Lawrence Livermore National Laboratory

March 2023

Science & Technology REVIEW

PREDICTING AND PREVENTING CORROSION

Also in this issue:

Livermore's Offsite Fellows

Software Builds for Supercomputers

Information Technology Resource Management

About the Cover

Corrosion damages and can ultimately destroy items from household appliances and personal vehicles to aircraft parts and reinforcing steel in bridges and roadways. As the article beginning on p. 4 describes, Lawrence Livermore researchers have developed capabilities for predicting the onset of corrosion in specific materials. Of particular interest to the Laboratory and its mission are impacts to weapon components stored in potentially corrosive environments. The cover illustration represents the worldwide economic, safety, and operational threat of unabated corrosion on households, communities, industries, and governments.

Cover design: Alii Diaz; Illustration: Eric Smith

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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Uranium Takes an Alternate Pathway

Under normal working conditions, radioactive materials such as uranium react in a predictable manner. However, under extreme conditions of high temperature, a short timescale, and rapid cooling, the reaction pathways and kinetics change dramatically. Until recently, scientists lacked a good understanding of the chemistry associated with the thermal decomposition of these reactive compounds under extreme conditions since their reaction rates are so fast and so different from equilibrium processes.

The October 21, 2022, *Inorganic Chemistry* cover story presents how Lawrence Livermore scientists have synthesized uranium-based compounds that are extremely air- and water-sensitive. The team was able to characterize the behavior of these compounds under extreme conditions using a custom-built laser chamber capable of handling radioactive material. The process used laser irradiation to thermally decompose UI_4(1,4-dioxane)$_2$ to form a thin layer of material containing a mixture of decomposition products. The extreme nature of the irradiation process is then observed in the production of vapor during the intense temperature cycling. This effort was the first application of laser-driven chemistry with a uranium-based compound containing organic ligands as the precursor.

"The knowledge can potentially be applied to materials manufacturing, stockpile stewardship, or even waste consolidation, processing, or storage," says Livermore radiochemist Maryline Kerlin, first author of the paper. "We could imagine storing a metal-containing compound under a stable configuration, and then react it under lasers to obtain a new product."

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Model Instantly Predicts Polymer Properties

Development of suitable polymer materials for use in a growing application space relies on accurately predicting the properties of candidate materials. Quantitative understanding of the relationship between chemical structure and observable properties is particularly challenging for polymers, due to their complex 3D structures. The molecular structure of polymers consists of numerous repeating chemical subunits, a characteristic known as periodicity.

A team of Lawrence Livermore materials and computer scientists developed a machine-learning (ML) model to demonstrate how subtle changes in a polymer's connectivity and periodicity can dramatically affect its predicted properties. The team developed a new method, described in the October 31, 2022, *Journal of Chemical Information and Modeling*, for explicitly encoding the polymer's periodicity into the ML model. "The results show that inclusion of periodicity in the model enables state-of-the-art accuracy for predicting polymer properties," says Livermore researcher Evan Antoniuk. The ML model can generate property predictions almost immediately. "The success of the model lies in a new polymer representation that compactly captures the polymers' structure, in combination with powerful graph-based ML techniques that autonomously learn how to describe the structure of the polymer," says Antoniuk. The team has also developed an interactive web interface to allow quick access to the ML models. Adds project co-leader Anna Hiszpanski, "This interactive model will allow polymer chemists to understand the properties of new polymer materials, enabling new concepts in polymer chemistry to be rapidly tested and iterated."

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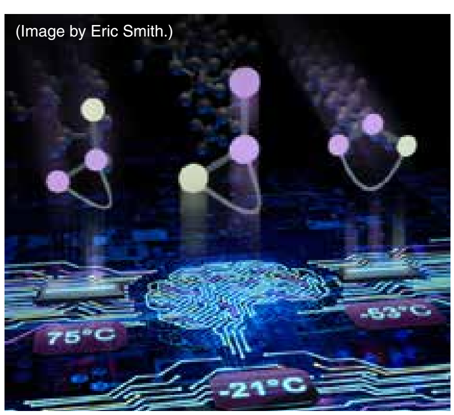

(Image by Eric Smith.)

New Technique to Analyze Fentanyl

A team of Lawrence Livermore scientists has developed a new method, published in the November 2, 2022, *PLOS One*, to analyze and confirm the presence of fentanyl and a related analog—acetyl fentanyl, a potent opioid as well—to aid in chemical forensics, toxicology, and medical diagnoses. The Livermore technique detects fentanyl in blood and urine at low levels still lethal enough to cause an overdose. Specifically, the researchers detected intact fentanyl in biological tissues to confidently identify and confirm fentanyl's presence in the sample by chemically modifying the opioid.

The team spiked blood and urine samples with levels of fentanyl and acetyl fentanyl obtained from human overdose cases. An organic solvent was used to extract the opioid from the samples. That organic extract was treated with the chemical reagent 2,2,2-trichloroethoxycarbonyl chloride (troc chloride). "The reaction between troc chloride and fentanyl breaks the compound into two products from the opioid: the first is 2-chloroethyl benzene and the second is troc-norfentanyl, both of which are easily detectable using standard forensic science equipment," says lead investigator Carlos Valdez. "The strength of this approach is that both products can be pieced together to identify any fentanyl-related substances, even unknown ones, that have been absorbed into the body." Along with applications for blood and urine analysis, the new fentanyl identification technique could be used for other biological tissues, including liver, kidney, and heart tissue.

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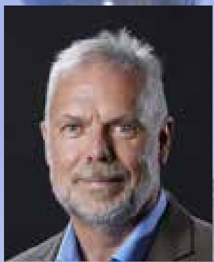
Commentary by Tony van Buuren



Accelerating Knowledge and Critical Timelines

LARGE in scope, with multidisciplinary, cross-organizational teams, Strategic Initiative (SI) projects supported by Lawrence Livermore's Laboratory Directed Research and Development (LDRD) Program advance the Laboratory's strategic goals through broad and deep research and development in key science, technology, and engineering expertise and capabilities. For Fiscal Year 2022, SI projects represented less than 8 percent of all funded LDRD projects but 34 percent of the program's total funding. As the saying goes, "Time is money." A successful SI project may accelerate the arrival of a long-term solution to mission challenges, achieving progress in a three-year timeline rather than a period twice as long.

This issue features an SI project studying corrosion that demonstrates how research can shorten real-world innovation timelines. Corrosion is a familiar and costly issue across industries, infrastructure, and even households. For the Laboratory's stockpile stewardship mission, improved understanding of corrosion's progression leads to more reliable aging models, codes, and certification standards. However, materials compatibility and corrosion tests can take considerable time, potentially slowing the progress of scientific discoveries in this area of science and affecting timescales for applying new findings to the mission.

As described in the article, three research thrusts applying Livermore expertise in multiscale simulation, multimodal characterization, microscopy, additive manufacturing, machine learning, and other disciplines resulted in new capabilities to understand the incipient phases of corrosion with an eye to one day predicting and preventing corrosion before it starts. The capabilities developed are a step to validate accelerated testing protocols as representative of real-time aging that would require 10 or 20 years to conduct, thus shortening design and testing timelines for materials used in infrastructure and transportation projects as well as nuclear weapon life-extension programs (LEPs). In a related long-term benefit that will far outlast the LDRD project itself, new postdoctoral researchers recruited for the initiative will offer the unique skill sets required to support LEPs over program lifetimes.

This research also promises to deliver results for pressing, short-term needs. Lawrence Livermore has established valuable expertise in materials degradation to support teams spinning out technologies that advance batteries, carbon capture technologies, and other clean energy initiatives. For example, the SI project's findings in hydrogen embrittlement inform the development of hydrogen-based fuels by addressing ways that hydrogen corrodes metal systems. The Laboratory can spin in industry expertise as well, exchanging knowledge as companies seek best practices for materials tied to their economic progress. Each new opportunity is a tendril emerging from the mission-related roots of this successful SI project.

Similar to spinning innovation in and out of the Laboratory, Lawrence Livermore experts assigned to positions in Washington, D.C., and other locations through the Offsite Fellows Program (OFP) provide their expertise to federal government agencies and, later, return to Livermore with a wealth of experiences that benefit other staff engaging with federal program managers. The first research highlight describes the assignments and accomplishments of six Livermore fellows along with lessons learned that have broadened their appreciation of budgets, policies, and decision-making across the national nuclear security enterprise. The OFP is further refining its assignment strategy to ensure diverse opportunities for future fellows.

The second research highlight presents the far-reaching effects of a open-source, high-performance computing package manager called Spack that speeds supercomputing center operations worldwide. Spack originated at Lawrence Livermore to support software building and integration projects relying on the coordination of software packages operating in intricate dependencies. A community of users has added thousands of lines of code to Spack in the last 10 years enabling the automated system to keep up with supercomputing's accelerated growth. Today, Spack is an essential part of the Department of Energy's Exascale Computing Project to support the massive computing demand for clean energy, materials, and other mission-related research.

The final research highlight goes behind the scenes of Livermore Information Technology (LivIT)—the networks, infrastructure, and service staff that support the entire campus and hybrid workforce. LivIT rose to meet rapidly changing workplace demands during the early months of the COVID-19 pandemic. System enhancements continue as LivIT leverages cloud computing and machine-learning tools to meet Laboratory needs.

Each story in this issue reinforces the value of Lawrence Livermore's expertise to our staff, the innovation community, and the nation. Opportunities for advancement continue to reach out like tendrils from our core, mission-related research.

■ Tony van Buuren is deputy associate director for Science and Technology in the Physical and Life Sciences Directorate.

STOPPING CORROSION BEFORE IT STARTS

Integrating experimental tests and high-performance computing models helps Lawrence Livermore understand the onset of corrosion and stop it before it starts.

CORROSION is a part of everyday life. From cars and home appliances that rust to roads, bridges, and other infrastructure that crack and pit, materials eventually begin to deteriorate and need to be replaced. Corrosion not only has a huge economic impact for households, industries, and governments, it is also a critical factor in nuclear weapons stockpile stewardship. Materials used for weapon components stored in potentially corrosive environments can crack, break, or fail over varying time frames.

Research has been largely focused on corrosion's later stage conditions rather than addressing the problem early on, when steps to mitigate the degradation can be most impactful and effective. In a new approach, Lawrence Livermore researchers recently completed a Laboratory Directed Research and Development Program Strategic Initiative project that focused on understanding the initiation of corrosion, specifically pitting initiation and chemical degradation in moisture- or hydrogen-rich environments at their earliest stages. The team integrated state-of-the-art multiscale computer simulations, in-situ characterization, and data science to paint a fuller picture of the timescales and evolution of corrosion.

Led by Brandon Wood, director of Livermore's Laboratory for Energy Applications for the Future, this project has filled many gaps in understanding the onset of corrosion in multiple materials. Wood says, "Looking at what's been done in the past for predicting and modeling corrosion over the lifetime of materials, the work has been mostly empirical. Data sets are collected under quasi-controlled conditions but result in many unknowns. The older studies also relied on traditionally manufactured materials as well as conventional processes and conditions, which aren't so relevant today given the advances in materials science and technology." To fill in the gaps, Wood and his team chose three research thrusts representing different materials classes and degradation modalities: aqueous corrosion of aluminum, hydriding of titanium, and corrosion of additively manufactured stainless steel. The team conducted experiments at the atomistic, compositional, and microstructural scales, using a variety of spectrometry and microscopy techniques to characterize the materials' surfaces as they corroded and degraded.

However, the experimental work only told one part of the tale. High-performance computing (HPC) simulations were developed to model the evolution and impacts of corrosion over time, and machine-learning (ML) tools were needed to analyze the data. The surprising results of the multidisciplinary project have attracted the attention and interest of many academic research institutions, national laboratories, and government and industry stakeholders also seeking to predict—and one day prevent—corrosion.

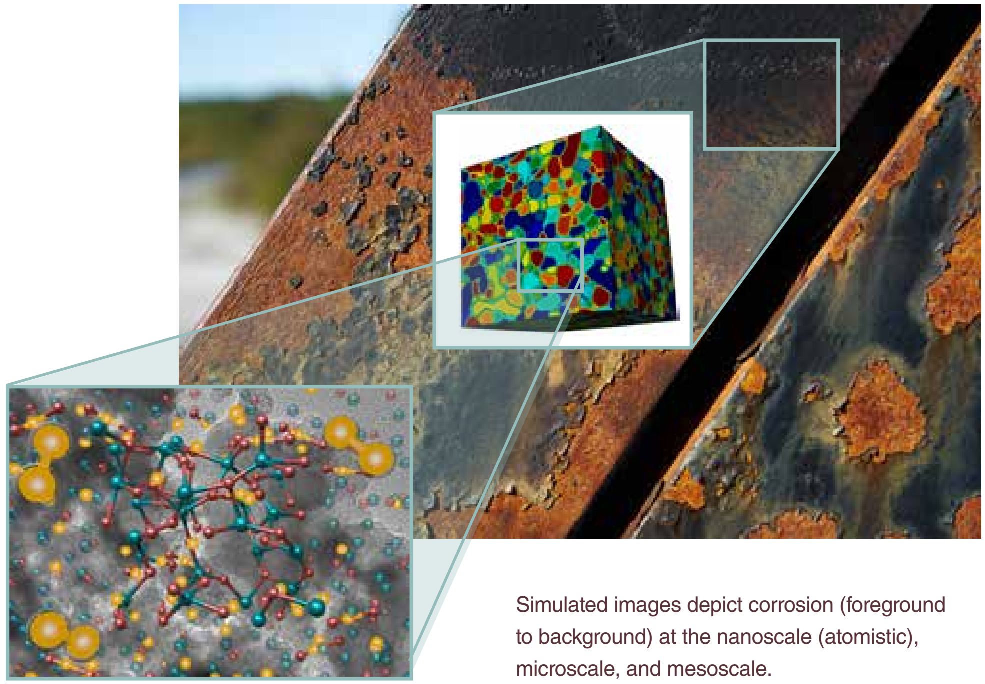
Aluminum Meets Acid

Aluminum is used across everyday and industrial needs, from aluminum foil and kitchen utensils to building materials and aircraft construction. As such, aluminum corrosion impacts nearly everyone in some manner, whether they realize it or not.

Lawrence Livermore's researchers sought to understand and predict several aspects of aluminum degradation such as aluminum's surface dissolution rate in corrosive solutions, the effect of aluminum's microstructure—which depends on processing conditions—on its susceptibility to corrosion, and the source of deterioration in surface oxides that form natively to protect the metal. While working with such a commonly used material with well-known properties may seem straightforward, the team realized early on that they would need to establish several parameters around the experiments and simulations to answer their questions. The team opted to work with pure aluminum instead of more commonly used aluminum alloys because alloys are much more complex systems with many more factors that are difficult to control in experiments and simulations. "We wanted to establish a baseline for aluminum's corrosion timescale and kinetics, which meant we needed to use the simplest system within the simplest environment," says Chris Orme, staff scientist. The simplest environment was determined to be the one in which the researchers could easily control and analyze the effects of changes to the corrosive solution on the material—varying only the pH of the solution in which the aluminum was submerged, in this case.

Orme and postdoctoral fellow Seongkoo Cho developed a titration system to adjust the pH levels of the solution by increasing and decreasing acidity levels on submerged aluminum samples. In doing so, they could measure corrosion rates in chemistries that develop in cracks and other occluded environments. Semi-closed environments, such as cracks, create a positive feedback loop of corrosion and acidity that leads to even more aluminum corrosion as the solution becomes increasingly acidic. The acidity produced during corrosion can worsen pre-existing cracks, pits, and crevices, exacerbating degradation. As the pH was lowered from neutral pH to acidic pH, the protective oxide normally present on the metal surface began to dissolve, and the corrosion rates increased. As the corrosion tests with different pH levels were taking place, electrochemical impedance spectroscopy was used to analyze the thinning oxide layer on the corroding aluminum, providing valuable insights into the variation of corrosion rates with changes in pH. At the lowest pH values, the metal was essentially bare, creating a good model system for comparisons to more detailed atomistic simulations.

One factor the team sought to better understand was the role that grain orientation, regions, and boundaries play during corrosion. Aluminum's grain structure is polycrystalline, meaning that it has a microstructure composed of randomly oriented grains separated by grain boundaries. Grain orientations can be viewed using a technique called electron backscatter diffraction, a method that maps grain orientations across the surface. Each grain orientation has a slightly different arrangement of atoms—some more tightly bound, others less tightly bound, depending on their number of nearest-neighbor atomic bonds—resulting in slightly different corrosion rates. Orme and her team were particularly interested in understanding the differences in corrosion rates between grain orientations, something that has been overlooked in the past. Orme says, "Typically, corrosion studies yield an average corrosion rate instead of looking closely at the differences between grain orientations. We wanted to know whether the corrosion rate tracked with the local bonding environment—the number of nearest neighbor bonds the atoms had due to their grain orientation—or whether something more complicated was going on."



Simulated images depict corrosion (foreground to background) at the nanoscale (atomistic), microscale, and mesoscale.

Neighborhood Effect

What the team found was rather unexpected. Under the aqueous corrosion experiments, the pure aluminum exhibited galvanic corrosion, an electrochemical process in which one metal normally corrodes preferentially when in electrical contact with a different metal due to the presence of an electrolyte. In Livermore's research, however, galvanic corrosion was occurring on a microscale between the grains of aluminum with no other metal playing a role.

The team correlated the grain orientation maps with confocal microscopy, an optical imaging technique that can measure height changes across a surface on the microscale, to know the corrosion rate of each grain of their metal surface. "We had expected to find that the grains with the best bonding environments would have the slowest corrosion rates because they have more nearest-neighbor atoms holding on to them, while the grain orientations with more isolated and loosely bound atoms would corrode more quickly," says Orme. "This is true of other metals, such as nickel-based alloys, but this was not what we found for pure aluminum." Instead, the team observed galvanic corrosion, where the dissolution rate of one metal grain was influenced by the presence of another metal grain in its neighborhood.

However, cooperative effects such as these are difficult to quantify. By converting the orientation and height maps into a spatial network and subjecting them to graph neural network ML algorithms, data scientist Tim Hsu was able to analyze interactions among hundreds of grains as the pH balance of the solution changed, enabling him to demonstrate how the grains interacted. Using the ML model, the team could compare corrosion rate predictions of any one grain when they either included or excluded information about the size and orientation of the neighboring grains. The team found they could significantly improve the ability to predict corrosion rates by including information about the surrounding grains, what they have called the "neighborhood effect" to mean that any given grain's neighbors had a strong impact on the corrosion rate. In addition to the surprise of galvanic corrosion with only aluminum, the team determined that their hypothesis about the relationship between bond strength and corrosion rates had been incorrect. Rather, galvanic corrosion reversed the relative corrosion rates making the grains with the highest local bonding the most likely to corrode.

The experimental research team partnered with Lawrence Livermore's HPC researchers to develop more predictive, physics-based models, but integrating the two fields was challenging. Anh Pham, researcher and quantum simulations expert, says, "Experiments are always more complex because the real systems are so complicated. Many factors, such as the different types of ions, solutions, and surface oxides, aren't typically included in computer simulations. Even though simulations offer tremendous insight into the corrosion process and what can be done to mitigate it, we also had to simultaneously make our computer models much more complex while simplifying and better controlling our experiments to find a middle ground that provides accurate information in a more cost-effective way than running many quantum simulations." The team developed new HPC capabilities and multiscale models to show how the grain orientation changed the corrosion rates and to directly predict rates of dissolution and oxide formation from quantum mechanics, going beyond simple textbook thermodynamics. These capabilities were used not only to recreate the surface height maps of locally varying corrosion, but also to reveal the key competing mechanisms and origins of the observed grain dependencies on corrosion rates. ML algorithms analyzed hundreds of grains at a time as the pH balance of the solution changed. By integrating atomistic modeling with data science and experiments, the team developed models that showed the rates of aluminum corrosion in solutions of varying pH. These simulations will be used in future research aiming at more accurately predicting the corrosion process.

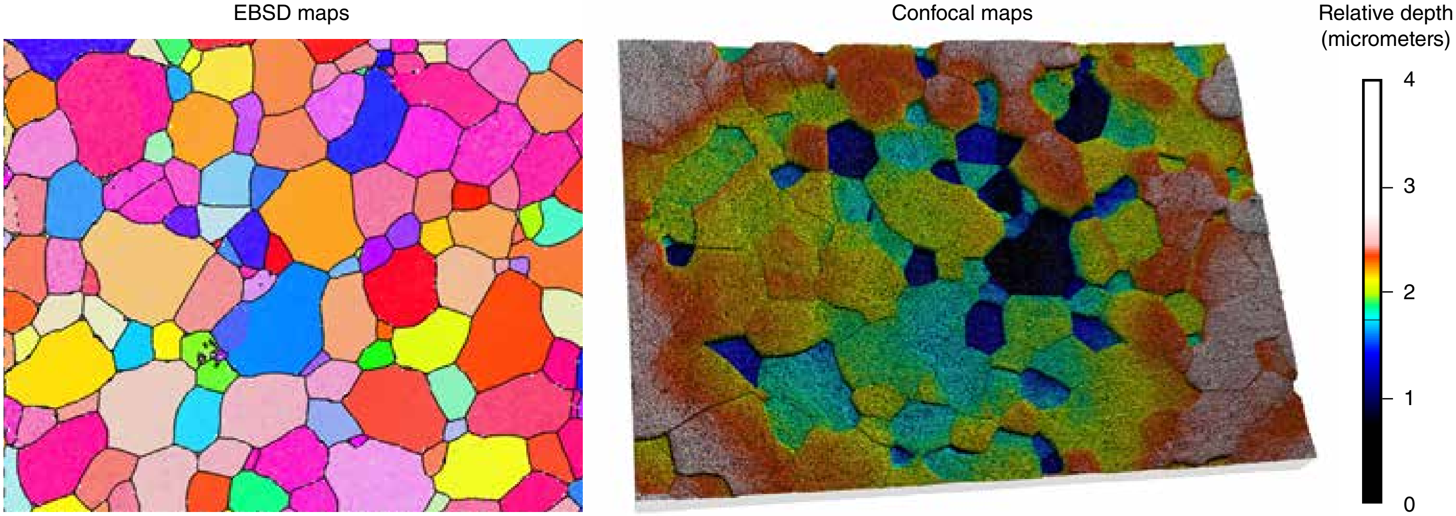
Hydrogen-induced Failure

Used for commercial and industrial applications such as spacecraft, automobiles, sporting goods, and mobile phones, as well as for military hardware, titanium is a material synonymous with strength and resilience. Yet titanium can fall prey to corrosion over time.

Livermore researchers placed their primary focus on the roles of surface oxide features and metal microstructure in initiating hydrogen-induced degradation of titanium as hydrogen permeates through the surface oxide layer and the formation of the undesired phase (i.e., hydride) is affected by the metal microstructure. While the oxide acts as a natural barrier to outside elements that can impact the chemistry of the metal, Wood says, "We needed to understand how the metal itself impacts what is in the native oxide film, and then how that native oxide film is impacted by the environment." Hydrogen-induced corrosion, or hydriding, can lead to embrittlement, fractures, cracking, and ultimately failure of titanium materials, which presents a serious problem for many of its uses, including national security and transportation purposes.

Because commonly used titanium alloys in industrial applications are too complicated to work with due to very complex surface oxide chemistry, Livermore researchers under the titanium

Through the use of electron backscatter diffraction (EBSD) and confocal maps, researchers track the surface height differences due to corrosion across aluminum samples. Each color in the maps represents a different surface height level. Areas of color or grain regions consist of multiple individual grains bonded together.



hydriding thrust worked with pure titanium that can serve as a representative model system. The team wanted to understand not just the initial hydrogen-surface interaction but also how hydrogen is specifically incorporated into the underlying metal at early stages. Tae Wook Heo, staff scientist, says, "What seemed like a simple question to answer was quite a big mystery, largely because the oxide on titanium has a very complicated and diverse structure at the atomistic level." That structure plays a role in how quickly or slowly the hydrogen can permeate the oxide and reach the titanium below, leading to material failure. Heo says, "We wanted to control the process of hydride formation, so it was vital to understand whether its onset depends on local microstructures and mechanical conditions and whether we could quantify the relationship between local features of the oxide and the onset of hydriding."

Like the aqueous corrosion thrust, an integration of experiments and computer simulations was necessary to capture the complex initial process of corrosion. However, the experiments were far more complicated and realistic than the early simulations. Heo says, "We needed to combine the two methods to fully understand hydrogen-induced corrosion at these initial stages, but we had to find an appropriate place where the two approaches can meet by simplifying experiments and incorporating beyond-ideal factors into simulations."

The researchers integrated a number of techniques and tools to evaluate and simulate the microstructure of the pure titanium, its surface titanium oxide layer, and the hydrogen distribution within both. First, Heo's team had to develop new multiscale models capable of resolving necessary features at both the microstructural and atomistic levels. ML and graph theory accelerated model generation, particularly for the disordered regions too complex to navigate using traditional approaches. The computational scientists incorporated advanced simulation techniques spanning molecular dynamics and kinetic Monte Carlo simulations, which simulate atomic arrangements directly with high accuracy, as well as continuum techniques that include phase-field modeling, in which atoms are approximated as continuously varying fields that evolve across much larger scales. Heo's team developed novel approaches to hand off parameters among these models, which then predicted how hydrogen should incorporate, distribute, and permeate upon contact with titanium and its oxidized surface.

To validate the model predictions, staff scientist Roger Qiu's team, including postdoctural fellow Yakun Zhu, used an ion beam sputtering deposition method and specialized thermal treatments to produce systematically varying titanium oxide films with physical properties resembling those of native oxides. The oxide layers and metal samples were imaged using multiple techniques, including transmission electron microscopy (TEM). In TEM, a beam of electrons is transmitted through a very thin (less than 100 nanometers thick) titanium sample to form an image, which is then magnified and focused onto an imaging device. TEM and companion techniques such as atom probe tomography, directly revealing atomic arrangements, provided exceptionally high-resolution images so the Livermore team could see the effects of corrosion on titanium and its oxide in much more detail than was typical in earlier research.

To study the local binding features of the titanium oxide and compare with the atomistic models, the Livermore team applied nuclear magnetic resonance spectroscopy, which observes local magnetic fields around atomic nuclei by exciting the atomic nuclei with radio waves. The resonance frequency changes based on the intramolecular magnetic field around the atomic nuclei, which tells researchers about the electronic structure of the molecule. The data generated from these techniques further refined the accuracy of the computer models and indicated how hydrogen interacts with the oxide layer at the atomistic, compositional, and microstructural scales.

Next, the Livermore team used a nuclear reaction analysis (NRA) tool, in collaboration with SUNY Polytechnic Institute, to study the hydrogen distribution and solubility. "Hydrogen is one of the difficult elements to probe experimentally due to its simple electronic structure," says Qiu. "A non-destructive nuclear reaction-based method such as NRA can provide accurate information of hydrogen depth distributions in materials without the need of a standard," says Qiu. These measurements were used to determine the dependence of hydrogen interactions with local structural features and defects. The results provided input for theoretical calculations and simulations to build a multiscale model of the way hydrogen inserts and permeates through the surface oxide, eventually forming a hydride in the metal underneath.

A major finding from the research was how the binding structure of oxygen determined the hydrogen interaction with the titanium oxide. Contrary to what the team expected, hydrogen did not distribute uniformly, but rather was very sensitive to the local chemistry and binding structure of the oxide. The surface oxides usually have a mixture of atomically ordered regions that are crystalline in addition to more disordered regions that comprise grain boundaries or amorphous layers. This complex, nonuniform structure contributed to a random initial onset of hydriding.

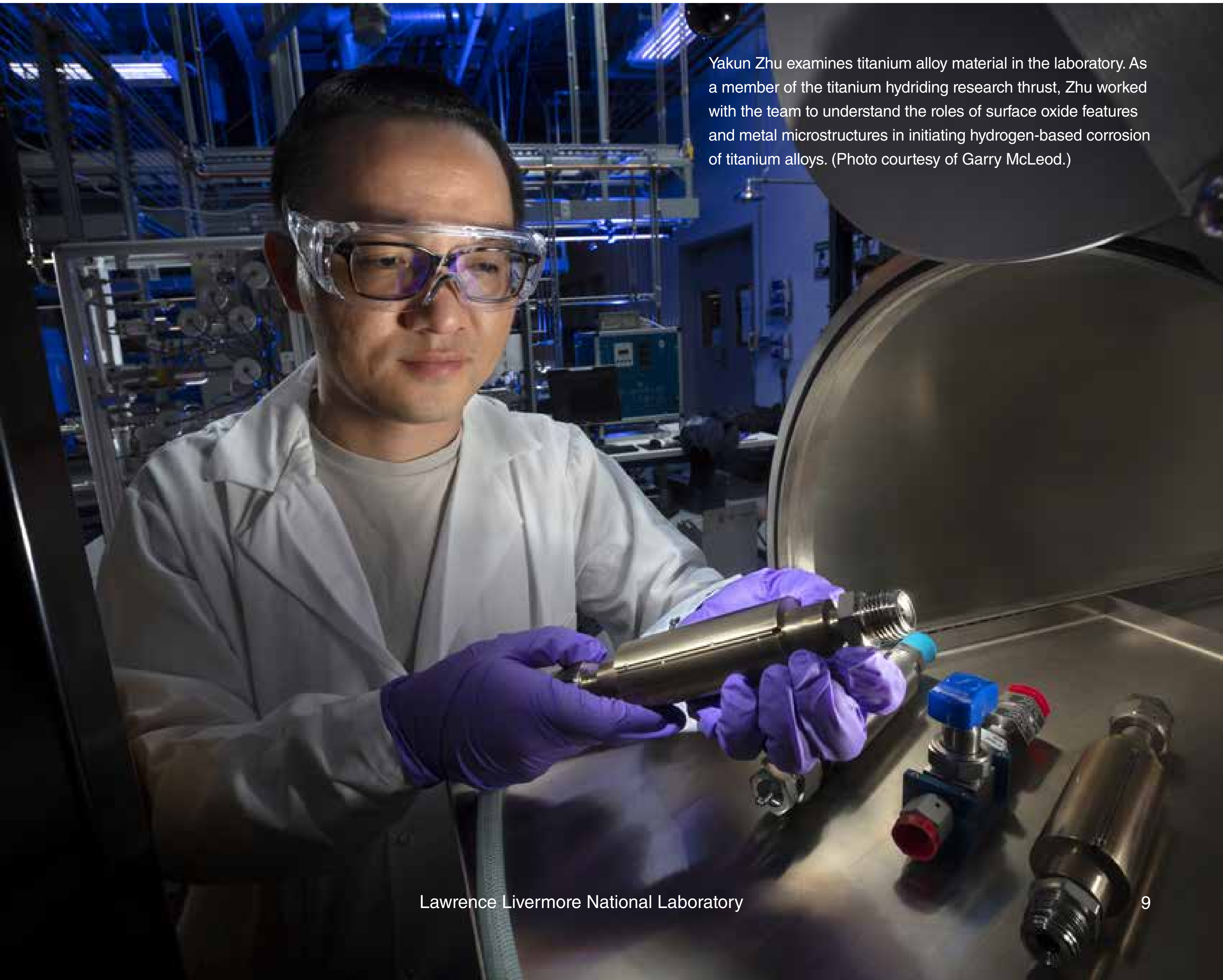
Sometimes hydriding happened very swiftly, while other times it took much longer. After the hydrogen permeated the oxide, the fracture and cracking of the metal itself could also be random, depending on the surface condition and internal microstructure of the metal. Despite this complexity, the team discovered certain patterns related to the local atomic arrangements. For example, the behavior of hydrogen within the surface titanium oxide is highly sensitive to local oxygen coordination geometries within the atomically disordered regions.

Certain arrangements of these local environments create "superhighways" for hydrogen to rapidly penetrate through the oxide into the metal, eventually leading to embrittlement and failure. The formation of the superhighways depends both on the ratio of titanium to oxygen atoms near the surface and to the microstructure of the surface oxide. This understanding implies that both the level of hydrogen incorporation and its rate of permeation through the surface oxide can be controlled by compositional and process modification, providing possible engineering guidance for improving durability of titanium and its alloys in hydrogen environments.

Strengthened Steel

Stainless steel, one of the most commonly used and most widely studied metals in the world, can be found in nearly every facet of people's lives. While very strong, stainless steel can still corrode. However, advances in additive manufacturing offer new ways to prevent corrosion and slow its onslaught.

In the stainless steel corrosion thrust, Livermore researchers studied corrosion of stainless steel 316L (316L SS) that was additively manufactured using a technique called laser powder bed fusion (L-PBF). L-PBF applies a high-power laser to a bed of powdered metal, and the extreme heat from the laser melts the powdered metal into a thin layer of material. Layer after layer of material is melted on top of previous layers until the item being manufactured is completed. Not only does this method open up the possibilities for additive manufacturing of complex shapes, it also can change the way that atoms within the material are organized. Thomas Voisin, staff scientist, says, "Because the laser beam is only about 100 microns in



Yakun Zhu examines titanium alloy material in the laboratory. As a member of the titanium hydriding research thrust, Zhu worked with the team to understand the roles of surface oxide features and metal microstructures in initiating hydrogen-based corrosion of titanium alloys. (Photo courtesy of Garry McLeod.)

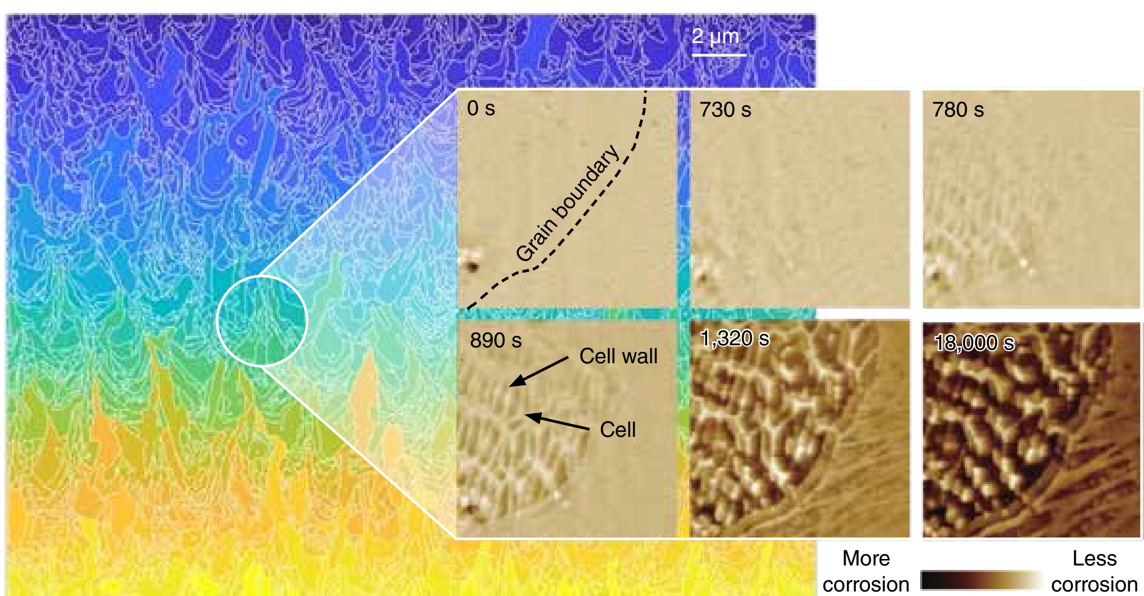
diameter, all melting is very local and very concentrated. Once the material has melted, it then cools much more rapidly than conventionally manufactured material. As a result, different atomic structures that form in the steel are maintained as they adapt to rapid solidification. These structures have significantly different properties than normal stainless steel." Among those properties is material strength two to three times greater than conventionally manufactured stainless steel with similarly improved resistance to corrosion.

In their work to understand corrosion of additively manufactured stainless steel, the team focused specifically on how the new surface oxide that forms under these extreme processing conditions can shield the material so well against degradation in saline water. They recreated a solution with the salinity of sea water in the laboratory, submerged the steel in the solution, and applied an electric current. Not only did the team recreate corrosion, they accelerated it, achieving years' worth of corrosion in just a few hours. Corrosion of steel in seawater takes the form of pitting, the formation of microscale craters in the material. This form of corrosion is difficult to predict and control. Although additively manufactured steel was certainly more resistant to pitting, the phenomenon still happened eventually.

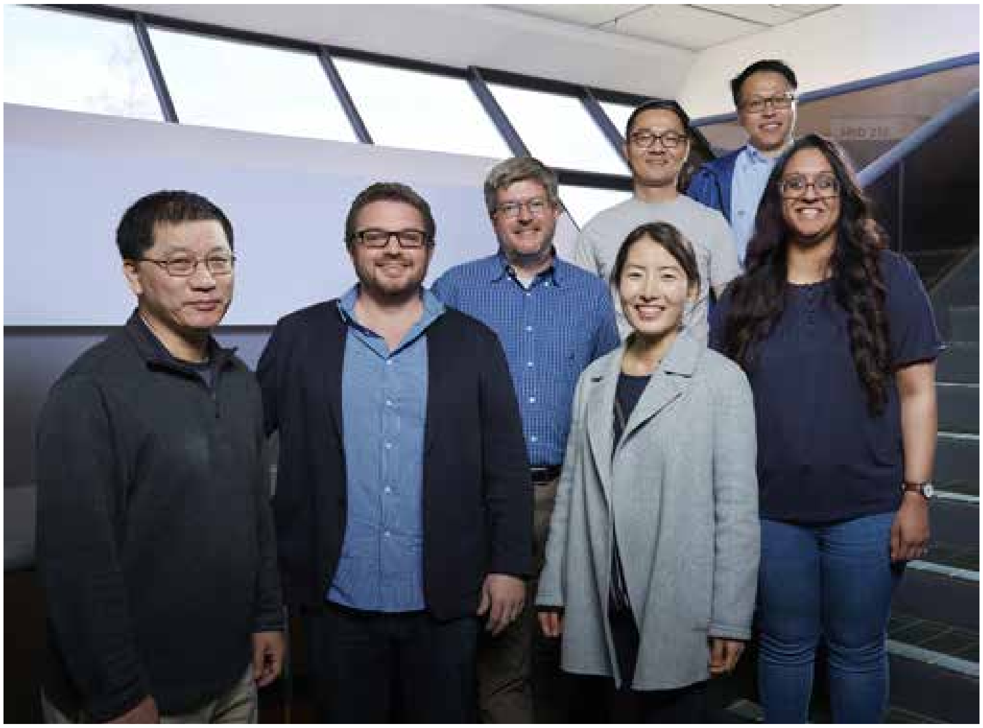
To study the corrosion effects in detail, a specialized high-speed atomic force microscopy (HS-AFM) was applied to scan the stainless steel's surface and form an image of the topographical in nanometer resolution. This technology was instrumental in helping the researchers visualize and track the evolution of corrosion's nucleation from its initialization. "The HS-AFM not only has the spatial resolution comparable to that of the conventional AFM, it also provides the temporal resolution needed for kinetics analysis. The unique combination allows us to identify the corrosion pitting site as well as the corrosion rate," says Qiu. Through the in-situ measurements, the correlation between corrosion and AM steel microstructure such as grain orientation, grain boundaries, cell wall, and cell interior can be revealed. For the ex-situ characterization, Voisin and his team conducted several TEM studies that investigated the additively manufactured steel surface structures down to the atomic scale. The chemical origin of the pitting in additively manufactured stainless steel was also identified through post-mortem characterization by TEM.

As with the other thrusts, experiments were only one part of the research, and computer simulations played a large role in helping to expand the picture of corrosion. Voisin says, "Not everything can be experimentally tested. Each experiment has its own limitations, leaving gaps where computer simulations became vital to better understanding corrosion. We used simulations to uncover the mechanisms behind some of our observations. An experiment and simulation integration approach was the only way to capture the full story about corrosion of additively manufactured stainless steel in seawater." Voisin and his team used computer models to simulate changes in atomic structure inside the stainless steel resulting from corrosion, in particular the manner in which the unique structures formed during additive manufacturing affect material behavior.

This integration of simulation and experiment has enabled the team to explain the nucleation of pits on the complex as-fabricated surfaces across several length scales, from macroscopic to atomic. Voisin says, "We were able to link processing to microstructures to corrosion mechanisms



Frames from in-situ dissolution measurement on an additively manufactured 316L stainless steel disc using high-speed atomic force microscopy. The scale bar is 2 micrometers (μm). Scan rate is 10 seconds (s) per frame. The dashed line indicates grain boundary. The cell wall and cell interior are highlighted with arrows. The colorful background represents the broader surface of stainless steel and different grain regions.



The stainless steel–additive manufacturing corrosion research team (from left to right): Roger Qiu, Thomas Voisin, Shin Young Kang, Brandon Wood, Shohini Sen-Britain, Yakun Zhu, and Yuliang Zhang.

to explain the additively manufactured stainless steel properties. In the future, we're aiming to develop a simulation that will tell us where corrosion will start, how fast it will degrade the surface of steel, and when we might expect a failure."

Opportunities for the Future

HPC has long been a pillar of Lawrence Livermore's research, leaving no surprise that developing multiscale model capabilities and integrating them with state-of-the-art experimental techniques has been a game changer for understanding the evolution and kinetics of corrosion. Wood says, "The message of integration was one we championed throughout this project. One was a scale integration—we did extensive work on the experimental and computational sides to understand what happens starting at the atomistic or nanoscale and moving up to the microstructure scale. Our hypothesis was that the experimental and computational sides were implicitly connected because corrosion is a chemical process that manifests in a macroscopic way." The birth of the HPC component of the research came from previous Livermore projects focused on the energy sector that looked at the effects of temperature on highly localized conditions, so many of the foundational elements behind the computer models for corrosion were already in place. By combining the experiments and computational models, the team has created the potential to unlock new opportunities for Livermore researchers and other stakeholders in materials science. "Now we can build a more reliable model to understand corrosion science," Pham says. "We're moving into an era where high-performance computing, machine learning, and computer simulations will play a very important role in explaining corrosion and its impacts, not only for the Stockpile Stewardship Program at Livermore, but also for wider industrial and commercial purposes."

The research team has already attracted the attention of other researchers and corporations. Livermore partnered with many academic institutions to conduct different components of the work, including Texas A&M University (aqueous corrosion thrust); SUNY Polytechnic Institute (metal hydride); George Tech University (TEM microscopy on additively manufactured thrust); Monash University in Australia (characterization of additively manufactured metals); Arizona State University (data science); University of Nebraska, Lincoln (electrochemical theory); and Ohio State University (simulation theory). Early in the project, Livermore began collaborating with Raytheon to understand the impacts of high temperature corrosion and oxidation, and the team has more recently been discussing opportunities with Boeing around modeling corrosion.

Livermore is also exploring research spin-off opportunities under federal government funding. The U.S. Department of Energy (DOE) has many areas of interest that overlap with the work that Wood and his team have done on corrosion, including hydrogen and fuel cells technology, as well as the DOE Advanced Materials and Manufacturing Technologies Office. As corrosion touches on so many levels of individual, household, commercial, industrial, and national security interests, Livermore's foundational corrosion research will undoubtedly expand to develop prediction and prevention solutions.

–Sheridan Hyland

Key Words: Additive manufacturing, aqueous corrosion, confocal microscopy, dissolution kinetics, galvanic corrosion, grain boundary, high-performance computing (HPC), high-speed atomic force microscopy (HS-AFM), hydriding, Laboratory Directed Research and Development Program, Laser Powder Bed Fusion (L-PBF), machine learning (ML), nuclear magnetic resonance (NMR), nucleation, pitting, stoichiometry, transmission electron microscopy (TEM).

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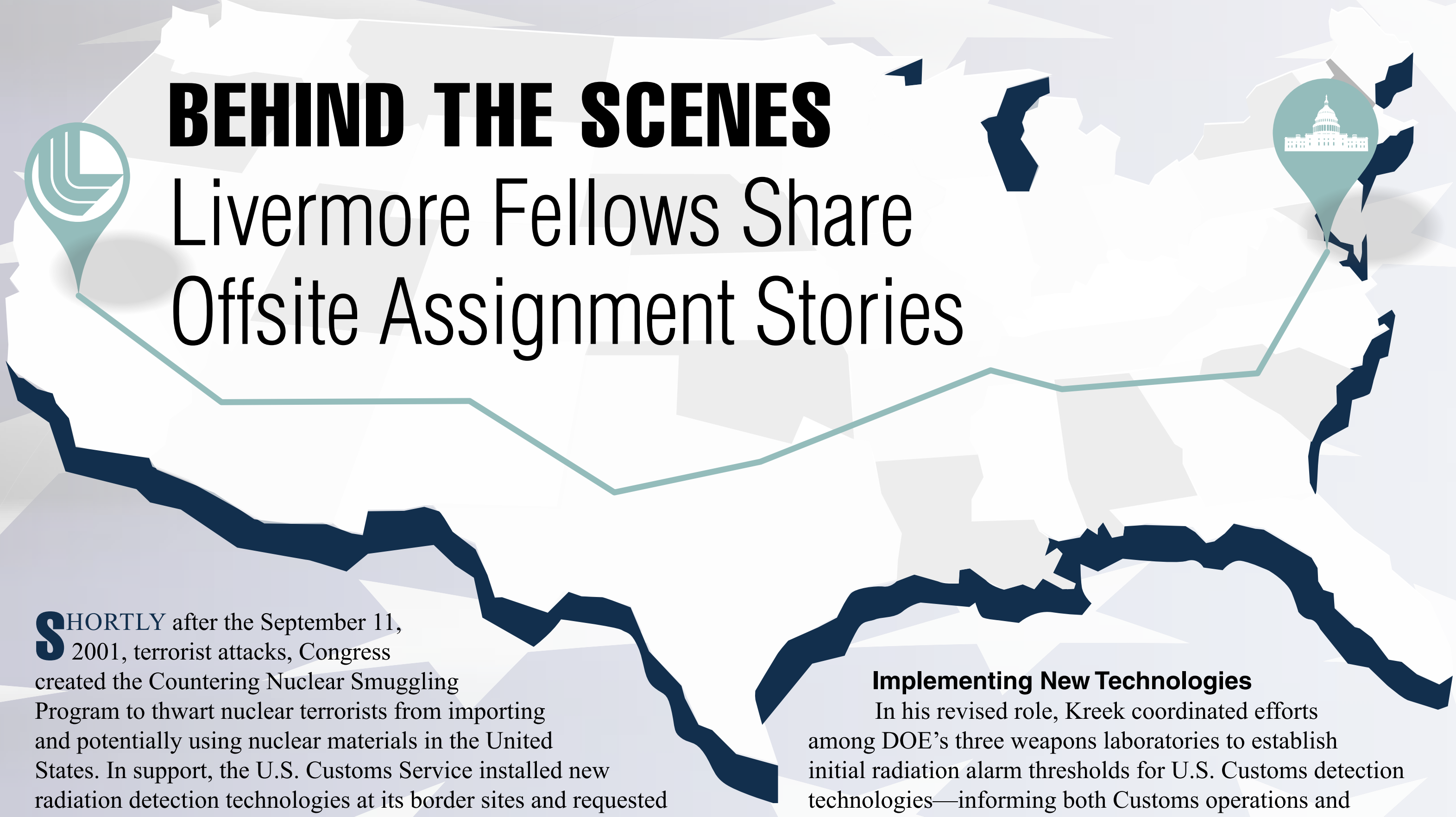

BEHIND THE SCENES

Livermore Fellows Share Offsite Assignment Stories

SHORTLY after the September 11, 2001, terrorist attacks, Congress created the Countering Nuclear Smuggling Program to thwart nuclear terrorists from importing and potentially using nuclear materials in the United States. In support, the U.S. Customs Service installed new radiation detection technologies at its border sites and requested Department of Energy (DOE) assistance in developing threat-based detection standards. With a background in radiation detection applications, Lawrence Livermore nuclear and radiochemistry expert Steven Kreek was well positioned to take on this task. In fact, Kreek had already been tapped for a temporary offsite assignment as a technical advisor for the National Nuclear Security Administration's (NNSA) Office of Defense Nuclear Nonproliferation (DNN) Research and Development (R&D)—known as NA-22.

Today, such assignments are part of the Laboratory's Offsite Fellows Program (OFP), offering Laboratory employees temporary roles with federal government agencies. (See *S&TR*, September 2019, pp. 12–15.) Offsite fellows learn to create and defend program efforts, engage with and advise federal program managers in Washington, D.C., and elsewhere, and gain a deeper understanding and appreciation for federal government operations from interagency, political, and budgetary perspectives.

While the general premise of an offsite assignment is similar for every fellow, unpredictable events can make for an unforgettable experience, which is exactly what happened to Kreek. He arrived in Washington, D.C., to begin his NA-22 assignment just before commercial aviation halted on the morning of September 11, 2001. The attacks shifted the focus of his original assignment, and ultimately his career at the Laboratory, from nuclear nonproliferation to domestic counterterrorism and homeland security.

Implementing New Technologies

In his revised role, Kreek coordinated efforts among DOE's three weapons laboratories to establish initial radiation alarm thresholds for U.S. Customs detection technologies—informing both Customs operations and new technology development within NA-22's Countering Nuclear Smuggling Program. Additionally, Kreek established an operational pilot program with the Port Authority of New York and New Jersey to better understand how radiation detection systems could be used and implemented across transportation vectors such as bridges, tunnels, and airports.

Following this work, DOE detailed Kreek to assist the newly established White House Office of Homeland Security in creating the Department of Homeland Security (DHS) and DHS's Science and Technology (S&T) Directorate. Once DHS was launched in early 2003, Kreek and the entire DOE/NNSA Nuclear Smuggling R&D Program were transferred to DHS S&T with Kreek named a Radiological and Nuclear Countermeasures R&D program manager. Kreek increased the program's emphasis on nuclear forensics research and developed essential partnerships between DHS, DOE, and the national laboratories.

At the end of his offsite assignment in 2004, Kreek returned to a leadership role within Lawrence Livermore's Counterterrorism and Incident Response Division. He says, "Once you have a behind-the-scenes view of operations in D.C., you can more easily set direction and strategy at the Laboratory."

In 2019, Kreek returned to Washington, D.C., for a second assignment, this time bringing his breadth of expertise to be a science advisor to NNSA's DNN Deputy Administrator. Among other projects, Kreek helped the Surplus Plutonium Disposition

Program speed up the disposal of 40 metric tons of excess plutonium by identifying areas of improvement and recommending existing technologies that could be converted to streamline the disposal process. His efforts are anticipated to shave years off the decades-long, multibillion-dollar program.

After this assignment ended in 2021, Kreek's Livermore career shifted once again. His returning role focused on operations and personnel, as he oversaw the Return to New Normal team responsible for launching the Laboratory's telecommuting program and communicating COVID-19 updates to employees. Today, Kreek is the Human Resources (HR) Deputy Associate Director, a position that draws on his diverse experiences and perspectives to shape, refine, and plan HR process improvements enabling staff to execute the Laboratory's mission.

Planning for the Future

A typical offsite assignment lasts around two years, but nuclear engineer Chris Ryan demonstrates that no two assignments are the same. Since 2017, Ryan has served in an extended assignment as a senior technical analyst with DOE's Office of Intelligence and Counterintelligence, supporting the nuclear terrorism and security branch. In this role, Ryan reviews papers on intelligence analysis, providing technical insights related to nuclear weapons, radiochemistry, nuclear forensics, and nuclear engineering; and coordinates these papers with other agencies and laboratories prior to publication. Ryan has also briefed the secretary of energy on pressing nuclear issues and written technical documents read by the highest levels of U.S. policy makers, including the president.

Prior to his offsite assignment, Ryan worked in the Laboratory's Nuclear and Radiochemistry Group, contributing to stockpile stewardship, post-detonation nuclear forensics, and intelligence analysis. "Working at the Laboratory has put me at a unique advantage," says Ryan. "Here, a researcher can experience so many different things under one roof. The breadth of knowledge I have to offer, thanks to my work at Livermore, has led to a long and prosperous offsite assignment."

Since 2021, Ryan has split his time between DOE and NNSA's Office of Nuclear Forensics. In fact, he helped DOE write a presidential memorandum on nuclear forensics and then later, in his second assignment as an NNSA science advisor, witnessed the document's implementation. "Seeing the results of my technical analysis play out in the real world and come full circle is surreal," says Ryan. "As someone who has worked in this field since graduate school, having a direct hand in revamping the government's approach to nuclear forensics and pushing forward the next generation of research and planning is an amazing feeling."

Not every assignment requires a scientific background; some require extensive knowledge in international relations and nuclear deterrence strategy. For example, the Department of Defense (DOD) depends on experts like Paige Gasser, with a strong background in nuclear deterrence, nonproliferation, and arms control, to inform the nation's military strategies. Gasser started her offsite assignment journey in February 2021 as a senior policy advisor within the DOD's Office of the Under Secretary of Defense for Policy. The greater part of her multiyear assignment was spent advising in the Joint Staff's Strategy, Plans, and Policy Directorate—better known as the J5. In the J5, she was responsible for advising the Chairman and Vice Chairman of the Joint Chiefs of Staff and other senior leaders on a range of nuclear deterrence policy and strategy issues, primarily concerning arms control, extended deterrence, and the North Atlantic Treaty Organization (NATO)—an international, intergovernmental political and military alliance.

In both roles, Gasser worked on key strategy documents, namely the National Defense Strategy, Nuclear Posture Review, and Countering Weapons of Mass Destruction Strategy. With the J5, Gasser supported the Chairman in preparing his best military analysis, options, and plans for the president and secretary of defense on matters related to U.S. nuclear force posture. Gasser explains, "Being an advisor means knowing your audience and their knowledge base, for example, how much background they need on the topic at hand to successfully make decisions and strategically address some of the most pressing deterrence issues."

Throughout her assignment, Gasser played a major role in addressing the nuclear dimensions and implications of the Russia–Ukraine war and Russia's noncompliance with the New Strategic Arms Reduction Treaty, the last standing nuclear arms reduction treaty between the United States and the Russian Federation. "This assignment has strengthened my understanding of the broader nuclear security enterprise beyond Livermore," says Gasser. "Being so closely involved in addressing some of the emerging and ongoing security challenges we face is a vivid reminder of why our national laboratories exist, especially as future leaders try to navigate this complex era of strategic competition."

Bridging the Gap

Shock physicist Dayne Fratanduono started an 18-month assignment in 2018 for NNSA's Office of Experimental Sciences, providing technical expertise in high-energy density physics and materials science to federal program managers within the Dynamic Material Properties (DMP) program. Fratanduono explains, "Federal program managers who run research portfolios oversee technical decisions but may not have a background in a specific scientific field. In my role as a fellow, I served as an advisor on topics related to my area of expertise."

Fratanduono helped stand up a new capability at Argonne National Laboratory's Advanced Photon Source (APS) in support of nuclear weapons research. Classified research had not been permitted at the facility, but Fratanduono ushered in classified experiments at APS, ultimately putting the DMP program on a better trajectory to utilize existing advanced light sources throughout the world.

Fratanduono says, "I spent a lot of time explaining and justifying to the federal government why enabling this capability would be of value and how it would advance the stockpile. To succeed, I conveyed messages that were simple, factually correct, and easy for the program managers to explain to their counterparts and up the chain of command." Upon returning to Livermore, Fratanduono was named the co-program working leader for Condensed Matter Physics (CMP) within the Weapon Physics and Design Program, applying his offsite experiences to help the CMP Program meet NNSA's needs.

While in Washington, D.C., Fratanduono crossed paths with Livermore experimental and nuclear physicist Dennis McNabb, serving in an offsite assignment for NNSA's Office of Defense Programs. Together Fratanduono and McNabb worked with members of Livermore's senior management team to educate federal stakeholders about the importance of the National Ignition Facility to the nuclear deterrent. McNabb focused on recommendations to improve the nuclear stockpile, speed up the modernization process, address production issues, and transform the enterprise to be more efficient and effective.

Additionally, McNabb served on the science council with other advisors, interfacing between the NNSA and JASON—an esteemed group of academics that provide national security advice to the government—putting together research requests for JASON to conduct on behalf of the NNSA and helping to facilitate those studies. "I had the opportunity to work with three other advisors, all from different DOE facilities. We truly bonded on the science council," he says. McNabb and his fellow council members also reviewed requests from the Committee on Foreign Investment in the United States, which handles export control, to ensure there were no potential national security issues.

"My time on assignment," says McNabb, "was a total change of pace from the normal day-to-day at Livermore. In D.C., my job was to explain the 'why' behind the science, to serve as a conduit between the federal government and the national laboratories rather than conduct hands-on, technical research." Upon returning to Livermore, McNabb was selected as Global Security's (GS) Deputy Principal Associate Director for Strategy and Programs. He remains a vital information conduit, working with external sponsors at the DOE and NNSA to ensure their priorities are reflected in the Laboratory's GS strategy.

Supporting Transformational Science

In October 2020, Heather Whitley entered a remote six-month assignment with NNSA's Office of Experimental Sciences (OES NA-113), within the Office of Research, Development, Test, and Evaluation (NA-11). OES NA-113 works closely with the national laboratories to deliver world-class experimental data, facilities, and expertise to support the needs of the Stockpile Stewardship Program. While on assignment, Whitley supported federal program managers in these endeavors by providing technical and advisory assistance on matters involving stockpile stewardship and applications of laboratory experiments and advanced simulations to problems of interest.

Along with NA-113, there are two additional offices under NA-11—the Office of Advanced Simulation and Computing and Institutional R&D Programs (NA-114) and the Office of Engineering, Stockpile Assessments, and Responsiveness (NA-115).


Steven Kreek


Chris Ryan


Paige Gasser

A major deliverable Whitley worked on was bridging these three offices in their strategic plan for artificial intelligence and machine learning (AIML). The efforts resulted in a draft AIML proposal geared toward exploring the use cases of AI and ML for improving information and data management processes, developing more efficient experimental designs, and building knowledge management tools to support knowledge transfer across the enterprise.

In a second deliverable, Whitley provided technical input to support the annual NNSA budget proposal. For this effort, Whitley helped break down technical details and summarize their importance to the program. In return, she gained a bird's eye view of the budget process. Upon completing her assignment, Whitley stepped into a new position with Livermore's Weapons and Complex Integration organization as Associate Program Director (APD) for High Energy Density Science. Whitley says, "Management is all about creating pathways and clearing obstacles to enable research, and my time on assignment taught me how to do this effectively in my role as APD."

Each offsite assignment story is different, yet all highlight the extreme value of the program to federal stakeholders and to scientists seeking career-broadening experiences. The experiences that fellows bring back to Livermore reflect how their offsite assignments have fundamentally altered their mindset and career, allowing them to become effective advocates for the sciences and embrace the meaning of nuclear stockpile stewardship. Fratanduono says, "A fellow on assignment is not advocating for Livermore or the other laboratories, but rather trying to do the right science for the enterprise and learning how science and policy come together."

Over the years, the number of Lawrence Livermore employees filling offsite assignment roles has increased tremendously. To better align the shared missions and priorities of the OFP, the Laboratory, and the federal government, the OFP board has conducted a strategic review of all assignments. As a result, the program has begun grouping assignments into one of three groups—those supporting relationships with current sponsors and partners, those developing new relationships with potential sponsors and partners, and one-off assignments that support an immediate and specific need at the request of a federal agency. The first two groups will be long-term assignments, filled on a rotating basis, while the final group will enable fellows to engage in unique assignments and are not intended to be backfilled after the original assignment is completed. This new strategy aims to equip Livermore employees with a diverse set of external opportunities, while ensuring the program is maximizing its resources.

–Shelby Conn

Key Words: Advanced Photon Source (APS); advisors; Committee on Foreign Investment in the United States; Countering Nuclear Smuggling Program; counterterrorism; Department of Defense (DOD); Department of Energy (DOE); Department of Homeland Security (DHS); Dynamic Material Properties (DMP); JASON; Joint Staff's Strategy, Plans, and Policy Directorate (J5); National Nuclear Security Administration (NNSA); North Atlantic Treaty Organization (NATO); nuclear forensics; Nuclear Posture Review; nuclear stockpile; Office of Defense Nuclear Nonproliferation (DNN); Office of Defense Programs; Office of Intelligence and Counterintelligence; Office of Nuclear Forensics; offsite assignment; Offsite Fellows Program (OFP); U.S. Customs Service; Washington, D.C.; White House.

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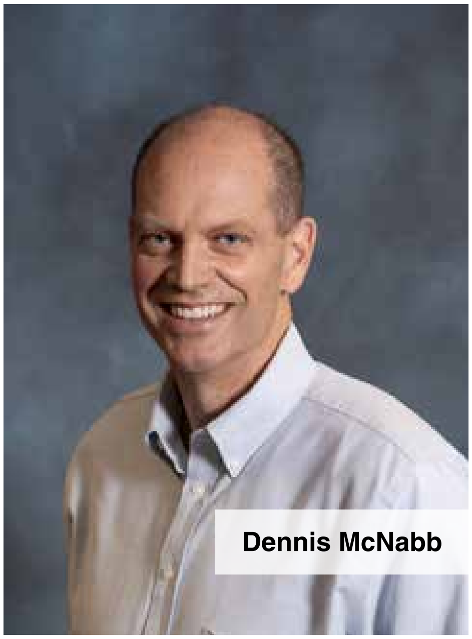


Expediting Research with SPACK

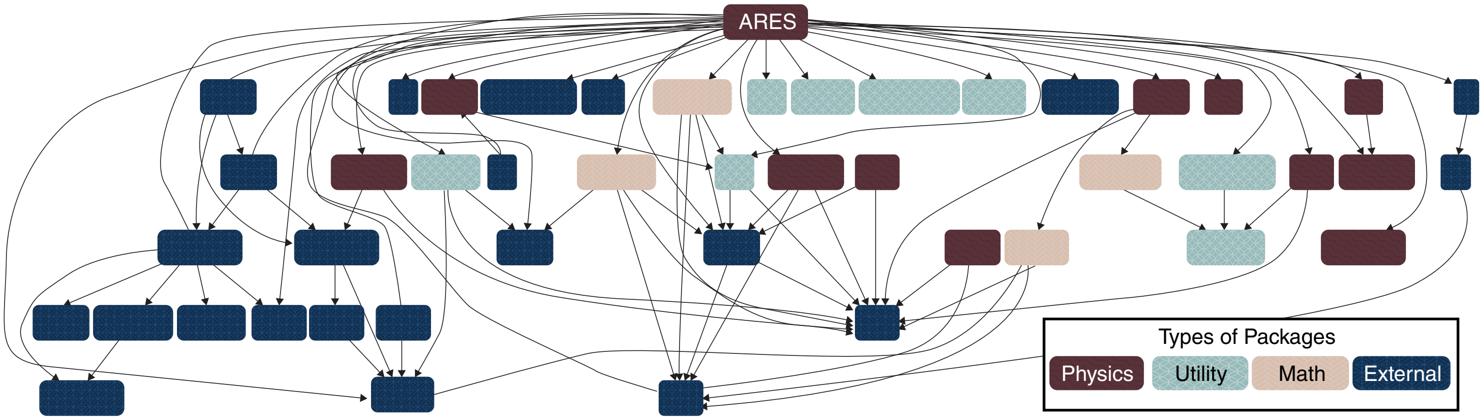
IN early 2013, Todd Gamblin was a staff scientist at Livermore mentoring graduate students as they struggled to build and integrate software on high-performance computing (HPC) systems. Seeing days and weeks of valuable research time lost to getting computing programs off the ground, Gamblin thought to automate the task of building and installing the disparate software elements HPC users required.

The solution, Spack (for Supercomputing PACKage manager), would go on to expedite operations across a community including top supercomputing centers, cloud providers, and individual users worldwide. "Fundamentally, Spack ensures all the software used by an HPC system is built in a compatible and efficient way," says Gamblin, now a distinguished member of technical staff in the Livermore Computing Division.

Laying Computing Foundations

Building software—that is, turning software code into usable applications—is a notoriously difficult computing challenge in its own right. Scientific programs used by HPC centers rely on a constellation of interdependent software packages that only function if software versions, languages, feature options, and other configuration options are properly coordinated.

"HPC users had done these tasks manually for many years," says Gamblin. "While package managers existed for other domains, the fine-tuning needed for HPC systems led most users to build software by hand. The software build process is painstaking and error prone even for experts." Since laying its foundation a decade ago, Gamblin's automated approach to building software has graduated from personal to global use. Recognizing potential to support stockpile stewardship, the Laboratory designated funding from its Advanced Simulation and Computing (ASC) Program to continue Spack's development. In 2019, the project received an R&D 100 Award (see *S&TR,* July



Spack automates the process to download, install, and manage scientific software packages. The application resolves package dependencies and user preferences to ensure operability of software stacks in ways not possible with manual integration. For example, Spack automates the build and deployment of the 46 dependency libraries (represented by interconnected boxes) that comprise ARES, a hydrodynamic simulation code used for fusion experiments at the National Ignition Facility.

2020, pp. 10–11), fueling even wider recognition and adoption within the HPC field.

Spack's automated approach to building, testing, and deploying software has reduced project software distribution times from several weeks to hours or even minutes, depending on the size of the stack. As preeminent computing systems (such as early access systems for Livermore's upcoming El Capitan exascale machine) come online, Spack ensures that users continents apart who employ different software, write in different programming languages, and execute asynchronous tasks can leverage each other's collective work to use HPC resources.

"Most people want to use a particular tool but don't care about its specific version or build options. However, getting the version right is crucial; a single incompatibility between packages could cause a project to fail to build," says Gamblin. With Spack, users can now create multiple versions of code and ensure compatibility before final deployment, averting experimental delays by preemptively resolving any inconsistencies. For example, Spack supports Livermore's proprietary radiation hydrodynamics codes, ARES and HYDRA, which aid inertial confinement fusion experiments at the National Ignition Facility (NIF) by incorporating dozens of software packages for modeling lasers, electromagnetic fields, and plasma physics. Purpose-built to model these experiments, HYDRA was used to design the December 5, 2022, NIF shot that achieved fusion ignition.

An Open Approach

An open-source project from inception, Spack is freely available on GitHub and actively seeks contributions. "The Spack community works to ensure that packages are integrated and kept up to date. When other organizations want to contribute updates to recipes, we welcome that. We benefit from the updates, and they benefit from having the needed changes integrated into Spack in a sustainable way so that future updates continue to include their revisions," says Gamblin. Other HPC sites benefit as well. For instance, deployment time for an extensive 1,300-package software stack on Oak Ridge National Laboratory's (ORNL's) Summit supercomputer was slashed from two weeks to 12 hours. The same stack has been ported and built on ORNL's Frontier system, the world's first exascale machine.

By enabling and expediting scientific research, Spack has cemented itself as an invaluable tool for the Exascale Computing Project (ECP) within the Department of Energy (DOE). ECP provides the next-generation computing software stack necessary to tackle challenges of national importance—including clean energy generation, stockpile stewardship, and materials discovery—to which Lawrence Livermore contributes significant computing resources.

What began as a library of roughly 100 software packages has grown into a trove of more than 7,000, contributed by researchers from other DOE laboratories, academic research institutions, industry, and international collaborators. The roughly 100,000 lines of code that comprise Spack's "core" are maintained by Lawrence Livermore and trusted members of the Spack community. Most of the remaining 250,000 lines originate from outside Livermore and form an expanding package repository for assembling software. Today, the community boasts more than 1,200 contributors and many thousands of users.

Rapid growth demands resources and external collaboration. While a handful of dedicated developers at the Laboratory manage core feature development and community contributions, extended core teams at subcontractors Kitware and TechX conduct build farm maintenance, Windows support, and continuous integration automation. Among GitHub contributors, roughly 40 users are trusted package maintainers authorized to merge pull requests; a broader set of more than 300 users helps to review submitted package recipes.

Software developer Greg Becker maintains Spack's functionality and supports its user base. In response to the tool's surge in growth, Becker and his colleagues spend significant time assessing code contributions and managing bug fixes to maintain consistency within Spack's repository. "Keeping up with all that growth is a challenge," Becker says, "but the great thing about open source is that anyone can jump in and help on a part of the project they care about." Despite the demands, Becker says, "Without all the work from the community, Spack wouldn't be nearly as capable as it is. The community is a huge force multiplier."

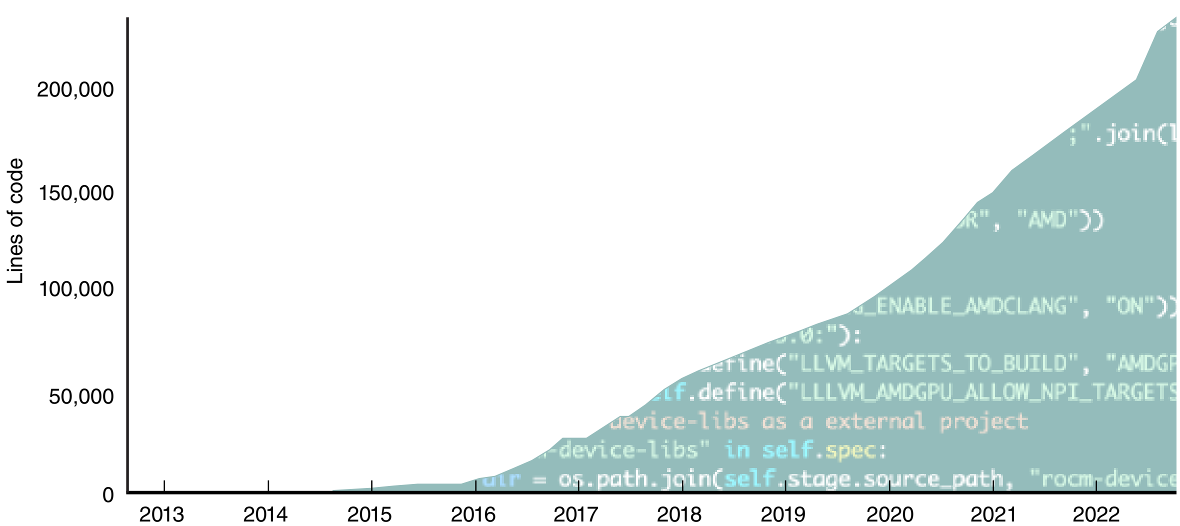
Spack's collaborative roots have spurred numerous partnerships. Amazon Web Services (AWS) invests significantly by providing cloud computing credits for Spack's community, enabling automated build testing and publication of a large cache of pre-built software. AWS has also hosted Spack-centered tutorials and hackathons with Livermore team members. Semiconductor developer AMD has contributed to ROCm™ software packages and the compiler that translates source code into machine code from high-level programming languages into computer-legible form. Intel helps to maintain and support packages for its oneAPI programming model. NVIDIA supports its NVHPC compiler recipes. HPE Cray performs continuous integration for Spack packages in its own supercomputing environment. Other open-source frameworks for software benchmarking and testing have emerged. For example, Ramble, written by Google Cloud staff, uses Spack to build benchmark programs, but adds a harness for running experimental performance campaigns. And in Japan, Spack was chosen as the deployment tool for the world's second-fastest supercomputer, Fugaku, manufactured by Fujitsu and Riken.

Current and Future Challenges

At the 2022 International Supercomputing Conference, the Spack team announced the latest release, v0.19.0, with a redesigned "concretizer," the component that resolves dependencies, versions, and other preferences for a software build. "Getting all the software packages to agree with one another is an NP-hard combinatorial problem," says Gamblin. NP-hard problems are the equivalent of searching for a needle in a haystack; an optimal solution must be located among millions of possible software configurations. The best known algorithms amount to guessing-and-checking solutions in the worst case, but they leverage sophisticated search techniques such as Conflict-Driven Clause Learning and multi-objective optimization to zero in quickly on good solutions. Nearly all package managers must contend with dependency resolution. "Like a game of Sudoku," says Gamblin, "Spack uses sophisticated criteria to make an educated guess, identify possible compatibility conflicts, and backtrack to quickly find a valid solution."

Resolving installation parameters is only the beginning. Computing's Tammy Dahlgren, a core Spack team member, puts the issue simply: "Just because you can build it, that doesn't mean it will run correctly." Dahlgren supports the ECP-funded Extreme-Scale Scientific Software Stack (E4S), which uses Spack to facilitate deployment of around 600 HPC software packages directly from source. "Once a package has been installed, E4S ensures the software remains functional while

Cumulative code contributions to Spack



Spack's open-source nature enables contributors worldwide—including Department of Energy national laboratories, industry, and academic institutions—to utilize Spack's resources and offer functional additions, accelerating support of new use cases. Contributions to Spack's GitHub repository over time (excluding those to the core) have dramatically increased in recent years.

Development team for Spack: (from left) Greg Lee, Matt Legendre, Todd Gamblin, Peter Scheibel, Greg Becker, and Tammy Dahlgren. (Photo by James Chalabi.)

underlying systems and package dependencies are constantly updated," she says.

Spack not only optimizes software build configuration, but also tests to ensure builds will operate as intended within a larger system before executing the immense task of deploying HPC programs. Utilizing "test recipes" included with software packages, Spack can assess package functionality in different configurations. Test recipes themselves can be customized to different versions and configurations. "That way, tests evolve with the software and adapt to the installation," says Dahlgren.

Although Spack has already expedited projects on several supercomputing systems, accommodating the complexity of Lawrence Livermore's El Capitan system—slated to be the world's most powerful supercomputer—is no easy feat. "The software stack for advanced supercomputers keeps getting more complicated, and some of the complexities of El Capitan will push the boundaries of what we can model with Spack," says Becker. The combination of compilers and other low-level tools necessary to meet heightened demands will require Spack to maintain consistency across distributed computing resources. To address the challenge, Becker says Spack's software package models continue to mature.

As an adaptable open-source tool, Spack is also well suited to bridging the gap between HPC and cloud-based workflows, the latter used to expand, diversify, and distribute computing loads. However, Becker explains, "HPC workflows are designed with static resources in mind: something is built once and meant to run for years. Cloud architectures instead focus on more ephemeral resources." Shorter lived systems can lean on Spack's ability to install quickly from binary caches rather than building from source. "Ultimately, we want an arrangement that rapidly gets us from a blank slate to doing science," says Becker. The team is currently working with scientists who use cloud resources for HPC to help them take advantage of the flexibility of cloud computing without forfeiting valuable research time to previously solved software installation problems.

"Spack's open approach to development is critical to its longevity," says Gamblin. "Large community efforts generate momentum, making the project easier to sustain in the long run." Dahlgren echoes Gamblin's view: "Spack is my first open-source software project, and I'm glad I joined. Interacting with talented people both at the Laboratory and across the world has been incredibly fulfilling."

–Elliot Jaffe

Key Words: Advanced Simulation and Computing (ASC) Program, concretizer, El Capitan, Exascale Computing Project (ECP), Extreme-Scale Scientific Software Stack (E4S), GitHub, high-performance computing (HPC), open-source, software package manager, Spack, supercomputing.

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LivIT Customer Service Center staff members (left to right): Ma'Lia Leines and Amanda Silveira.

LivIT Self-service Pickup staff member Glenn Mahan.

LivIT Computer Build Center staff member Brad Rodrigues.

LivIT Meets the DEMAND

THE children's book *If You Give a Mouse a Cookie* simplifies the universal truth that one need opens the door to another need and so on, in a cascading fashion. Similarly at Lawrence Livermore, the best and brightest researchers require access to the most capable and cutting-edge information technology (IT) resources. Access to such high-level resources requires an elite IT team such as the Livermore Information Technology (LivIT) group to keep the Laboratory's crucial computing infrastructure operating smoothly.

Led by the guiding principles of simplicity, agility, and capability, LivIT regularly improves operations to better equip and empower users. The group partners with users in divisions and directorates across the Laboratory, learning from them and anticipating their needs to help accomplish the Laboratory's goals.

Five-Program Structure

To optimize scope and maximize competencies, LivIT deploys 450 staff across five programs. Business Enablement (BE) oversees 250 customized applications such as the timekeeping and training platforms TIME, LAPIS, and LTRAIN, familiar to all Laboratory employees. The Workforce Enablement (WE) group supports end users by keeping Webex, video teleconferencing support, email, and other collaboration tools up and running. The Customer Service Operations Support (CSOS) team performs myriad support functions for many of LivIT's customer-facing services such as the Service Desk, desktop and infrastructure support, cyber security support, mobility, and communications. The Cyber Security Program (CSP) provides vital defense for network, desktops, infrastructure, and intellectual property. The Systems and Network Technology (SNT) program oversees the Laboratory's data center, networking, hardware, and Webex and video teleconferencing infrastructure.

The five-program structure maximizes LivIT's ability to respond to changing needs. As Matthew Myrick, Chief Information Security Officer, explains, "While LivIT is a service organization, some people aren't aware that we offer many amazing services beyond our Service Desk. LivIT often operates transparently to better modernize, transform, and protect all aspects of the Laboratory's IT ecosystem, which permeates virtually every mission area and task performed here." The five programs have their own unique responsibilities yet operate in concert. Principal Deputy Chief Information Officer Mark Pettit adds, "All LivIT program areas work collaboratively to deliver services—not unlike the way organs of the human body provide specialized functions so the body can operate effectively as a whole."

Pandemic Demand Management

LivIT's overall function relies on demand management: as the demand for Laboratory capabilities increases, so does the need for IT resources to help empower mission-driven work. The Laboratory's range of teams, programs, and directorates requires automation and efficiency in business processes, strategic mission and business enablement solutions, enhanced communications and collaboration, and data availability. Sue Marlais, Livermore's Chief Information Officer, says, "Users rely on IT more and more to do their jobs with very little tolerance for down time. We invariably have a significant amount of new scope to incorporate as we continue to manage with ongoing operational IT."

When an elite IT team must function throughout a pandemic, demand management takes on new dimensions. Kristin Ruley, CSOS Program Leader, sums up the earliest technical hurdle of the pandemic: "Our biggest challenge was ensuring that the transition from onsite work to offsite work felt seamless for Laboratory employees. We had to be certain that people could access their systems and tools remotely and effectively carry on with work virtually, something the Laboratory population hadn't been that familiar with. Because LivIT has an eye on the future, we already had many of the necessary tools and processes in place to do just that, in a matter of days."

Not all pandemic-related challenges to LivIT's infrastructure were simple to solve. Teams rapidly scaled up remote access capability to provide additional capacity while mitigating the risks from being unable to access crucial data. Once LivIT personnel understood that most in-person work would cease, they had to quickly evaluate and implement new digital collaboration capabilities such as Webex and MS Teams while expanding capabilities within OneDrive and the Office 365 space. To ensure successful continuity of support operations, the LivIT Service Desk, which handles an average of 6,000 contacts each month, transitioned to fully remote work a week ahead of the rest of the Laboratory.

"If luck occurs when preparation meets opportunity then, in many ways, the Laboratory got lucky," says Myrick. "We

Amazon Web Services facilitated Laboratory employees' use of hands-on machine-learning tools and a cloud-based 3D racing simulator during the Fall 2022 "hackathon."

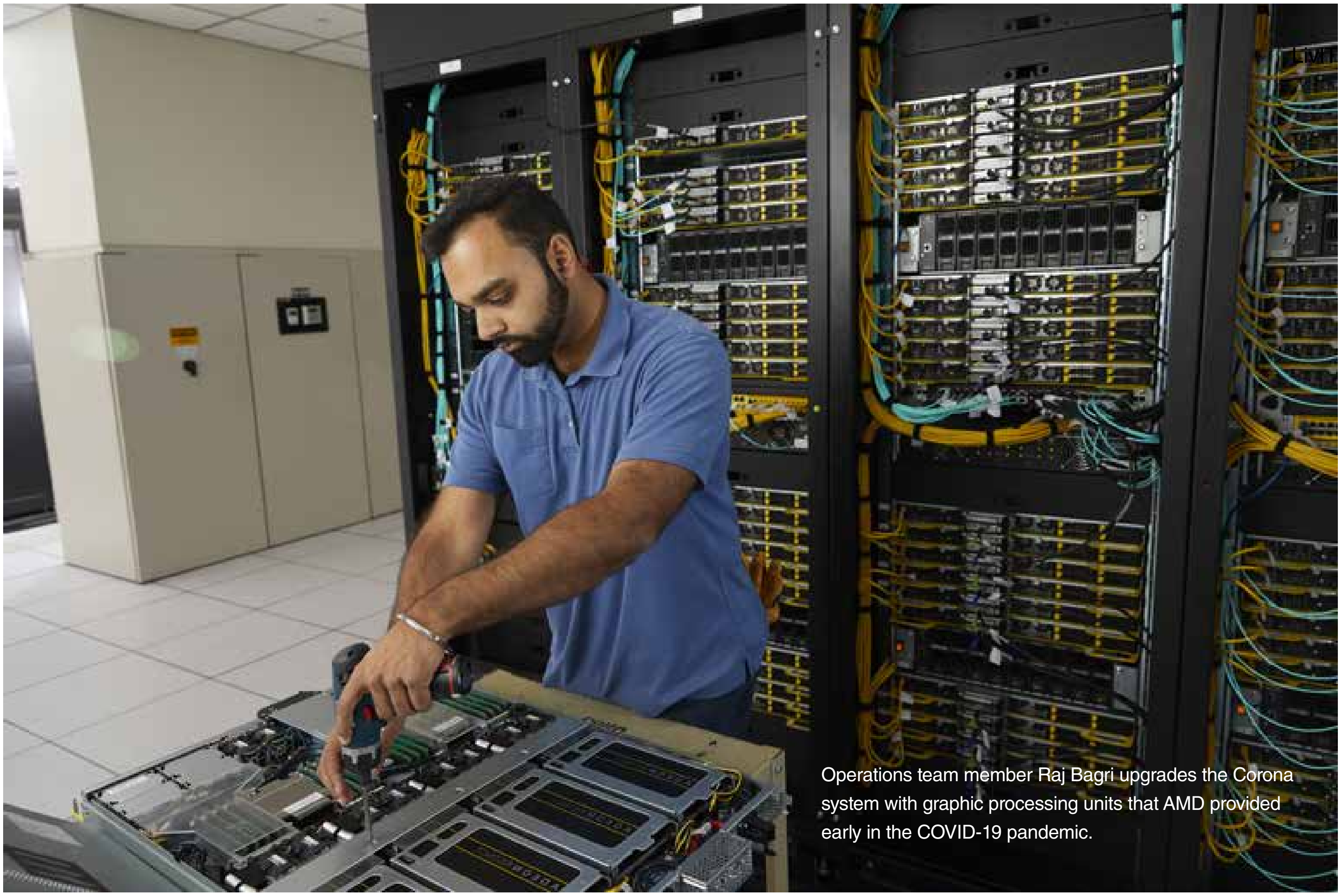
had already been piloting a new virtual private network (VPN) system, which could easily be operationalized to help sustain the load of the entire Laboratory population. We had recently deployed a best in class, cloud-based Endpoint Detection and Response software on all Lawrence Livermore systems, which allowed us to extend system protection whether onsite or offsite."

While Livermore employees focused on the technology they "touch" every day—softphones, laptops, peripherals being mailed home in the early days of the pandemic—many crucial IT issues were tackled behind the scenes. Content classification and approved usage of collaboration tools, including cyber security risk mitigation, was a major concern. LivIT also reduced VPN access requirements, provisioning accounts for all Laboratory employees and bypassing thousands of hours of administration and approvals.

Hybrid Workforce

New requirements led LivIT to develop or modify applications to provide, for example, onsite employee tracking and contact tracing, vaccine card validation, and development of a workspace methodology to support a first-ever virtual summer student intern program. Navigating onsite–offsite collaboration issues was trickier for classified work. The Weapons and Complex Integration organization sponsored LivIT to architect and implement a classified Webex-like meeting capability—Meet@LLNL—enabling the safe, effective continuation of classified program mission work. Given pandemic travel restrictions, the Meet@LLNL platform provided for appropriate social distancing and ongoing collaboration.

Once technological guardrails were put in place, IT business processes were adapted to support an increasingly hybrid workforce, from enhancements to distance support methodologies and practices, to equipment deployment and delivery. Pettit notes, "The pandemic and the hybrid nature of our workforce has created a sense of urgency to access all things digitally, all the time, from any platform, anywhere. Remote access is now a necessity and one that drives much of the work we do. We demonstrated our ability to adapt and become agile in responding to emerging needs in a rapid and meaningful manner." Pettit also notes that as IT professionals, the LivIT staff may have been able to transition to hybrid work more rapidly than most. "The tools and capabilities are more familiar, since we use them to support and interact with Laboratory employees every day," he says. "If anything, a hybrid workplace has dramatically accelerated the pace of the work that we do as well as the speed with which we do it." Ruley agrees, "Because we leverage modern technology and capabilities, LivIT as an organization can perform a lot of its work remotely, therefore enabling our staff a greater work–life balance through a healthy telecommuting posture."


Operations team member Raj Bagri upgrades the Corona system with graphic processing units that AMD provided early in the COVID-19 pandemic.

When it comes to lessons learned and best practices, the LivIT team has no shortage of examples. Marlais is especially proud of LivIT's mastery of improved collaboration tools. "Live events, like the Director's All-Hands meetings, are comparable to producing a TV show with many moving parts. LivIT has done an exceptional job delivering this type of service."

Another major pandemic-era achievement was the launch of the LivCloud, enabling Laboratory employees to conduct scientific research and IT development work in the cloud. More than 90% of LivIT's computing infrastructure migrated to cloud platforms such as Amazon Web Services (AWS), with the production environment moved in a single weekend. "Cloud migration significantly reduced LivIT's onsite computer infrastructure and increased our resiliency by leveraging highly redundant and more capable cloud resources," says Myrick. Pettit adds, "Cloud migration was the very first step toward a capability maturity that will enable us to become more agile and adaptive to the emerging needs of our program customers. The goal is to deliver solutions and capabilities quickly while also being able to adapt as needs change."

The team also leveraged AWS's machine-learning tools to validate COVID-19 vaccination cards for Laboratory staff. Using an image recognition tool, a model was created to discern vaccination card images submitted by employees. If the image was recognized to be a valid vaccination card, then an optical character recognition tool extracted the employee's information from the image. "With these tools the team was able to quickly validate and process the information," says John Lee, LivCloud technical lead.

In looking ahead to meet the Laboratory's increasing need for new solutions and capabilities, the LivIT team will retain a focus on demand management while maximizing agility. Pettit says, "One of our primary goals is to deliver innovative solutions that enable our customers to realize or exceed their mission goals beyond what they had even imagined. This requires a significant investment in LivIT as a key mission enabler. We can bring so much more to the table."

–Stephanie Turza

Key Words: cloud migration, cyber security, demand management, LivCloud, Livermore Information Technology (LivIT), remote work, Service Desk, virtual private network (VPN).

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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 (uspto.gov).

Patents

System and Method for Forming Material Substrate Printer
James A. Demuth, Andrew J. Bayramian, Bassem S. El-Dasher, Kevin J. Kramer
U.S. Patent 11,446,741 B2
September 20, 2022

Non-Destructive, In-Situ Evaluation of Water Presence Using Thermal Contrast and Cooled Detector
Mihail Bora
U.S. Patent 11,448,555 B2
September 20, 2022

Shape Memory Polymers
Thomas S. Wilson, Jane P. Bearinger
U.S. Patent 11,453,740 B2
September 27, 2022

Surface Modification of Polymer Foams Using Plasma
Landon D. Nash, Duncan J. Maitland, Nicole Docherty, Thomas S. Wilson, Ward Small, IV, Jason Ortega, Pooja Singhal
U.S. Patent 11,459,439 B2
October 4, 2022

Wavelength Selective Transfer of Optical Energy
Graham S. Allen, Diana C. Chen, Matthew J. Cook, Robert P. Crist, Derrek R. Drackenberg, Jay W. Dawson, Victor V. Kitrov, Leily Kiani, Michael J. Messerly, Paul H. Pax, Nick Schenkel
U.S. Patent 11,460,639 B2
October 4, 2022

All Solid Hybrid Arrow Fiber
Paul H. Pax, Diana C. Chen, Michael J. Messerly
U.S. Patent 11,462,878 B2
October 4, 2022

Methods for Cytotoxic Chemotherapy-Based Predictive Assays
Paul Henderson, George D. Cimino, Chong-Xian Pan, Ralph William de Vere White, Maike Zimmermann, Kenneth W. Turteltaub
U.S. Patent 11,474,106 B2
October 18, 2022

Antigenic Combinations against Francisella Bacteria and Related Nanolipoprotein Particles, Compositions, Methods and Systems
Nicholas Fischer, Amy Rasley, Terry Wu, Julie Lovchik
U.S. Patent 11,491,215 B2
November 8, 2022

Mitigation of the Harmful Effects of Stray-Light Reflections in High-Energy Laser Systems
Lynn G. Seppala, Alvin C. Erlandson
U.S. Patent 11,493,756 B2
November 8, 2022

Localization Based on Time-Reversed Event Sounds
Jim Candy, Karl A. Fisher, Christopher Roland Candy
U.S. Patent 11,495,243 B2
November 8, 2022

Synchronized Electric Meter Having an Atomic Clock
Liang Min, Can Huang
U. S. Patent 11,496,143 B2
November 8, 2022

Awards

Two Livermore-led teams received **SciVis Test of Time awards,** recognizing articles that continue to impact scientific visualization. The first paper describes a framework for computing structures that extract and visualize data. Livermore co-authors included **Attila Gyulassy**, then in the Student Graduate Research Fellowship program, computer scientist **Peer-Timo Bremer**, and former computer scientist **Valerio Pascucci**.

The second paper, by **Mark Miller** and former Livermore scientist **Mark Duchaineau**, describes a terrain visualization method enabling accurate images of large data sets at high frame rates with less computational work.

Livermore developers of the Suite of Nonlinear and Differential/Algebraic Equation Solvers (SUNDIALS), an open-source software library that solves mathematical equations critical to modeling and simulating physical phenomena, received the 2023 **Society for Industrial and Applied Mathematics (SIAM)** and **Association for Computing Machinery (ACM) Prize** in **Computational Science and Engineering.** The SUNDIALS team includes **Carol Woodward, Cody Balos, David Gardner, Peter Brown,** guest scholar and retiree **Alan Hindmarsh**, and former Laboratory staff **Daniel Reynolds** and **Radu Serban**.

Optica selected two Lawrence Livermore scientists as fellows, based on their distinguished contributions to the optics and photonics community. **Félicie Albert** was named for pioneering research on x-ray sources driven by laser-Wakefield acceleration and for leadership in the LaserNetUS initiative. **Craig Siders** was selected for contributions to research, application, and development of high-intensity lasers in both basic and applied sciences.

Japan's prime minister awarded **Brad Roberts,** director of the Laboratory's Center for Global Security Research, the **Order of the Rising Sun** for strengthening U.S.–Japan cooperation on extended nuclear deterrence and in mentoring the emerging generation of officials and scholars. The award, one of the highest honors bestowed by the Government of Japan, is rarely awarded to non-Japanese citizens.

Abstract

Stopping Corrosion Before It Starts

Researchers at Lawrence Livermore National Laboratory have developed a new capability for predicting the early onset of galvanic corrosion and hydriding of metals by integrating multiscale simulations, advanced characterization, and data science. Their findings address key shortcomings in empirical corrosion models to create a comprehensive, physics-based model of corrosion initiation in support of stockpile stewardship as well as national infrastructure and manufacturing interests. The research effort, funded by the Laboratory Directed Research and Development Program and conducted as a Strategic Initiative project, has also demonstrated successes in the areas of workforce development, partnership building, and the potential for follow-on scientific discoveries that further contribute to the Laboratory's mission.

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U.S. Government Printing Office: 2023/ 770-075-20029

Coming Next Issue

Double Asteroid Redirection Test (DART)

Lawrence Livermore contributed multiphysics simulations supporting NASA's successful experiment to divert an asteroid.

Also in an upcoming issue…

- *Livermore's capabilities in flight dynamics simulations define the effects of warhead design prior to flight testing.*
- *Sidney Fernbach Postdoctoral Fellows contribute computational science research and attract new talent for the future.*
- *Laboratory additive manufacturing expertise yields a training resource for bomb-sniffing dogs.*

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