagnostic tools to the full extent of their capacities. As we continue this quest, we seek to either reach ignition or establish what's needed to achieve it in the next-generation facility. We embarked on this journey without guarantees that the destination is within our grasp. But that is the nature of science, particularly science conducted at the frontier. Science is a process of trying, learning, adapting, trying again. Failure—that dreaded "f" word—is an essential and unavoidable part of the process. In failure, we learn, and from learning we move forward.

We have come a long way since the early days of stockpile stewardship. Our understanding of weapons physics, material properties under extreme conditions, and even the data collected from long-ago nuclear testing, has increased tremendously due to our more sophisticated tools and capabilities. The progress that we have made in addressing the ignition challenge has brought a new generation of extraordinary people to the Laboratory: people who will carry stewardship of the stockpile into the future.

With every step along the way—every new experiment, diagnostic, design, or code—we accumulate new knowledge and insights into the heart of the systems that form the foundation of the nation's nuclear deterrent. The nation benefits from every new steward who is attracted to join our team, and is then retained and challenged by the world-class science and technology we seek and develop. The pursuit of ignition is perhaps our most ambitious undertaking yet. These gains, in and of themselves, are worth the journey.

■ Kim Budil, former Principal Associate Director for Weapons and Complex Integration, was named the director of Lawrence Livermore National Laboratory on February 1.

FUSION SUPPORTS THE STOCKPILE

From providing data that sheds light on the complex physics of a nuclear weapon to providing a valuable training ground for the next generation of stockpile stewards, Livermore's Inertial Confinement Fusion program brings unparalleled value to the nation.

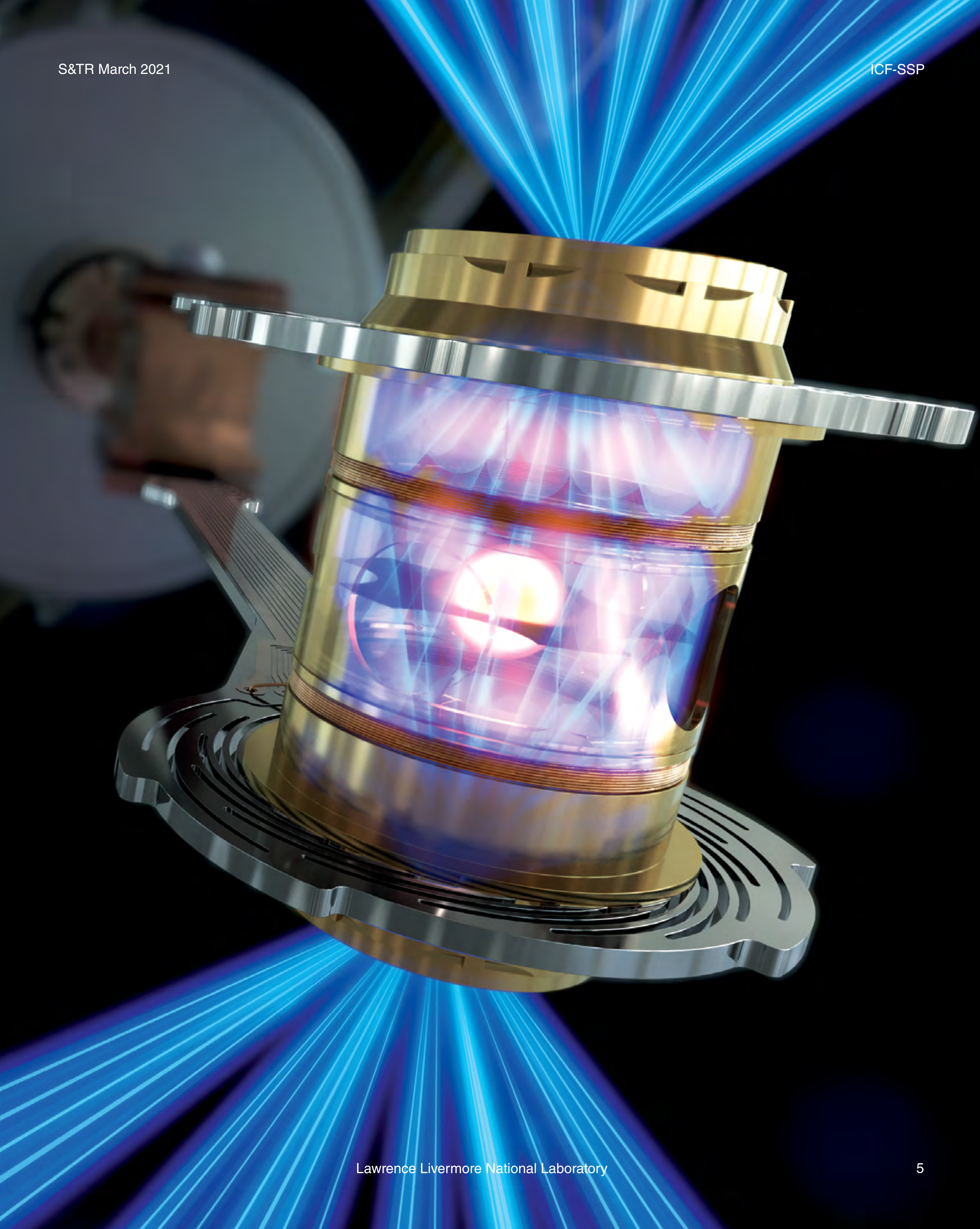
THE last U.S. underground nuclear explosive tests, which were key to assessing the design and viability of the country's nuclear weapons, occurred over 27 years ago. However, the need for deeper understanding of the complex physical processes that drive nuclear weapon performance and for putting stockpile design and assessment on a solid science-based foundation continue to be of utmost importance to the nation.

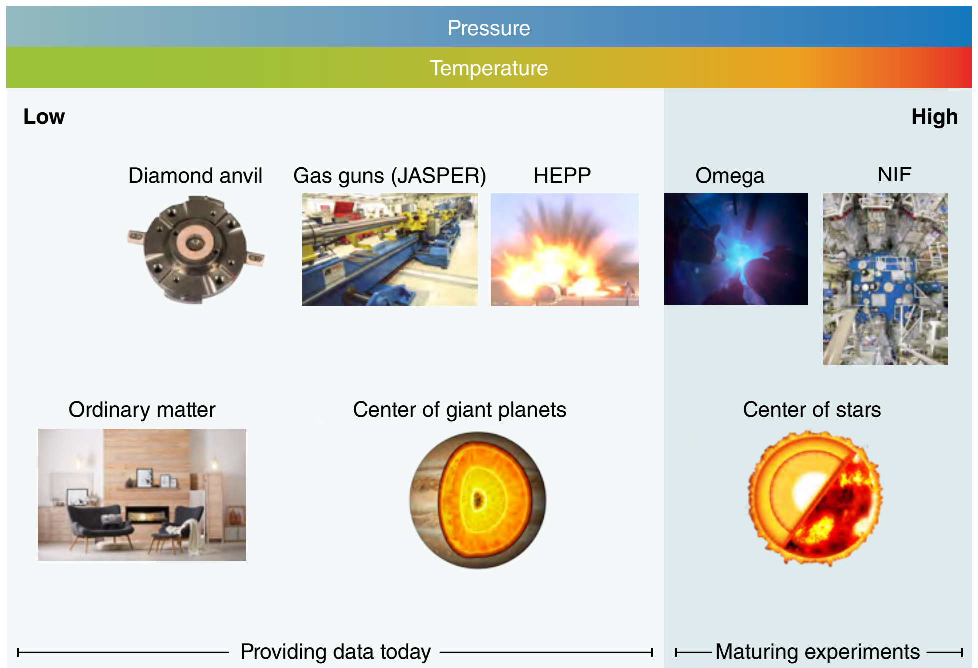
A core mission of the Department of Energy's (DOE's) National Nuclear Security Administration (NNSA) is to ensure this stockpile remains safe, secure, and reliable, without further underground testing. Lawrence Livermore's Inertial Confinement Fusion (ICF) program supports the Stockpile Stewardship Program (SSP) mission by seeking to recreate and examine the processes that occur in the heart of burning stars and nuclear weapons, through heating a tiny amount of encapsulated fusion fuel and compressing it to the point that nuclear fusion reactions occur. The data from experiments at ICF facilities help to refine computer models used to better understand and assess the performance of the stockpile's aging nuclear weapons. These experiments also provide an opportunity for weapon designers, experimentalists, engineers, and staff to tackle challenging design problems in the absence of underground nuclear explosive testing, thereby developing and refining the skills needed to support the SSP. This dedicated workforce turns to platforms of immense energy and engineering prowess, such as the world's largest and most energetic laser—the NNSA's 192-beam National Ignition Facility (NIF), located at Livermore—to meet the SSP mission, now and in the future.

Science Reveals the Stockpile

The end of underground testing and DOE's creation of the science-based SSP significantly increased the need to have a detailed scientific understanding of nuclear weapons and how they work (See p. 7: "The Quest for Fusion Ignition and the Birth of Science-based Stockpile Stewardship"). This requirement ushered in an era of large-scale experimental platforms and high-performance supercomputing facilities, paired with cutting-edge diagnostic capabilities. A detonating nuclear weapon passes through many regimes of temperature and pressure, requiring myriad tools and facilities to study the different regimes. However, the overwhelming majority of the energy yield from a nuclear weapon is produced in the high-energy-density (HED) state, with temperatures and pressures ranging from those found at the center of the earth to those at the center of the sun. These extreme conditions of temperature, pressure, and material densities can only be created in unique experimental facilities. Three NNSA facilities provide the energies and diagnostics to help scientists delve into this challenging environment: Sandia National Laboratories' Z-Machine (the world's most energetic pulsed-power facility), the University of Rochester's Omega laser facility, and NIF. Livermore's Deputy Program Director for Fundamental Weapons Physics Mark Herrmann notes, "NIF provides us with experimental data in the higher-end temperature, pressure, and density regimes to measure our computer models against and provides insights into weapons performance."

Bradley Wallin, program director of the Weapon Physics and Design Program,





Different tools are required for the various temperature–pressure regimes experienced by a nuclear weapon. Experiments at relatively low pressures and temperatures are conducted with diamond anvil cells (See *S&TR* July/August 2019, pp. 20–23). The conditions that reflect those at the centers of giant planets can be reproduced in gas-gun experiments in facilities such as the JASPER gas gun (See *S&TR* April/May 2013, pp. 20–23) and high explosive pulsed power (HEPP) experiments. Setting experiments at the fusion conditions created in stars and nuclear weapons requires facilities such as the pulsed-power Z machine, the Omega laser facility, and ultimately, the National Ignition Facility.

says, "As we reach into higher and higher areas of pressure, temperatures, and densities of materials in our experiments, we learn much along the way that is applied to many areas of stockpile stewardship." HED experiments and research provide data for design codes that aid in assessment of the stockpile. (See p. 11: "Simulations: A Powerful Tool in the SSP Toolbox.") For example, the combination of modeling and HED experiments helps researchers to better understand a weapon's survivability when facing possible hostile encounters in the stockpile-to-target sequence: the order of events involved in removing a nuclear weapon from storage and assembling, testing, transporting, and delivering it on the target. "The goal is to keep the nation's nuclear deterrent strong and viable," says Wallin. "A strong deterrent helps keep the peace." Additionally, some HED experiments at NIF focus on determining materials' equation of state (EOS)—the relationship between pressure, temperature, and density. Accurate EOSs for key elements are essential for generating the computational models that underpin simulations critical to SSP efforts such as life extension programs (LEPs), which aim to add 30 years of service life to aging nuclear warheads.

NIF is the only U.S. facility designed to perform experimental studies of fusion ignition and subsequent thermonuclear burn, the phenomenon that gives rise to the immense energy of modern nuclear weapons. For the ICF experiments at NIF, a capsule filled with deuterium–tritium (DT) fuel is seated inside a gold or depleted uranium hohlraum, which is a cylindrically shaped device with open ends. NIF's laser light enters through these open ends and strikes the hohlraum walls, generating a bath of x rays that causes the capsule to implode while heating and compressing the DT fuel into a central hot spot. Fusion reactions within the hotspot produce energetic alpha particles (also known as helium nuclei) and neutrons. The energetic alpha particles deposit their heat in the fusion fuel. For ignition to occur, enough heat must be deposited to generate a propagating burn wave from the hot spot into the cold fusion fuel. The yield of the fusion experiment can be measured by counting the number of neutrons generated.

NIF Director Doug Larson explains, "Achievement of ignition is critical since once the fusion fuel is ignited, higher fusion yields can be generated, opening a gateway to even higher energy densities that are needed for the SSP." In an experimental campaign that took place over several months in 2017 and 2018, scientists at NIF successively produced record numbers of fusion neutrons, culminating in a January 2018 shot that produced 1.95×10^{16} neutrons and 55 kilojoules, the highest yield to date (See *S&TR* April 2019, pp. 12–15). Recent results from a 2019–2020 campaign improved upon that, increasing the neutron yield by 4 percent at a much lower implosive velocity. LLNL's Chief Scientist for ICF Omar Hurricane explains, "The real significance of these results is that we can now drive the new target design to a higher implosion velocity using more laser energy, achieving greater fusion yield."

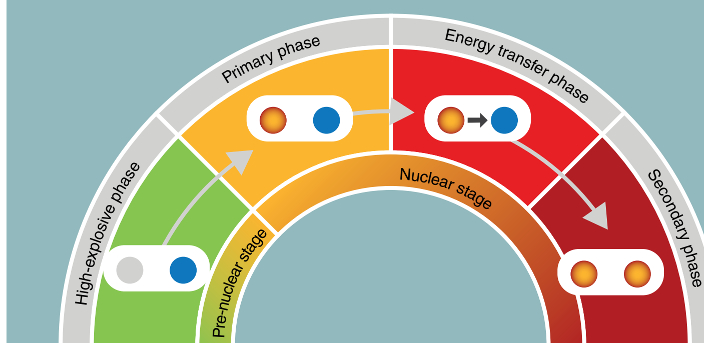
Addressing Ignition Challenges

Hurricane adds, "We've made incredible scientific progress over the past decade. Our understanding of the

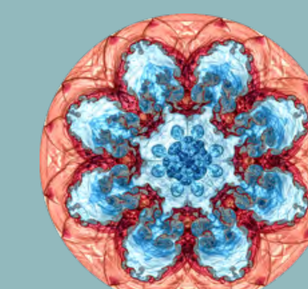
The Quest for Fusion Ignition and the Birth of Stockpile Stewardship

Soon after the invention of the laser in 1961, Livermore physicists John Nuckolls, Ray Kidder, and Stirling Colgate used Livermore-developed codes to study whether laser light might be able to trigger fusion reactions. Their results led to the launch of a small laser fusion project in 1971, which grew to develop a series of increasingly powerful lasers: Janus in 1975, Shiva in 1977, and Nova in 1984. The 1980s also saw the growing interplay between computer simulations and experiments, along with the birth of supercomputers.

Meanwhile, well before the 1992 underground nuclear test ban, DOE recognized that ICF could provide an alternative to underground tests for exploring radiation hydrodynamics—the study of the flow of matter that is strongly coupled with electromagnetic radiation, including x-ray radiation. Such radiation plays a critical role in the detonation of a nuclear weapon. After 1992, the question became, how would the nation maintain a deterrent in the absence of testing? Since modern thermonuclear weapons rely on fusion to perform, weapon researchers needed a platform upon which to explore fusion ignition and thermonuclear burn. Fusion in a weapon was one of its least-understood processes, so having the capability to reproduce this process in a laboratory setting has become one of the grand challenges for the science-based Stockpile Stewardship Program.



There are roughly four phases in a two-stage nuclear detonation. In the first "high-explosive" phase, high explosives compress special nuclear material, creating a supercritical assembly. The "primary phase" comes next, when the supercritical assembly fissions and initiates fusion reactions, ultimately creating a burst of neutrons and x-ray energy. Those x rays travel from the weapon primary to the secondary in the third "energy transfer" phase. Finally, the weapon secondary produces energy, explosion, and radiation in the "secondary phase."

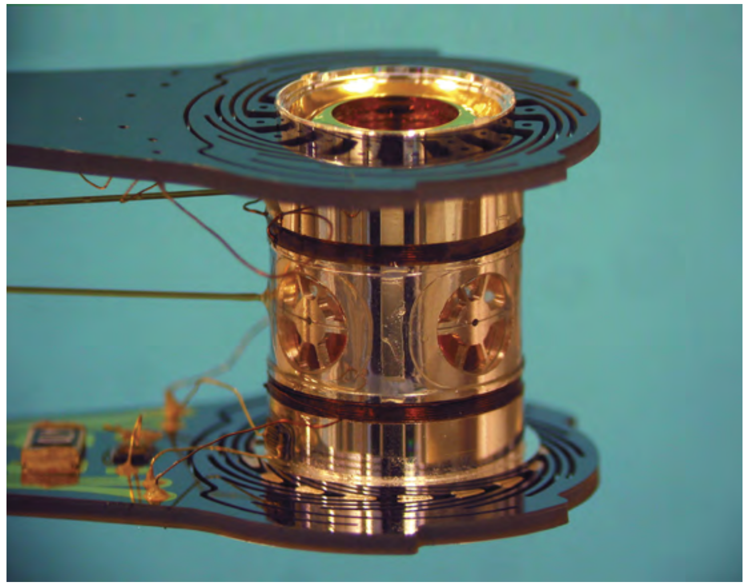


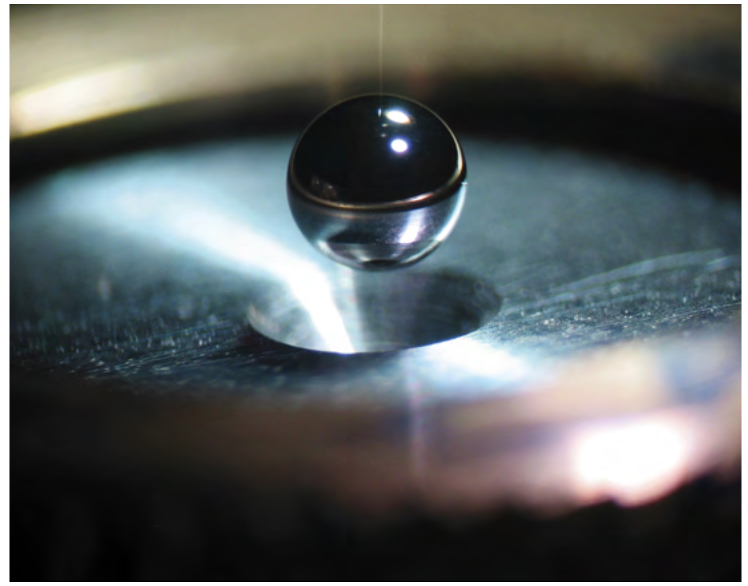
Modern-day stockpile stewardship depends on experiments, historic test data, and high-performance computing to ensure the long-term viability of the U.S. deterrent without additional underground nuclear tests. Left: Before each NIF experiment, a technician uses a positioner to precisely center the target inside the chamber. The positioner serves as a reference to align the laser beams. Right: This simulation shows hydrodynamic instability of two fluids mixing in a spherical geometry. Such simulations provide valuable data sets for understanding turbulence models important to ICF and stockpile stewardship applications.

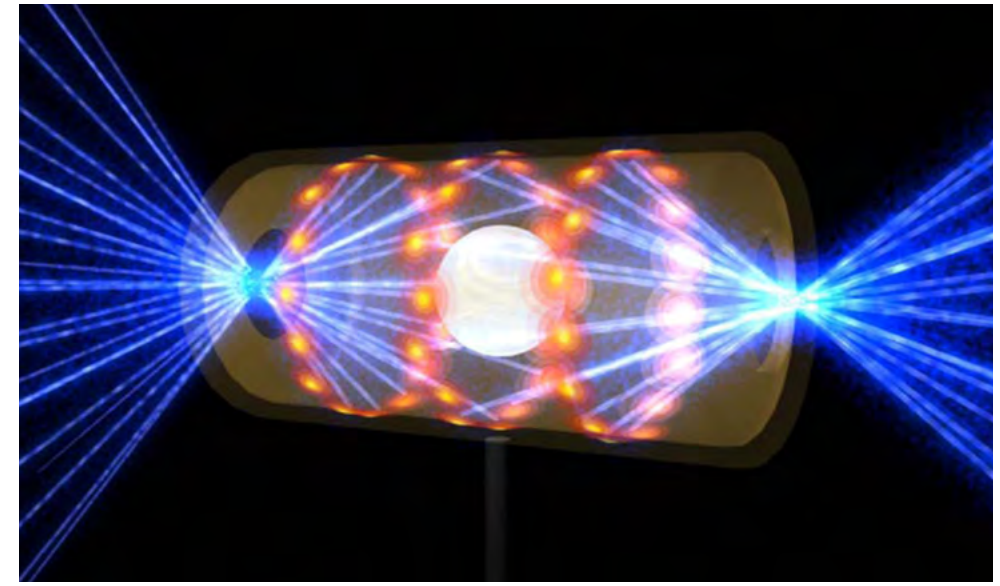
physics involved on the path to ignition increases with each step we take." Researchers have focused on such challenges as addressing hydrodynamic instability. "The first trick was to determine the one thing we could do that would make a significant improvement. The intuition and judgment of the weapon designer came into play as we evaluated different options. In this case, the 'fix' involved changing the shape of the NIF laser pulse, which improved the yield by a factor of 10." (See *S&TR*, June 2014, pp. 4–10). The resultant "high-foot" pulse, which lasts 15 nanoseconds and has three main shocks (instead of the 20-nanosecond pulse and four shocks used in low-foot shots), creates a stronger first shock in the foot, or early part, of the pulse. Experiments using this pulse shape proved more forgiving of imperfections in the fuel capsule and less susceptible to implosion instabilities that decrease fusion reactions.

Once these hydrodynamic instabilities were removed, other issues emerged that had been masked by the larger problem. "It's like peeling away the layers of an onion," says Hurricane.

The next challenge to tackle was implosion asymmetry. Implosions act as amplifiers, taking 100 million atmospheres of pressure and increasing it to many hundreds of billions of atmospheres. Any asymmetries caused by, for instance, a tiny material defect in a capsule or a variance in







Left: Traditionally, fusion target capsules are about 2 millimeters in diameter and filled with cryogenic (super-cooled) fuel. Capsules are composed of plastic, diamond, or beryllium. Center: The capsule is held inside a hohlraum—a metallic case. Target handling systems precisely position the target and freeze it to cryogenic temperatures of 18 kelvins (-427 degrees Fahrenheit) to enhance the fusion reaction. Right: When NIF laser beams strike the internal walls of the hohlraum, they are converted to x rays that irradiate the capsule inside. The outer wall of the capsule rapidly ablates, or burns away, while the adjoining fuel layer implodes and compresses the capsule core.

one of the 192 laser pulses, gets amplified. "This is why we all work so hard to minimize any defects," says Hurricane. For instance, the "tent," or membrane that holds a capsule in place in the hohlraum, contributes to instability in implosions. This plastic support membrane, only 30–110 nanometers thick, touches the capsule along rings at the top and bottom of the capsules. Those tiny areas of contact are enough to perturb an implosion's symmetry by perforating the ablator and shooting annular jets of material into the implosion (See *S&TR* March 2018, pp. 16–19; January/February 2016, pp. 4–11). Another feature that affects the implosion is the tube used to inject fuel into the capsule. "This tube, which is 1/10th the diameter of a human hair, was causing a jet of ablator material to shoot into the hot spot, cooling it down as we were trying to compress the capsule to heat the hot spot up," says Hurricane. The target fabrication team at NIF shrank the tube to 2 micrometers in diameter, which reduced the jet, and are exploring whether a 1-micrometer fill tube might be feasible, if needed.

The work addressing these challenges and others continues. Notes Herrmann, "The data quality and diversity we now get from NIF is unprecedented and has given us a good idea of the limiters. We can't quite compress the capsule as much as we need to, so we're trying to figure that out, and also we are looking at how efficient we can make the hohlraum so we can drive bigger capsules that are more resistant to imperfections."

In more recent ICF experiments, the research team fired a three-shock laser pulse (less than half the duration of pulses used in the high-foot campaign) lasting about 7 nanoseconds at the target. The precisely timed series of shocks propagated through the fuel capsule as it imploded. Some experiments adopted a strong initial shock, deemed the "big-foot" pulse, to drive a high-velocity implosion. A somewhat different strategy based on a more traditional pulse shape used a roughly 2-millimeter-diameter, high-density carbon (HDC) capsule that contained a thin layer of DT fuel located just inside the outer shell. HDC, or diamond, has a higher density than the plastic and beryllium shells previously used in ICF experiments and allows for a shorter pulse that still reaches the same kinetic energy. Recent record neutron yields have stemmed from the use of HDC capsules, a shortened laser pulse, a lower concentration of helium gas fill in the hohlraum, and a thinner fill tube, as well as enhanced understanding of the implosion process.

Scientists are also exploring different hohlraum shapes to increase the amount and symmetry of x-ray energy on the capsule, including a novel hohlraum shaped like a rugby ball (See *S&TR* July 2020, pp. 12–15).

Igniting a Passion for Stewardship

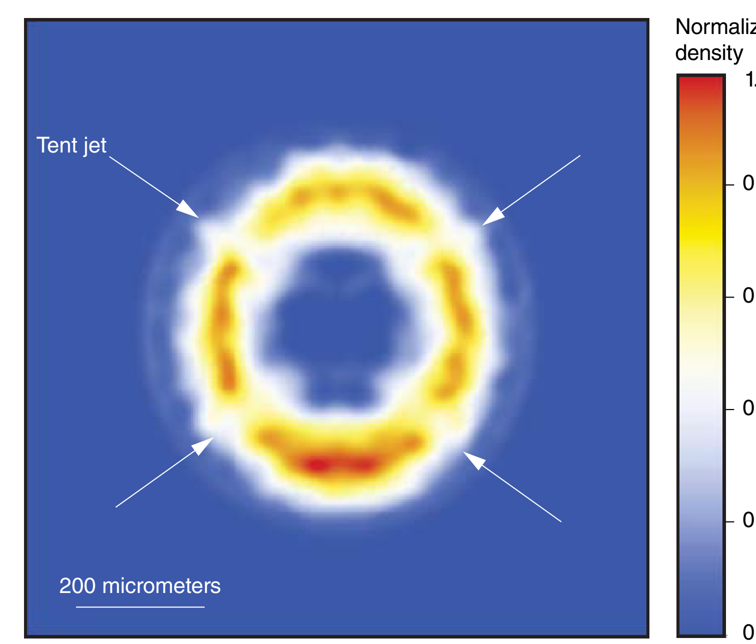
During the Cold War, underground nuclear testing at the Nevada Test Site was the centerpiece of the development and deployment of the U.S. nuclear stockpile. The tests were "final exams," not only for the nuclear warheads themselves but for the laboratory scientists and engineers, who were continually experimenting with new ideas, apparatuses, and diagnostics.

With underground testing now in the past, the venue has changed, but the challenges remain. Debbie Callahan, deputy for integrated experiments and associate division leader for HED-ICF in design physics, explains that the ICF experiments conducted today at NIF and elsewhere serve as the same training ground for today's researchers. "We are training the designers and experimentalists to make decisions and hone their intuition."

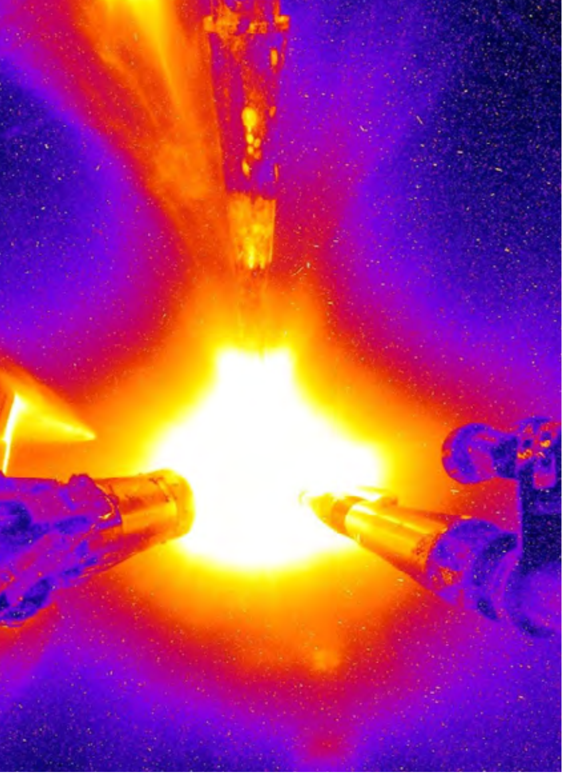
Just as with the underground experiments of decades before, ICF experiments are complex, requiring much time and coordination. Designers and experimentalists work in tandem on an ICF experiment that can take a year or more from concept to the final shot. Designers use codes and theories to develop an experimental design that will address a particular challenge; experimentalists determine the diagnostics that will best capture the test results and analyze the data. But the lines of responsibility are often blurred, with experimentalists and designers working together to address the challenge.

A case in point is designer Andrea Kritcher and experimentalist Dan Casey. Kritcher, a designer in the ICF program, came to the Laboratory in 2009 as a Lawrence Fellow. In one of her projects, she used x-ray Thomson scattering to characterize fusion targets for ignition experiments at NIF, diagnosing the compression-phase temperature and density conditions of the implosion capsules. (See *S&TR* June 2011, pp. 4–12.) Casey arrived at LLNL in 2012 and became lead experimentalist for several NIF and OMEGA campaigns supporting NNSA programs, including the Big Foot campaign. Two and a half years ago, Kritcher and Casey teamed up as lead designer and lead experimentalist for the ICF program's Hybrid-B campaign. Now completed, this campaign was one of several focused on taking the best elements of past designs and using data-based understanding of the key physics factors that control symmetry and performance. The goal of such "hybrid" implosion design work is to field large-scale, ignition-relevant implosions using NIF's full power and energy capacity.

The Hybrid-B campaign sought to determine how big a capsule would fit in a traditional hohlraum and how it could be driven to relevant velocities. "Ultimately, we wanted to determine if we could field bigger implosions using our existing hohlraums by optimizing several design parameters including the size of the capsule compared to the size of the hohlraum," says Kritcher. Casey adds, "There was a lot of effort involved, from developing the initial design, to the design and building of the target, preparing the diagnostics, conducting preliminary 'tuning' shots that help us better grasp the



The "tent" that holds the hohlraum capsule in place affects the quality of the implosion. Where the capsule touches its "tent" in a ring shape, as depicted in this x-ray snapshot of the imploding capsule, the points of contact cause upper and lower ring jets to penetrate the shell as it implodes and quench the yield of inertial confinement fusion experiments.



In February 2016, the ICF program conducted its first layered deuterium-tritium (DT) fusion implosion using the “big-foot” three-shock pulse with a sub-scale diamond ablator and a thinner DT ice layer, and a low-gas fill to limit laser–plasma instability and cross-beam energy transfer. Credit: Don Jedlovec.

implosion shape, shock trajectories, and so on, before we can conduct the final, integrated shots.” The Hybrid-B campaign included seven tuning experiments and six final integrated experiments using three different case-to-capsule ratios, including a capsule with the largest radius fielded to date: 1.2 millimeters.

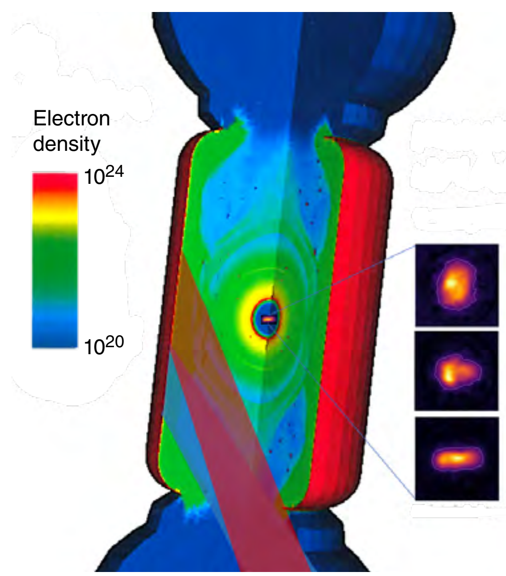
For the lead designer and experimentalist, the day when a full integrated NIF test shot is to occur is imbued with much of the same anticipation and tension that was present in the legacy underground test shots. “Final tests are both exciting and gut-wrenching,” says Casey. “It’s the moment of truth.” A year or two of effort has gone into the design. An enormous number of instruments, sensors, control systems, and diagnostics are involved, as well as hundreds or thousands of person-hours. Right before the shot, sirens and alarms sound for clearing the NIF target bay. The physicists stand by in the control room, waiting. From the control room, the shot is heard as a faint “pop.” “Ten, fifteen minutes go by before you know what has happened,” says Casey. “You keep hitting ‘refresh’ on the data download.” The data trickles in over the next few days, so it takes a while for the final results to arrive. Kritcher adds, “We always look forward to the data that tells us the quality of the implosion—particularly how symmetric it was—and how well the results match the predictions. And we are always eager to see the results of the many nuclear diagnostics that provide a wealth of information about how well the fuel came together at the end of the implosion, although the first question we usually get asked is ‘what was the yield?’!”

The shot’s neutron yield is determined from data gathered from a variety of diagnostic instruments, including the neutron time-of-flight (nTOF) detector, which records the neutron energy spectrum; fuel temperature; bang time (the time of peak neutron emission); and areal density, which is a measure of the combined thickness and density of the imploding frozen fuel shell. For ignition to occur, the fusion fuel must have a high enough areal density and temperature, as well as a symmetric shape at the time of peak compression (See *S&TR* December 2012, pp. 15-17).

Kritcher notes that working on ICF on NIF is a major part of the excitement of working at the Laboratory. “It’s a unique opportunity to work hands-on in an experimental campaign, solve problems in real time, and engage in real-time decision-making. There are the models, and there are the experiments… they don’t always agree, and testing gives us a chance to hone our intuition and learn why our models don’t always agree with the experiments. We can set the models to reflect results obtained in past shots, but once you change the designs, you often need the data from new experiments so you can incorporate new features in the models.”

Of course, the lead designer and experimentalist in a campaign are not working alone. There are 15 to 20 physicists who take on various roles in a campaign, split between designers and experimentalists. To bring an experiment to fruition requires an army of others who have responsibilities in the facility, in building and assembling the required targets, and in setting up the experiments.

With Hybrid-B behind them, Kritcher and Casey are involved in testing a different target design. “Experimentally, we’re still not getting the areal densities we want,” says Kritcher. “So, for this campaign, the capsule will have a thicker DT ice layer, which should increase the areal density and be less susceptible to capsule imperfections. To drive the thicker ice layers to relevant implosion velocities, we will use high-temperature hohlraums.” The initial design phase and reviews are complete; experiments began in summer 2020 and extend into fiscal year 2021.



Left: A simulation of electron density during implosion of a target for the Hybrid-B campaign, created by LLNL’s HYDRA radiation hydrodynamics code. ICF design physicists use HYDRA to simulate the entire ignition target in 3D, including the hohlraum and capsule. Areas of higher electron density correlate to areas of higher-density plasmas. Right: The measured hot spot x-ray emissions of three different shots using capsules of different diameters, captured by x-ray penumbral imaging, showed the impact of case-to-capsule ratio on hot-spot symmetry.

The Future Beckons

As Callahan notes, when it comes to training the next generation, it’s a journey. “We are training people to be the future leaders and stewards for a stockpile that must stay viable for the next 30 years,” she says. “We are training them to develop good judgment and intuition, so whether they are designers or experimentalists, they can apply their knowledge on the very difficult problem of inertial fusion for a better understanding of the behavior of the stockpile in these very high-energy regimes.” Through experiments and simulations, the understanding improves. Experimental data informs new codes, adding and validating the models that underpin the simulations. Conversely, the models inform the experiments, providing guidance for what to expect, tools for pushing the limits of the known.

“The end goal of the ICF mission is to create the high yields that are the gateway to the high energy densities in nuclear weapons in which the stockpile stewards of the future can test their ideas under conditions that closely approach those of operating nuclear weapons. As to the first step of ignition, we’ve come a huge distance over the past decade in our understanding and capabilities,” says Herrmann. “There are certainly challenges remaining, and we can’t say for sure we will get there. Some of the issues we think we know how to fix. Others, we need to get a better understanding.” He points out that 10 years ago, the energy required to reach ignition was more than a factor of 10 away. He adds, “Now it’s about a factor of two or three, and we’re working on how to close the remaining gap.”

— Ann Parker

Simulations: A Powerful Tool in the SSP Toolbox

Along with experiments and legacy data, stockpile stewardship requires advanced supercomputer facilities that can conduct simulations at scales of interest. As LLNL retiree Dick Fortner, a former associate director during the underground testing era, explains, “Even during the test era, physical experiments and computer modeling went hand in hand, and the results balanced and reinforced each other. Experimental data was needed to do the calculations. And you get the calculations to see if you understand the data. It’s still true today, as we continue to test the codes and models. If the results or predictions from the models doesn’t fit the experimental data, then you have to fix the models.”

The Sierra supercomputer is the latest in a series of NNSA’s leading-edge Advanced Simulation and Computing (ASC) program supercomputers, whose predecessors include Sequoia, BlueGene/L, Purple, White, and Blue Pacific. Sierra is helping to solve the most demanding computational challenges faced by the ASC program in furthering its stockpile stewardship mission (See *S&TR* August 2020, pp. 12–15). At peak speeds of up to 150 petaflops (a petaflop is 10^{15} floating-point operations per second), Sierra provides at least four times the performance of Sequoia.

Data analysis is also benefitting from the explosion in computing power that comes with bigger, faster machines, such as Sierra and the Trinity supercomputer at Los Alamos National Laboratory. Machine learning (ML) uses computers to learn from data and make predictions about the environment (See *S&TR* March 2019, pp. 4–11). For example, one project leveraged ML to analyze the largest-ever data set from ICF implosions on NIF, pointing the way toward new laser target designs (See *S&TR* September 2018, pp. 16–19). Another group is developing an innovative cognitive computing platform that combines ML with graph analytics and other areas of artificial intelligence to improve ICF simulation efficiency.

From past to present, Livermore has employed the most powerful computer systems available to support stockpile stewardship design and test efforts. Left: The Univac, Livermore’s first supercomputer, had 5,600 vacuum tubes, a 6-kilobyte memory, and a code stored on magnetic tape. Right: LLNL’s newest supercomputer system, Sierra.

Key Words: Advanced Simulation and Computing (ASC) Program, big-foot, deuterium-tritium (DT) fuel, fusion ignition, high-density carbon (HDC), high-energy density (HED), high-foot, hohlraum, Hybrid-B campaign, HYDRA, implosion asymmetry, inertial confinement fusion (ICF), life-extension program (LEP), National Ignition Facility (NIF), nuclear deterrent, nuclear weapons, plasma instability, Sierra supercomputer, Stockpile Stewardship Program (SSP), target, underground nuclear test.

For further information, contact Mark Herrmann at (925) 423-5719 or herrmann9@llnl.gov.

Evaluating Patients in the HARSHEST Environments

As NASA prepares to send astronauts beyond low-Earth orbit for the first time since 1972, scientists are working to better understand and mitigate the potential health risks associated with long-distance space travel. Rapid medical diagnosis will help ensure astronauts stay healthy and productive. To that end, Lawrence Livermore and NASA researchers, with colleagues from Uniformed Services University; University of Arizona; Michigan State University; the University of California at Davis; Sandia National Laboratories; and Travis Air Force Base, are developing a hand-held diagnostic instrument that can rapidly evaluate the effects of radiation exposure, weightlessness, and other astronaut health concerns.

David Loftus, medical officer for the Space Biosciences Research Branch at NASA's Ames Research Center and Lawrence Livermore collaborator, notes, "The International Space Station (ISS) is close enough to Earth that it's easy to bring people back if they get sick, so we don't need to do much health monitoring, but we will need monitoring devices for missions to the Moon, Mars, and beyond." While a rescue from ISS can be executed within a day, Mars is eight months away, and travelers will need to be equipped to manage on their own.

This work was supported by Livermore's Laboratory Directed Research and Development Program and builds on Laboratory strengths in radiation effects research, additive manufacturing, and bioengineering along with NASA Ames expertise in astronaut health research and nanotechnology. Researchers ultimately envision the low-cost, easy-to-use, accurate, and robust tool's use in other austere environments as well, such as disaster sites, developing countries with limited medical resources, and on the battlefield.

Conditions that can be diagnosed with a single biomarker:

Analyte	Diagnosis
Troponin	Myocardial infarction
DDX46	Chronic lymphocytic leukemia
NO	Lung inflammation
Breath acetone	Diabetes mellitus
Myostatin	Muscle wasting

Conditions requiring multiple biomarkers:

Analyte	Diagnosis
Breath volatiles	Pneumonia
IMP-1, CEA, CA19-9, serum YKL-40	Early colon cancer
CD14, SEPP1, SELL, TNXB, LUM, PEPD, QSOX1, COMP, APOC1	Tuberculosis (versus ordinary pneumonia)
CBC, IL-6, IL-10, IL-12, CRP	Radiation exposure

Biomarker targets developed at Lawrence Livermore will be used as part of the microarray panel for blood plasma analysis.

Taking It for a Spin

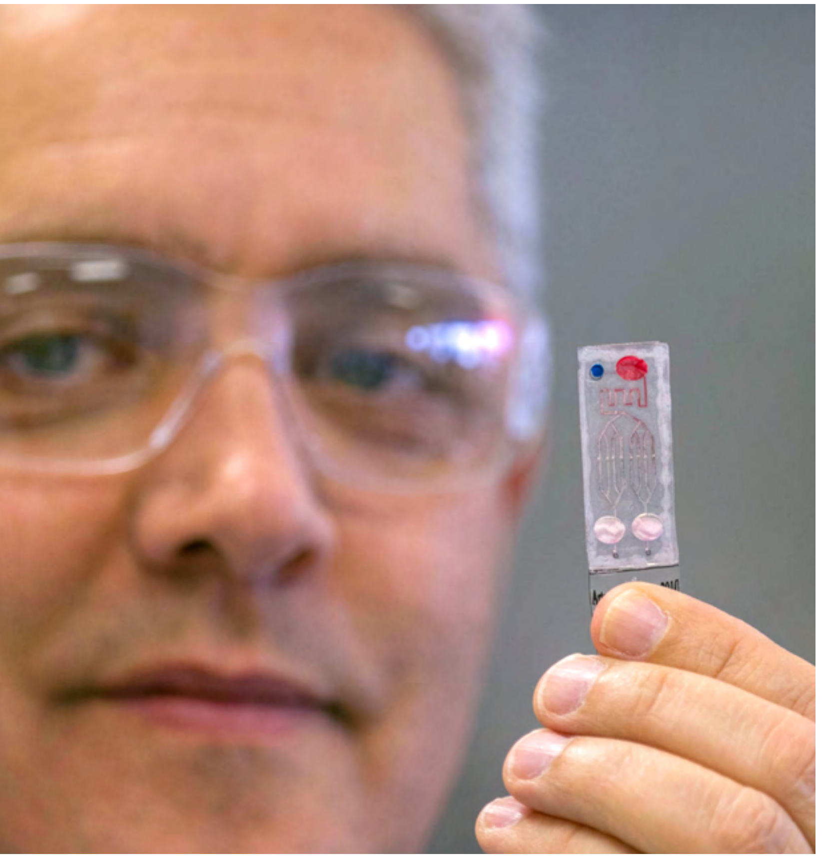
Flexibility is central to the device's design. While "blood is the gold standard for understanding a person's health," according to Livermore bioengineer Erik Mukerjee, volunteering a breath sample is simpler and less invasive, so this tool will be engineered to harvest data from either or both sources. Further, while the team's initial focus for blood analysis has been establishing a capability for identifying radiation exposure biomarkers—building on previous Laboratory efforts to characterize biomarkers that could inform and improve radiation-based cancer treatment—the device could be used to search for almost any set of biomarkers. (Biomarkers are any measurable biological characteristics that provide information about current or future health status.)

Hampered by stringent limitations on power usage and instrument size and weight, most medical diagnostics intended for extreme environments focus on identifying a single biomarker. This device could thus be among the first multifunctional health diagnostic tools used in space. The team's innovative spinning cartridge design for blood and saliva analysis is mechanically simple, robust, and has modest power requirements, as it uses only centrifugal force to manipulate fluid. "Typically, such devices will have pumps and valves—two types of mechanical parts," explains Mukerjee. "We have just one mechanical part, the motor, so if the motor works, the system will work." Importantly for an instrument destined for space, the design does not depend on gravity to function.

It Only Takes a Drop

The tradeoff for mechanical simplicity is the complexity of the microfluidics—the network of channels and nonmechanical valves only tens to hundreds of micrometers wide—on the cartridge itself. These channels function like tiny test tubes and work in conjunction with the motion of the cartridges as they spin around a central axis to move, control, order, and layer elements of the fluid sample. "By changing the speed at which the cartridge spins, we can move fluid in specific ways and perform different analysis steps. The design of the valves means that we can temporarily control the location of all fluids with just one parameter," notes Mukerjee.

The researchers' design efficiently separates the liquid and solid elements of blood so they can undergo different tests. Measurements of the relative quantities of blood's cellular components—the red blood cells, various types of white blood cells, and platelets—can provide critical information regarding inflammation, infection, radiation exposure, and cancer. The liquid portion, the plasma, is shuttled to the microarrays for identification of metabolites and proteins of interest. (Certain



Radiobiologist Matt Coleman displays a disposable protein detection assay similar to those that will be used in the medical diagnosis instrument he is helping to develop. (Photo: Julie Russell)

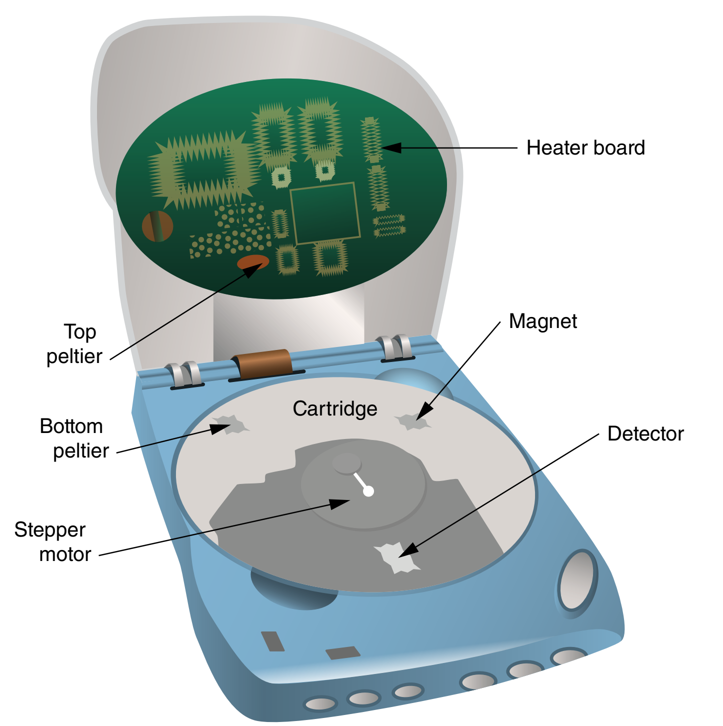
metabolites form as a biological reaction to environmental conditions, like exposure to radiation or a pathogen.) Searching for a different set of biomarkers will be as simple as switching to a cartridge targeting another set of metabolites and proteins.

One of the many attractive features of microfluidics systems is that they require far smaller samples than conventional clinical assays—200 times less than the amount needed for a standard panel of blood tests, for instance. Laboratory radiobiologist and project principal investigator Matt Coleman says, "For our project, we aim to work with less than 100 microliters of blood. That's just a drop or two. Clinically, it's easier to get the blood from a finger prick rather than finding a vein. It limits the trauma, pain, and inconvenience." Further, the biomarker assay tests can be performed in just 15 minutes, far faster than conventional tests. "The beauty of this technology is that it's at the point of care—the analysis happens where the patient is," adds Coleman. "That's more efficient."

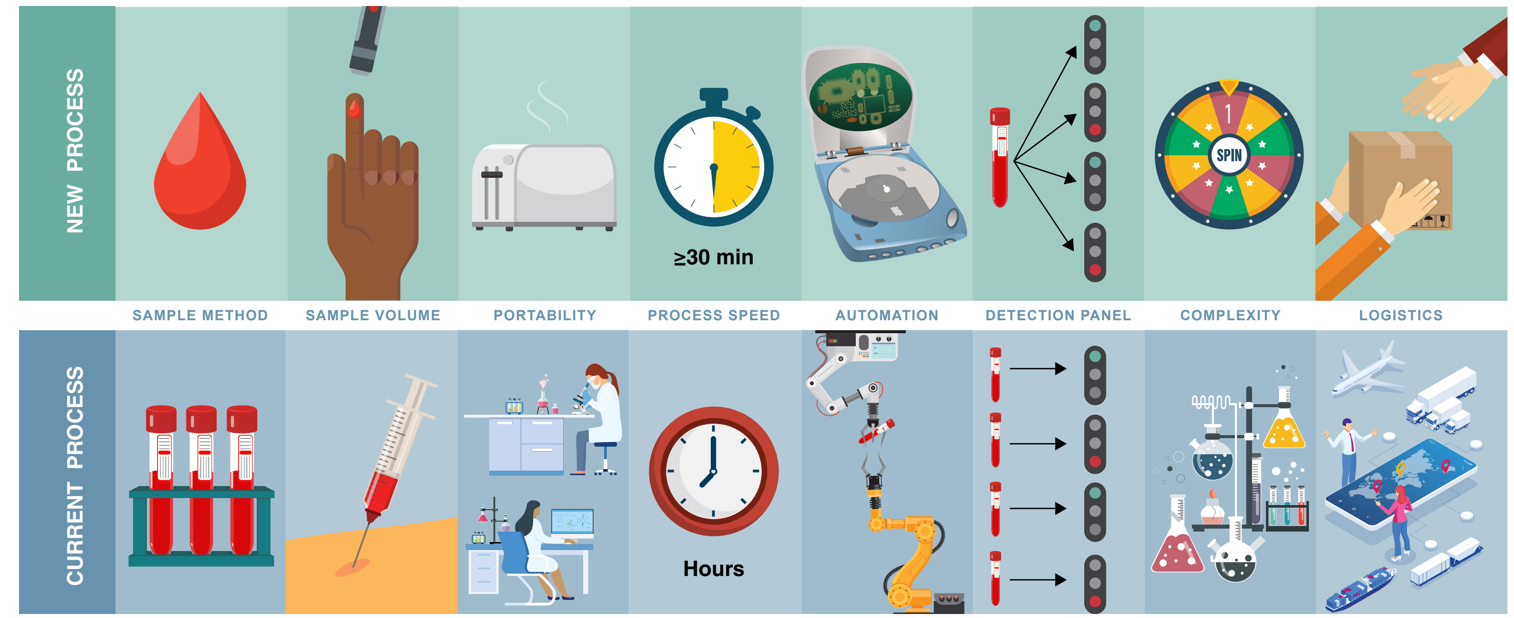
(Not) Breaking the Mold

Livermore scientists and engineers—Coleman, Mukerjee, engineer Michael Triplett, physicist Matthias Frank, and graduate student Kristen Reese—have taken the lead on designing and refining the system's microfluidics. Given that everything about the material and dimensions of the cartridge and channels affects performance, this has proven challenging. The team has made major strides, though, thanks to the Laboratory's rapid prototyping capabilities. "We can revise and print a new design in one day," says Triplett, "and new technology enables complex microfabrication shapes."

After generating a cartridge design, the Livermore team employs a 3D printing technology—stereolithography—to create a reverse mold of it from a fairly stiff plastic. They then fill the reverse mold with a softer silicone rubber to create a stamp and press it into a heated, harder plastic. The rubber shape serves as the actual stamp for the cartridges. This method of pressing a flexible stamp into a hard surface to create a three-dimensional structure is known as hot embossing, and the team



Early concept for the portable microfluidics-based analysis tool, which uses centrifugal force to move and separate sample components. The design originally called for disposable discs for fluid analysis, but the researchers have since moved to rectangular cartridges arrayed around the center like spokes on a wheel. The cartridges weigh less and are interchangeable for a more customized assessment.



The standard laboratory process for collecting and analyzing blood (lower row) is more complicated than the simplified system developed by the research team (top row).

hopes to incorporate it into future microfluidics projects. Before adopting this approach, the team struggled with making high-resolution parts without the mold breaking. After test printing a design, the team sends it to University of Arizona technicians, who manufacture larger quantities of the cartridge for testing and analysis.

The prototype cartridges are integral to animal model studies performed in conjunction with the Air Force, which supplies the team with baseline samples of healthy subjects for comparisons between standard assays and assays performed with the microfluidics system. Future studies will validate system performance for subjects with injuries, environmental exposures, or disease. Eventually, the project team will conduct human clinical trials.

Excitement Is in the Air

The researchers will ultimately integrate automated data analysis technology, the microfluidics element, and instrumentation for analyzing breath biochemistry into one compact, simple-to-use unit. The latter diagnostic, which has been under development for 15 years, employs carbon nanotube-based sensors to capture and separate breath and saliva for biomarker analysis. Liquid components will be passed to the microarray, while a miniature spectrometer will identify individual chemical compounds in exhaled breath.

Says Coleman, "E-nose is a NASA technology we're very excited about. It's a gas-phase chemical analyzer that detects volatile compounds in breath. If an astronaut needs urgent evaluation, it's easier to have them breathe into the device than to take a blood sample." However, because biomarker research for breath is still in its infancy compared with blood, explains Loftus, "the integrated device is key. We can take advantage of the best of both analysis approaches and share specimens across platforms."

The research team hopes to have a diagnostic platform ready for NASA moon missions in the late 2020s—or possibly even sooner for the ISS, where it could help expedite ongoing animal research. But their vision is broader than that. The researchers recognize that rapid analysis of radiation exposure effects, for example, would be as valuable for first responders after a nuclear accident as for astronauts en route to Mars, and they are eager to explore and encourage other such uses for their new diagnostic tool. "The more we think about terrestrial applications for this technology, the more excited we get," says Loftus.

—Rose Hansen

Key Words: astronaut health, biomarker assay, blood cell, carbon nanotube, E-nose, International Space Station (ISS), Mars, medical diagnostic, microarray, microfluidics, National Aeronautics and Space Administration (NASA), platelet, radiation effects, stereolithography, three-dimensional (3D) printing.

For further information, contact Matt Coleman at (925) 423-7687 or coleman16@llnl.gov.

Hydrogen Vehicles Get a QUANTUM BOOST

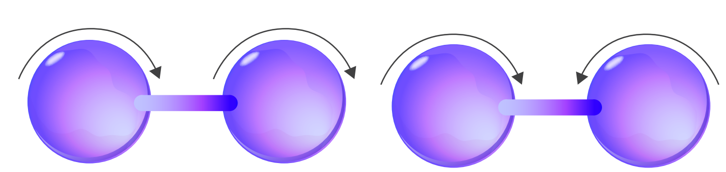
HYDROGEN fuel cell electric vehicles are a clean and potentially sustainable form of transportation. However, researchers must overcome significant technological and economic challenges before these vehicles become a practical alternative to gasoline-powered cars. Funded by the Department of Energy's Office of Fuel Cell Technology, Lawrence Livermore is addressing some of the challenges facing hydrogen vehicles.

Sal Aceves, a Livermore mechanical engineer and the project's principal investigator, says, "Although battery electric vehicles have the advantage of more infrastructure, hydrogen has certain advantages too, especially for large vehicles where heavy batteries are a limitation. A hydrogen vehicle can refuel in about five minutes, and hydrogen fuel tanks are cheaper and lighter than batteries."

Seeking technologies that could make hydrogen fuel cell electric vehicles (FCEVs) more practical, Lawrence Livermore researchers developed and tested a fuel tank designed to fit into personal vehicles, and a high-pressure process to refuel FCEVs quickly (See *S&TR* September 2016, pp. 20–22). The thermally insulated tank stores the hydrogen fuel as a liquid or cryogenic fluid under high pressure at low temperature. Much more hydrogen can be stored in a tank at low temperature compared to a gas at ambient temperature, substantially increasing the range of a hydrogen-powered vehicle.

A fundamental quantum mechanical property of cryogenic hydrogen (H2) gives drivers of H2-powered vehicles an added range boost, according to studies performed by Lawrence Livermore researchers and colleagues. The effect, called para- to ortho-hydrogen (H2) conversion, increases the storage capacity of cryogenic H2 tanks. To confirm the magnitude of the effect, the researchers had to calculate first-of-their-kind quantum mechanical properties based on measurements of samples from an automotive fuel tank-sized volume of hydrogen. The para- to ortho–H2 conversion is a rare example of a phenomenon from quantum mechanics having an impact on a mechanical engineering problem at the scale of everyday life.

In ortho-hydrogen (ortho-H2), the two protons of the hydrogen molecule are spinning in the same direction. In para-H2, they spin in opposite directions.



Orthohydrogen Parahydrogen

The tests demonstrated that the cryogenic tank could keep cryogenic H2 at high pressure with no hydrogen venting under all but the most extreme driving conditions. Fuel is most likely to vent while the tank sits idle and gets warmer, wasting fuel and reducing fuel economy. After these tests, the research team decided to investigate the para- to ortho-H2 conversion when they suspected that the effect had a materially positive impact on the tank's ability to store H2.

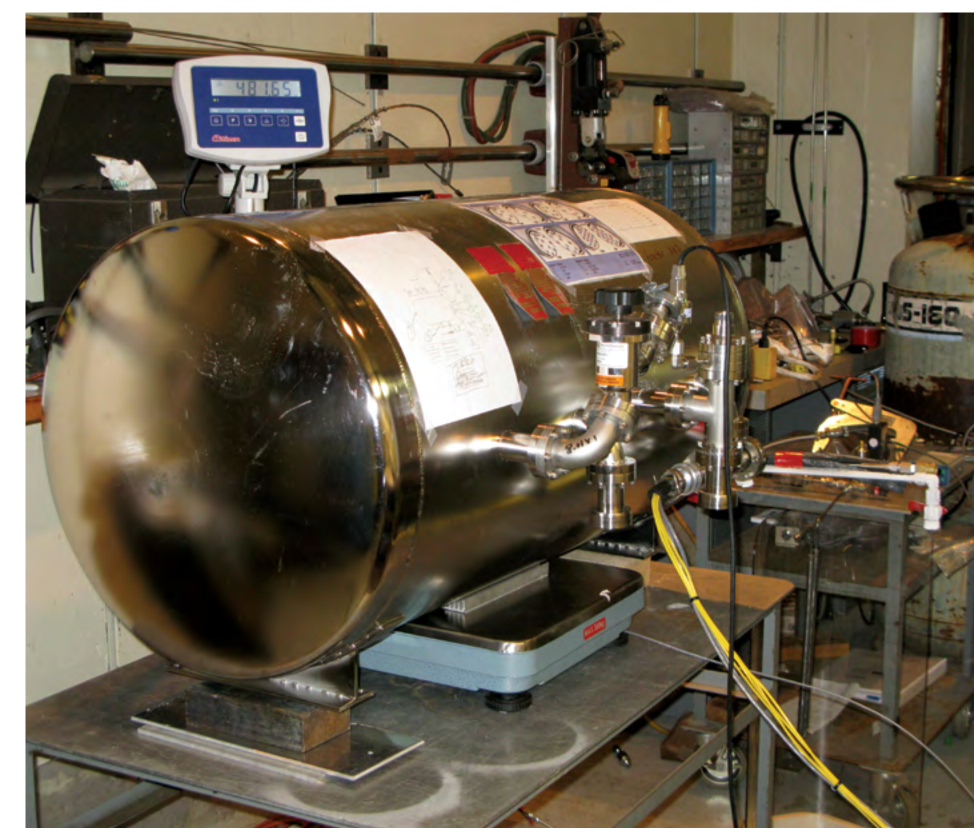
Quantum Versus Everyday Mechanics

Elementary particles like protons and electrons possess a property called "spin." Molecular hydrogen consists of two protons and two electrons, any of which can exist in an up or down state (sometimes referred to as clockwise or counterclockwise spin from classical mechanics, as defined by looking down on the axis of the particle). When the two protons in molecular hydrogen possess opposite spin states, the molecule is called para-H2. When they possess spin in the same state, it is known as ortho-H2. These are known as the spin isomers of hydrogen. Ortho-H2 exists in a quantum-mechanical state that has higher energy than para-H2.

At room temperature and higher, the equilibrium mass of hydrogen is about 75 percent ortho-H2 and 25 percent para-H2. As the temperature drops, the abundance of para-H2 molecules increases and heat capacity decreases. At about the liquefaction temperature of air, 77 kelvins (K), the number of para- and ortho-H2 molecules is about equal, and the transition continues as the temperature drops lower. H2 liquifies at a chilling 20.3 K. At this temperature, it exists as greater than 99.7 percent) as para-H2. Moving in the opposite direction, as para-H2 absorbs heat from the environment and becomes a gas, it converts back to a predominantly ortho-H2 form.

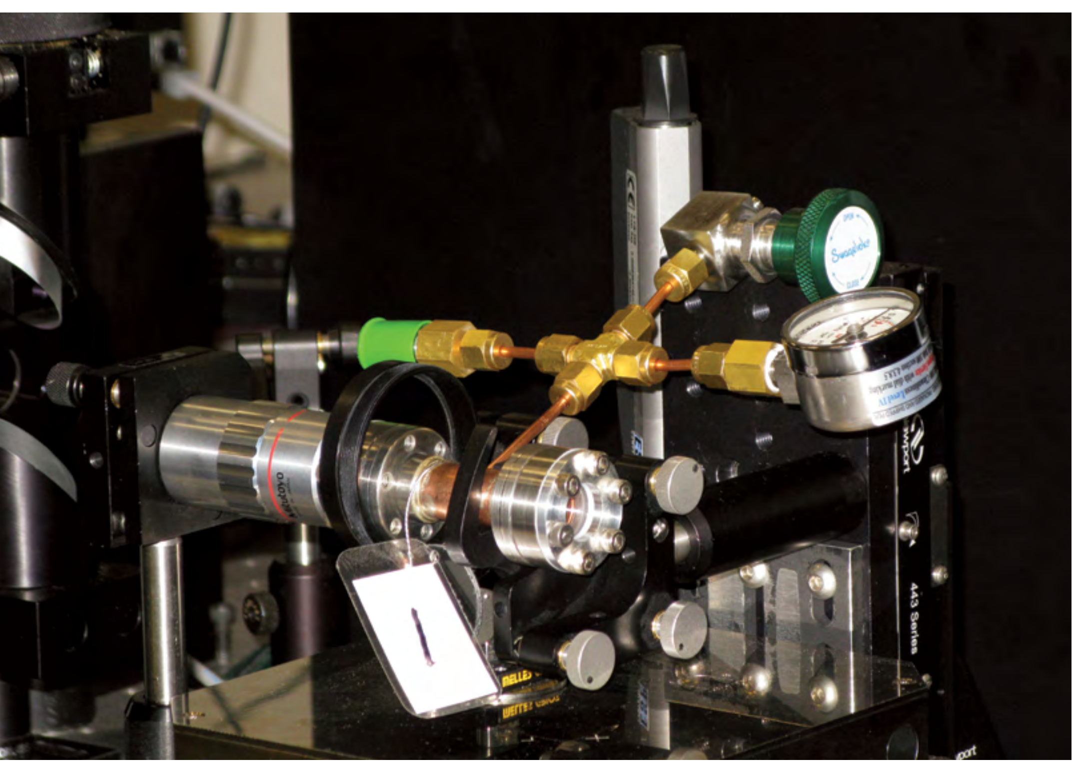
"This is good for the car," says Aceves, "because you have to worry about what happens to the pressure in the tank as H2 heats up." When the car is not in use, its hydrogen tank slowly heats up due to heat transfer from the environment, and the hydrogen pressure within the tank increases. When the pressure gets too high, some of the hydrogen must be vented to prevent damage to the tank. The para–ortho conversion absorbs energy, which uses some of the thermal energy in the tank that would otherwise contribute to increasing the hydrogen pressure. This keeps the tank cold and delays the onset of venting. The time interval until venting is defined as the tank's dormancy period.

Retired Laboratory technician Tim Ross fuels up a cryogenic tank with hydrogen at the Laboratory's Cryogenic Hydrogen Test Facility.



Instruments measure H2 storage density in a cryogenic fuel tank.

Above: Tim Ross draws a sample of hydrogen from an in-vehicle cryogenic fuel tank. The sample will be taken to Livermore's Raman spectroscopy lab to measure the ratio of para- to ortho-hydrogen.
Below: The Raman spectroscopy apparatus. The sample container is visible in the center-right as a pair of brass-colored crossed pipes with a green knob.



To measure the magnitude of the para–ortho effect, Aceves, Guillaume Petitpas (now at Air Liquide, France), Ibo Matthews, and Ray Smith conducted 15 experiments in which they filled the cryogenic tank with H2 at different densities. To determine how much of the hydrogen existed in para- and ortho-states at varying conditions, Aceves turned to Matthews to apply Raman spectroscopy to the problem.

Measuring the Spin State

Raman spectroscopy can measure the vibrational modes of solids and molecules as well as the rotational modes of gaseous molecules. Rotational Raman spectroscopy provides information about rotational populations of molecules which, for certain molecules like H2, can be related to their nuclear spin states. Matthews first established his optical spectroscopy lab at Livermore with a focus on studying National Ignition Facility (NIF)-related optics and targets using Raman and photoluminescence spectroscopies. Later, the lab scope was expanded to include techniques that allow NIF staff to find, understand, and repair laser-induced damage (See *S&TR* April 2017, pp. 17–20). He and his NIF colleagues are now working to develop commercial applications for this optical repair technology and push the boundaries of other laser material-processing techniques such as laser-based additive manufacturing. "Sal came to me asking whether we could use Raman spectroscopy to reliably and accurately measure differences in para- and ortho-H2 concentration. We came up with a plan to do time-dependent experiments to determine the reaction kinetics that drive how the para/ortho ratio was changing in these vessels," says Matthews.

During each experiment, the research team drew a sample from the tank at the Laboratory's Cryogenic Hydrogen Test Facility every day and rushed it over to Matthews' lab to measure the fraction of para-H2 in the sample. These were the first such measurements of para- and ortho-H2 sampled from large tanks. Prior investigators took measurements from much smaller volumes of hydrogen under less relevant conditions for hydrogen vehicles.

The Livermore team discovered that para–ortho H2 conversion usually became active after 10 to 15 days of parking, when the internal tank temperature reached 70 to 80 K. The conversion approached completion after 25 to 30 days when the vessel reached 100 to 120 K at a density of 50 grams per liter. The practical consequence of their finding is that vessel dormancy, the time the vessel can absorb heat from the environment before venting fuel to the environment, increased by three to seven days as a result of the conversion effect. It also means that the tank has greater capacity than expected as it warms.

In addition to its practical implications, the research also had a basic-science impact. The team's conversion measurements differed from the different diagnostic technique used in an earlier Ukrainian study, which found that the para–ortho conversion rate increased with increasing temperature. The Livermore measurements showed a slight decrease in conversion rate with temperature. This is consistent with a theory of paramagnetism proposed in 1933 by distinguished physicist Eugene Wigner, providing a quantum mechanics-based explanation for the conversion.

Driving with Hydrogen

In a follow-up study, Aceves and Livermore, University of Guanajuato, and Worthington Industries colleagues modeled all of the factors affecting cryogenic tank fill density to evaluate the performance of a hydrogen vehicle. The team modeled the effects of average daily driving distance on hydrogen density in the tank under different scenarios, such as driving distances ranging from 10 to 80 kilometers per day with and without refueling.

They found that the fill density of hydrogen gas in the tank increases linearly with driving distance. In consequence, increased driving distance depletes the fuel more rapidly, reducing the time available for heat transfer and leading to colder vessels that fill to higher density. Frequently driven vehicles need more tank capacity for hydrogen refueling. The tanks in these vehicles are refueled more frequently, are colder (they have had less time to heat up), and therefore can be filled with more hydrogen at a higher density. A side benefit is that at cold temperatures, the walls of the stainless steel vessels grow stronger and stiffer, increasing the safety of the tanks.

The results also show that the para- to ortho-H2 conversion is responsible for a significant increase in fill density, up to 5.3 percent. The conversion is most active for vehicles driven 20 to 60 kilometers per day—about the average distance traveled per day of most passenger cars. By managing the conversion process, hydrogen FCEVs will be more effective for the average driver thanks to quantum mechanics. "As a mechanical engineer, I feel bad that we don't usually get to join in the fun of quantum mechanics," says Aceves. "Here for a change, is one effect where we mechanical engineers can work on a quantum-mechanical phenomenon that has an impact on daily life."

—*Allan Chen*

Tim Ross (right) watches as a technician delivers hydrogen to the Laboratory's Cryogenic Hydrogen Test Facility.

Key Words: Cryogenic Hydrogen Test Facility, cryogenic tank, Department of Energy's Office of Fuel Cell Technology, Eugene Wigner, hydrogen fuel cell electric vehicles (FCEVs), National Ignition Facility (NIF), para- to ortho-hydrogen (H2) conversion, paramagnetism, quantum mechanics, Raman spectroscopy, spin isomer, University of Guanajuato, vessel dormancy.

For further information, contact Salvador Aceves at (925) 422-0864 or aceves6@llnl.gov.

TRACKING PLUTONIUM through the Environment

PRIOR to World War II's Manhattan Project, plutonium existed naturally only in trace amounts on Earth. Today, the worldwide inventory of this element, a component of nuclear weapons and a byproduct of fission reactors, is estimated at 2,850 metric tons. About one percent of this amount has been released into the environment. Some of the released plutonium has been deposited underground at nuclear test sites around the world, where weapons were detonated during the nuclear testing era. Plutonium also resides at sites of reactor accidents such as Chernobyl and Fukushima, in accidental releases from nuclear waste reprocessing facilities, and in radioactive waste dumping from the early nuclear era.

Roughly half of worldwide nuclear detonations took place during the era of nuclear testing at the Nevada National Security Site (NNSS), formerly called the Nevada Test Site. Approximately 2,775 kilograms of plutonium are dispersed underground at the NNSS.

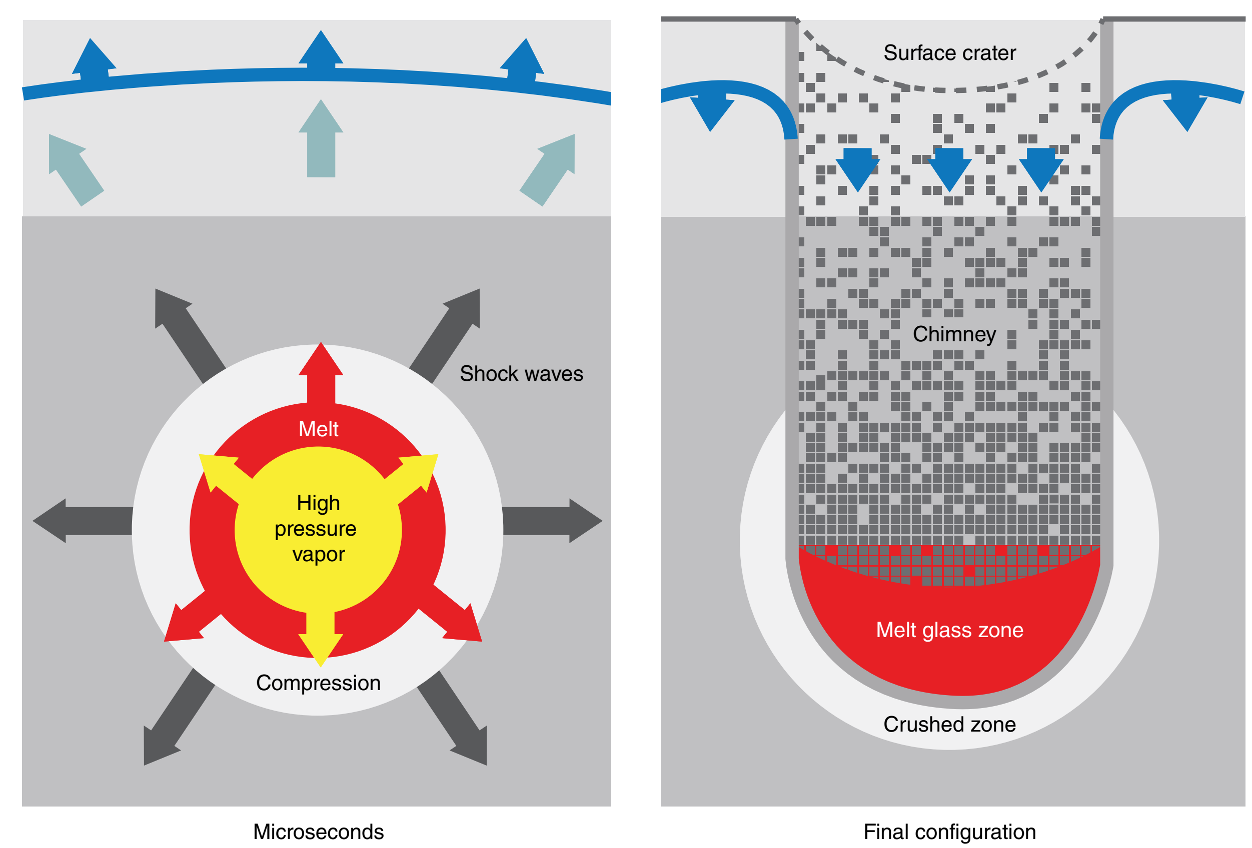
The transport and fate of plutonium in the environment is an ongoing concern. Will it stay confined to the immediate surroundings of contaminated areas? Or does plutonium move? If so, how far, how fast, and at what concentration? Researchers at Lawrence Livermore's Glenn T. Seaborg Institute have been studying these questions for more than 20 years and have developed insights into the natural biogeochemical processes governing plutonium's migration.

Plutonium sits in the lowest row of the periodic table, home of the actinide elements, the heaviest and most persistent elements in the universe discovered to date. Plutonium is both highly toxic and long-lived, therefore needing to be safely isolated from the biosphere. For example, plutonium-239 has a half-life of 24,100 years, so it will be present in the environment for millions of years.

Commercial nuclear reactors produce some 70 metric tons of plutonium per year as nuclear waste and, along with the plutonium from the U.S. nuclear legacy, serves as motivation for ongoing research. "As a National Nuclear Security Administration (NNSA) laboratory, we have a knowledge of the inventories and chemistry of actinides in the environment, and we have always been at the forefront of monitoring actinide concentrations for NNSA programs in nuclear safeguards and nonproliferation," says Mavrik Zavarin, director of the Seaborg Institute. Zavarin is also principal investigator on a Department of Energy (DOE) Office of Science Biological and Environmental Research Program studying the behavior of plutonium in the environment. The Institute has engaged over a ten-year effort to identify and quantify the biogeochemical processes and underlying mechanisms that control mobility of plutonium and other actinide elements to reliably predict the cycling and migration of actinides in the environment. Seaborg Institute staff conduct collaborative research with universities and encourage students and postdocs to develop careers in actinide environmental chemistry.

Surprisingly Mobile

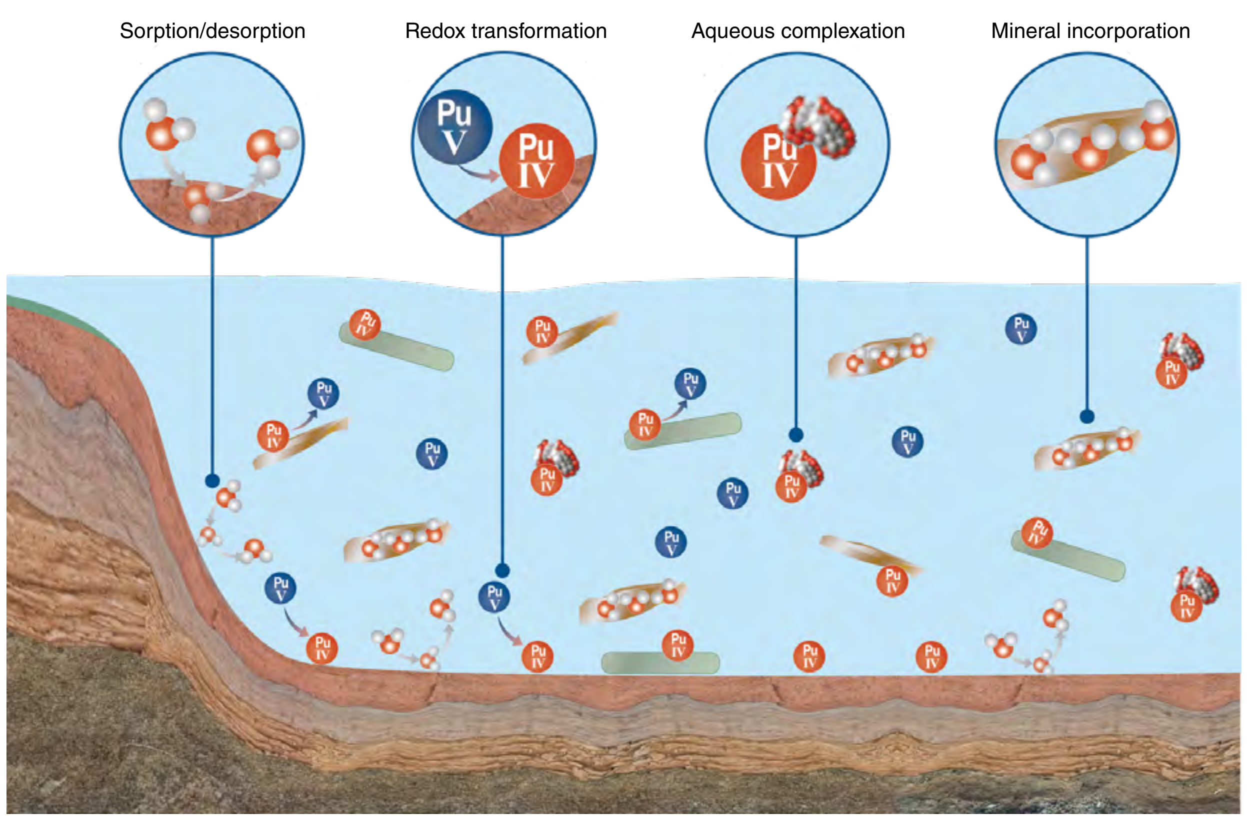
In 1998, Annie Kersting, former director of the Seaborg Institute, now Livermore's director of University Relations and Science Education, analyzed contaminated groundwater collected downgradient from a nuclear test at the Nevada National Security Site (NNSS, formerly the Nevada Test Site). Kersting's research team found low levels of plutonium and associated isotopic ratios that uniquely matched a test 1.3 kilometers from the contaminated well. During a detonation, residual plutonium is thought to be trapped in melt glass that



Schematic of a nuclear test and the subsequent formation of nuclear melt glass.

forms when the heat of the explosion vaporizes surrounding material that then solidifies into a glass. As a result, actinides such as plutonium were thought to remain isolated from the environment. Kersting's work was the first documented proof that plutonium can migrate significant distances and associates with small, naturally occurring particles, called colloids, in the groundwater. The results surprised scientists in the field. "Everyone had thought plutonium was relatively immobile," says Kersting. "It has low solubility in ambient groundwater and sticks strongly to minerals and organic material of the host environment." Other research groups working in contaminated locations worldwide have now confirmed the plutonium transport phenomenon under varying biogeochemical conditions.

At least four processes govern how plutonium interacts with its environment (from left): its sorption to and desorption from micron-size particles in the water; its chemical transformation between more and less mobile chemical species; its ability to form complexes with other species dissolved in water, including organic molecules; and its tendency to be incorporated into minerals that have broken down through the action of high-temperature geothermal fluids. Many of these processes may be mediated, directly and indirectly, by microbial activity.



Colloid-facilitated transport is now accepted as an important mechanism that allows plutonium to migrate in the environment. The NNSS effort was supported by the long-standing LLNL Underground Test Area program, currently led by Andy Tompson, focused on the fate of radionuclides from underground nuclear testing at NNSS.

In recent years, Seaborg Institute staff have focused on understanding the biogeochemical mechanisms that associate plutonium with colloid surfaces, whether mineral, organic, or microbial, as well as identifying the conditions of potential mobility under different hydrologic and geologic environments. The figure below shows several possible mechanisms the team has investigated using a combined field, laboratory, and modeling approach.

Finding Partners for Plutonium

In recent years, the Seaborg Institute research team has been exploring the mechanisms by which plutonium can adsorb (attach) to and desorb from common minerals such as clays and iron oxides. In specialized flow-cell reactors, researchers pumped water with different concentrations of plutonium into cells containing clay colloids and monitored the rates of reaction between plutonium and the colloids. These experiments

"A complex picture of interrelated processes governing plutonium's disposition is emerging."

showed that plutonium will desorb from colloid particles over a timescale of years to decades. The research helped resolve key issues that have frustrated the DOE's Underground Test Area Environmental Management project at the NNSS.

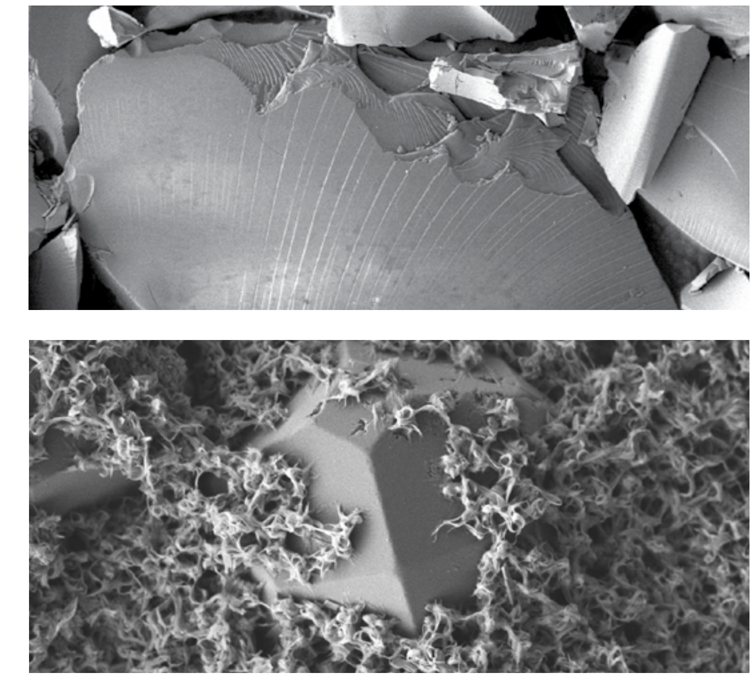
In addition to plutonium adsorption–desorption, plutonium forms chemical complexes with large organic molecules in water through aqueous complexation. Results of a 2016 Seaborg Institute study showed that a strain of *Pseudomonas* bacteria isolated from well water at the NNSS can generate a complex residue of organic material called extracellular polymeric substances that can react chemically with and adsorb plutonium.

Seaborg Institute researchers also investigated direct incorporation of plutonium into minerals. In research published in 2019, Zavarin and colleagues studied how hot hydrothermal fluids can alter nuclear melt glass at NNSS by placing samples of nuclear melt glass into pressure vessels with hydrothermal fluids heated to 25°, 80°, 140°, and 200°C for up to three years to study long-term colloid formation. Follow-on experiments led by Enrica Balboni, a geochemist who began as a postdoc with the institute and is now a staff scientist, demonstrated that in the 140°C samples, plutonium desorption rates matched previously measured colloid desorption rates, suggesting that simple adsorption–desorption could be the mechanism. However, in the 200°C samples, the desorption rates were significantly slower. This suggests that plutonium may be incorporated into the mineral structure as the colloids form and, as a result, be transported much farther in the environment.

Complex Interactions

A complex picture of interrelated processes governing plutonium's disposition is emerging. "How do we grapple with these multiple mechanisms and long timescales in a lab setting?" asks Zavarin. "One way is to rely on field observations where contaminated sources have evolved over decades." Extending the research to additional field sites with longer timescales is a current focus of the institute.

Seaborg Institute researchers are heading to new field sites. Balboni is working on a project at the Ravenglass Estuary on the Irish Sea, near the U.K.'s Sellafield nuclear site. Samples will provide insights into how plutonium and other radionuclides interact with their environment in coastal wetland sediments, a



Scanning electron microscope images of hydrothermally altered melt glass (140° and 200°C) after 994 days of reaction showing increased colloid formation with increasing temperature.

very different environment from that of the NNSS. "We're going to new sites to apply what we've learned in the lab and look at plutonium's behavior at various field conditions and longer timescales—years instead of weeks to months," she says.

Postdoc Nancy Merino studies plutonium migration and its association with microbes at the DOE's Savannah River site in South Carolina. She observes, "With an element as complex as plutonium in the environment, you must expect that many factors will affect its mobility." The next generation of actinide scientists in Livermore's Seaborg Institute are leading the effort to untangle its complex behavior and persistence in nature.

—Allan Chen

Key Words: actinides, adsorption, biogeochemistry, Chernobyl, colloid, desorption, extracellular polymeric substances, Fukushima, Glenn T. Seaborg Institute, groundwater, hydrothermal fluid, Manhattan Project, National Nuclear Security Administration (NNSA), neutron, Nevada National Security Site (NNSS), nuclear melt glass, plutonium, radionuclide, Ravenglass, redox, Savannah River Site, Sellafield, sorption.

For further information, contact Mavrik Zavarin at (925) 424-6491 or zavarin1@llnl.gov.

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 (uspto.gov).

Patents

Electrostatic Generator Electrode-Centering and Seismic-Isolation System for Flywheel-Based Energy Storage Modules
Richard F. Post
U.S. Patent 10,541,586 B2
January 21, 2020

Solvent Depression of Transition Temperature to Selectively Stimulate Actuation of Shape Memory Polymer Foams
Anthony J. Boyle, Keith Hearon, Duncan J. Maitland, Landon D. Nash, Thomas S. Wilson
U.S. Patent 10,548,608 B2
February 4, 2020

Pulse-Train Drive System for Electrostatic Generators and Motors
Richard F. Post, Edward G. Cook
U.S. Patent 10,554,151 B2
February 4, 2020

Accelerating Fissile Material Detection with a Neutron Source
Mark S. Rowland, Neal J. Snyderman
U.S. Patent 10,557,950 B2
February 11, 2020

System and Method for Portable Multi-Band Black Body Simulator
Nicholas Calta, Gabe Guss, Manyalibo Joseph Matthews
U.S. Patent 10,564,039 B2
February 18, 2020

Ion Conductive Inks and Solutions for Additive Manufacturing of Lithium Microbatteries
Eric B. Duoss, Patrick G. Campbell, William C. Floyd, III, Julie A. Mancini, Matthew Merrill, Conner T. Sharpe, Christopher M. Spadaccini, Michael Stadermann, Cheng Zhu
U.S. Patent 10,566,595 B2
February 18, 2020

Awards

Lawrence Livermore National Laboratory physicist **Yuan Shi** has earned the **American Physical Society's Marshall N. Rosenbluth Outstanding Doctoral Thesis award** for his work in plasma physics. Shi's thesis, entitled "Plasma Physics in Strong Field Regimes," was conducted at Princeton University. His award is cited "for elegantly describing three-wave coupling in plasma modified by oblique magnetic fields, identifying applications including plasma-based laser amplifiers and adapting quantum field theory to describe plasma physics in the strong-field regime."

The award recognizes exceptional young scientists who have performed original thesis work of outstanding scientific quality and achievement in plasma physics.

Three scientists from Lawrence Livermore, **Hye-Sook Park, Steven Ross**, and **Dmitri Ryutov**, are recipients of the **2020 John Dawson Award for Excellence in Plasma Physics Research** from the **American Physical Society**. The honor recognizes a recent outstanding achievement in plasma physics research.

The scientists are part of an international team of researchers that was cited "for generating Weibel-mediated collisionless shocks in the laboratory, impacting a broad range of energetic astrophysical scenarios, plasma physics, and experiments using high energy and high-power lasers conducted at basic plasma science facilities."

The award recognizes nearly a decade of the team's work in frontier laboratory astrophysics, encompassing plasma physics theory, large-scale numerical simulations and experiments on some of the world's premier high-energy laser facilities, including Livermore's National Ignition Facility.

SPIE, the International Society for Optics and Photonics, recently announced the election of Lawrence Livermore National Laboratory research engineer **Richard Leach** as a **senior member** of the organization. The designation honors Leach for his technical and scientific contributions to a variety of optics and photonics fields, including seismic detection, satellite communications, medical devices, first responders, homeland security, and large high-power laser systems. SPIE recognizes senior members based on exceptional professional experience, active involvement with the optics community, and/or significant performance that sets them apart from their peers, according to the organization.

Abstract

Fusion Supports the Stockpile

The National Nuclear Security Administration's Stockpile Stewardship Program (SSP) uses a science-based assessment of the reliability of nuclear weapons to assess and certify the stockpile, without nuclear explosive testing. Lawrence Livermore's Inertial Confinement Fusion (ICF) program supports the SSP mission by seeking to re-create and examine the processes that occur in the heart of burning stars and imploding nuclear weapons. In ICF experiments conducted at the National Ignition Facility (NIF), scientists heat a tiny amount of encapsulated fusion fuel and compress it to the point that nuclear fusion reactions occur. Data from these experiments help refine models used to assess the performance of the U.S. stockpile. Progress toward ignition, where the outgoing energy from an implosion is greater than the incoming energy, is being made through experimental campaigns designed to investigate how different target and laser configurations affect the rate of fusion. Simulations of NIF capsule implosions are being run on the new Sierra supercomputer to try and predict how a certain experimental configuration will perform. The ICF program also offers valuable training for a new generation of stockpile stewards. Executing ICF experiments allows these future stewards to tackle challenges important to maintaining the safety, security, and reliability of the nation's nuclear deterrent.
Contact Mark Herrmann at (925) 423-5719 or herrmann9@llnl.gov.

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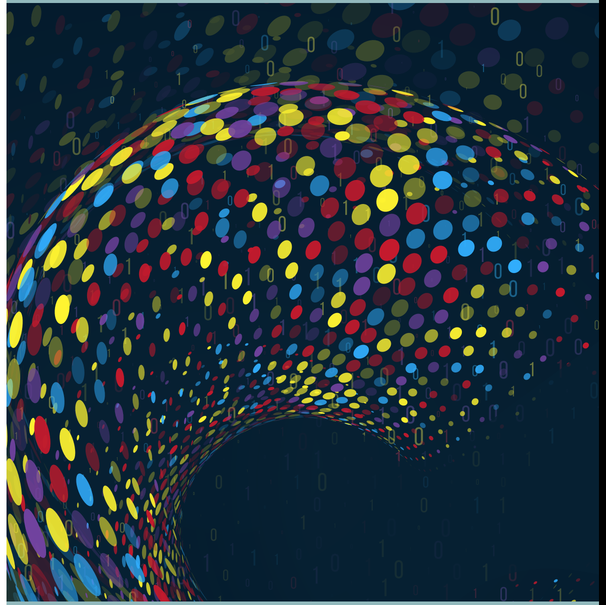
A Nuclear Needle in a Haystack



Machine learning is speeding up and expanding researchers' ability to identify patterns and find useful avenues forward. Lawrence Livermore is paving the way.

Also in the next issue:

- *Software for high-performance computers helps discover new materials.*
- *A fresh look at plutonium, thanks to Scorpius.*
- *A window into pathbreaking science with Laboratory legend Johnny Foster.*

Coming Next Issue

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