Lawrence Livermore National Laboratory

# Science & Technology REVIEW

April/May 2025

# OPTIMIZING POWER GRID INVESTMENTS

*Also in this issue:*

Physics of the Planets and Stars

3D-Printed Target Capsules

AI Advances National Security

## About the Cover

Increasing energy demands from expanded manufacturing, computing demands to support AI resources, and new communities call for a more reliable, resilient electrical grid. As described in the article beginning on p. 4, Lawrence Livermore researchers and university partners, drawing on disparate sources, developed a capability to optimize power grid investments that includes consideration of likely weather threats. The cover design represents the sophisticated modeling and data science integration required to model the power grid.

Cover design: Heather Chandler

## 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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# Science & Technology Review

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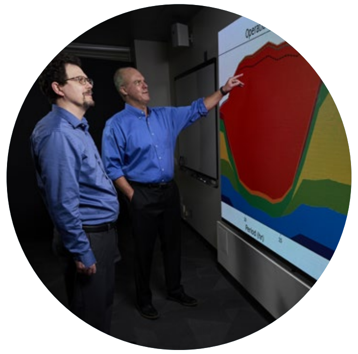

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### Sample Configuration for Ultrahigh Pressure Experiments

Livermore’s development of the toroidal diamond anvil cell has been revolutionary in pushing the static pressure limit in condensed-matter sciences. However, sample fabrication is nontrivial for very small anvils, and no standardized methods have been in place for such complex experiments. A global team, including researchers at Lawrence Livermore and Argonne national laboratories and Deutsches Elektronen-Synchrotron, have developed a new sample configuration that enables more reliable equation-of-state measurements in a pressure regime not previously achievable in diamond anvil cell experiments. Their results are published as an Editor’s Pick in the August 21, 2024, issue of the *Journal of Applied Physics*.

The team used the toroidal diamond anvil cell with a sample chamber diameter of approximately six micrometers. In this small sample chamber, the researchers microfabricated a sample package in a 10-step process whereby the target material is embedded in a uniform capsule of soft metal, which serves as a pressure-transmitting medium. This compression environment, in turn, improved the quality of equation-of-state data.

The new sample package solves the standing difficulty of static compression experiments to pressures higher than 300 gigapascals. Says Livermore scientist Claire Zurkowski, the paper’s first author, “We anticipate that this sample-encapsulation method will readily push static equation-of-state calibrations in physics, chemistry, and planetary science materials into the multi-megabar range—conditions where static compression data is very limited at present.”

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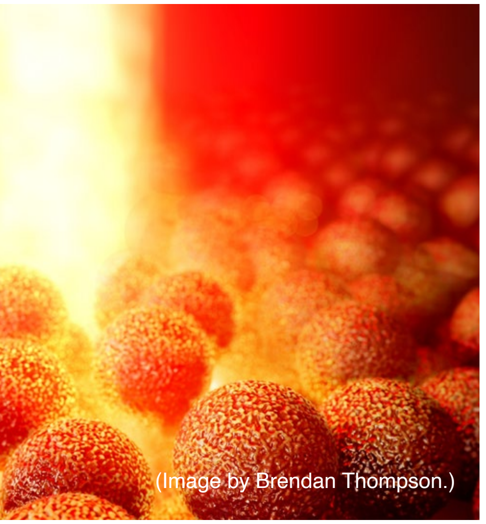
### Enhanced Powder Absorptivity in 3D Printing

One of the persistent challenges in laser powder bed fusion (LPBF) 3D printing is the high reflectivity of certain metals, which can lead to inefficient energy absorption and inadequate print quality. Lawrence Livermore researchers in collaboration with scientists from Stanford University and the University of Pennsylvania have introduced a wet chemical etching process that modifies the surface of metal powers, enabling a more effective energy transfer during laser melting. Their study appears on the cover of the September 6, 2024, issue of *Science Advances*.


(Image by Brendan Thompson.)

The new process creates nanoscale grooves and textures that increase absorptivity of metal powders used in LPBF without compromising purity or properties, such as high thermal and electrical conductivity, that make copper and other metals desirable for 3D-printed objects. The team printed high-purity copper and tungsten structures using lower energy input: less than 100 Joules per cubic millimeter (J/mm$^3$) for copper (a value closer to the typical range for high-density titanium and stainless-steel alloys), and approximately 700 J/mm$^3$ for tungsten (about one-third of the energy typically used).

Enhancing metal powder absorptivity is a promising step toward reducing additive manufacturing costs as well, particularly as the demand for more efficient manufacturing processes continues to grow. “With standard commercial laser-based machines, high-quality pure copper metal additive manufacturing is considered infeasible,” says co-author and Livermore materials scientist Philip DePond. “We are enabling copper printing without the risk of damaging existing machines or the expense of building new machines to process highly reflective materials.”

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### A New Treatment for the Effects of Fentanyl

Fentanyl’s lethal effects have killed more than 210,000 Americans in the last three years. The primary drug used to treat fentanyl overdoses, Naxolone (or Narcan), is effective but has a half-life of between 30 and 80 minutes, so it must be readministered to maintain activity in the body. A team of Laboratory researchers has discovered a new treatment to counteract the effects of fentanyl and related opioids. Called Subetadex, the drug has a half-life of 7.5 hours. Their results are published in the October 23, 2024, issue of *ACS Central Science*.

The Livermore team used nuclear magnetic resonance (NMR) to test the binding of various potential treatment compounds to opioids. These researchers were the first to test the compound Subetadex, discovered in 2002, against fentanyl, finding that Subetadex encapsulated fentanyl and prevented it from binding to receptors in the body. Recovery times for in vivo experiment models exposed to sublethal fentanyl doses were significantly reduced when Subetadex was administered.

This discovery of Subetadex’s effectiveness offers potential for the development of a medical countermeasure against the effects of fentanyl. “Using NMR, we found that the Subetadex binds to fentanyl quite well and does not let go of it,” says Carlos Valdez, principal investigator for the fentanyl medical countermeasure initiative. “That was a big moment. Finding a compound that already offers benefits is an exciting discovery because, as chemists, we know we can modify the compound to make it perform even better.”

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## Commentary by Huban Gowadia

# Mission First, People Always

In today’s evolving landscape, Lawrence Livermore National Laboratory’s scientific research and development efforts are more critical than ever. From energy security to AI, high-energy-density physics to additive manufacturing (AM), we are advancing solutions that address immediate national security needs, and we seek to anticipate over-the-horizon global security challenges and create strategic advantage to address them.

Energy security remains a cornerstone of national security. As future energy demands grow and as threats increase, Lawrence Livermore leads efforts to ensure that the nation’s critical power infrastructure remains reliable and resilient. The feature article in this issue of *Science & Technology Review* presents the work of a multidisciplinary Laboratory team to develop models and data-integration methods to anticipate and optimize grid investments in light of low-frequency, high-impact threats such as wildfires and floods. California’s dynamic geophysical features, varying weather patterns, and expanding energy demands provide the perfect test bed for applying the team’s predictive modeling and uncertainty analysis. Statistical bias correction and high-resolution data analysis enable more accurate predictions of these high-impact weather events and pave the way for actionable solutions to secure the nation’s power grid beyond the state’s borders.

The National Ignition Facility (NIF) Discovery Science Program exemplifies the Laboratory’s commitment to advancing fundamental scientific knowledge while investing in workforce development. By setting aside a portion of NIF’s experiments for basic science campaigns, we provide opportunities for external partners and early-career scientists to explore high-energy-density regimes that push the boundaries of physics. As the first research highlight in this issue describes, these experiments not only yield groundbreaking data but also serve as a recruiting tool for the Laboratory. Two scientists featured in the highlight—Alison Saunders and Max Boehme—began their Livermore careers through the Discovery Science Program, demonstrating how the initiative fosters the next generation of scientific expertise.

The Laboratory further drives transformational change, embraces meaningful risk, and demonstrates agility in the field of AM. The second research highlight presents how AM-crafted inertial confinement fusion target capsules required for NIF laser shots open new possibilities for faster, affordable, and more flexible production options. Application of the Laboratory’s dual-wavelength two-photon polymerization printer and utilization of complementary photo resin has optimized target capsule quality and printing speed, promising to meet NIF’s increasing demand for high-repetition shot rates. Further, the technology unlocks new opportunities for innovation in fusion energy as researchers adapt target capsule designs on the fly.

The final research highlight explores how Lawrence Livermore stands at the forefront of leveraging AI for its national security mission. Through initiatives such as the opening of our AI Innovation Incubator (AI3) we are forging public–private partnerships with industry leaders including OpenAI, Microsoft, NVIDIA, and Hewlett Packard Enterprise to scale up AI technologies for national security missions. These collaborations ensure that Lawrence Livermore remains connected to cutting-edge advancements while providing value to the national security community by addressing their real-world challenges. Complementary to AI3, the Laboratory’s Data Science Institute cultivates a partnership with the University of California system to engage students in solving challenging, real-world data science and AI problems—a relationship that further develops Lawrence Livermore’s data-science workforce pipeline. The Laboratory’s internal AI education platform, aiEDGE, empowers the workforce to harness AI tools for scientific innovation, operations, project management, and communications, among other applications, through accessible training and shared success stories.

The Laboratory’s mission is clear: to enable U.S. security and global stability by empowering multidisciplinary teams to pursue bold and innovative science and technology. This mission drives us to prioritize innovation and embrace meaningful risk while maintaining a steadfast commitment to addressing the world’s most pressing challenges. Whether ensuring energy security, advancing fundamental physics, revolutionizing AM, or leveraging AI, we strive for agility in fulfilling the Laboratory’s national security mission and remain dedicated to the development of our excellent workforce.

My mantra, “Mission First, People Always,” encapsulates an effective approach to tackling these challenges facing our nation and the world. Together, we are not only safeguarding the nation but also inspiring the next generation of scientists and engineers to dream big, innovate, and achieve the impossible.

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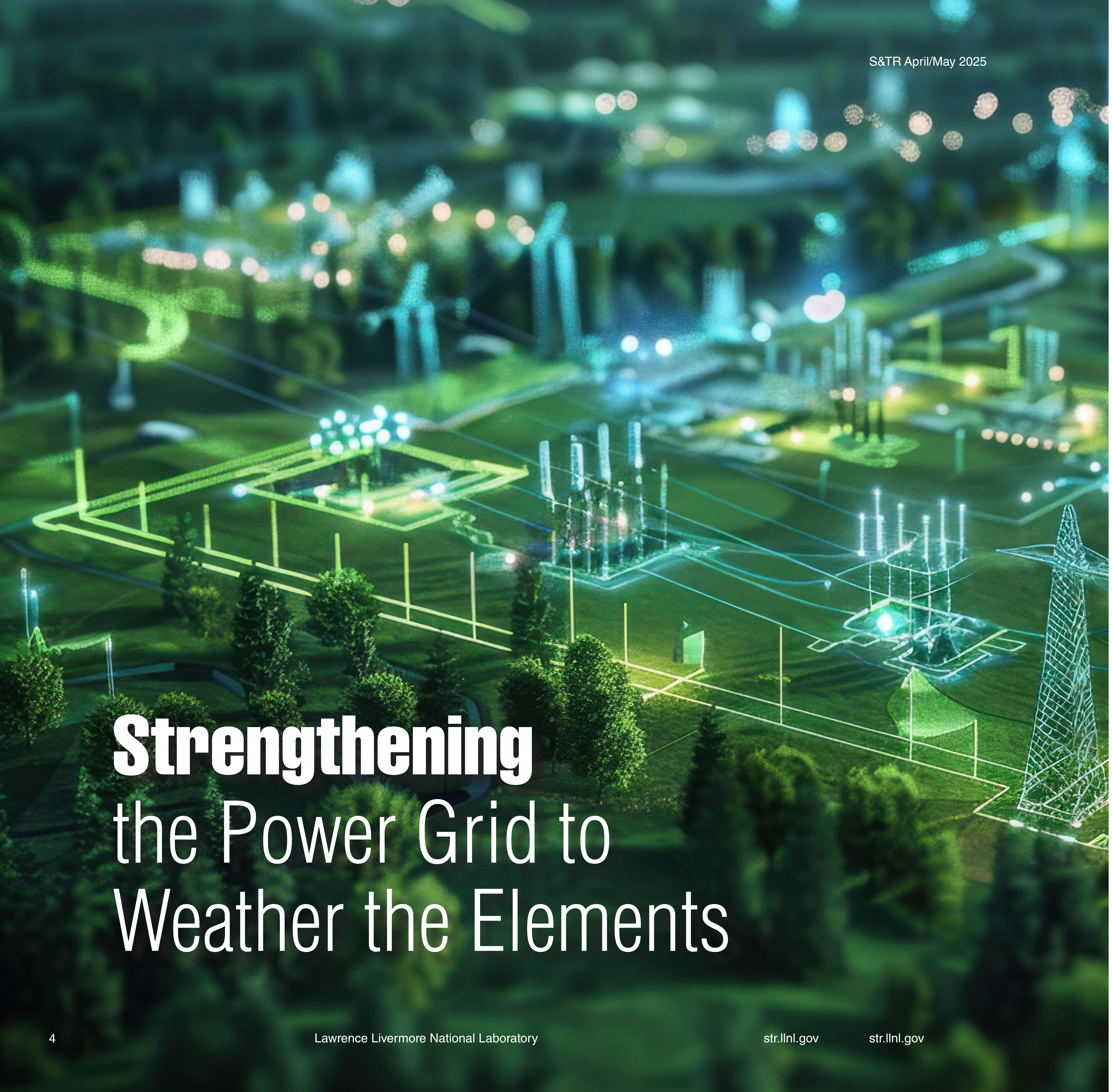
■ Huban Gowadia is principal associate director for Global Security.



# Strengthening the Power Grid to Weather the Elements

,Severe winter storms fed by a polar vortex swept across Texas in February 2021, plunging temperatures below freezing for days on end in regions such as Austin and Houston better known for extreme heat. Residents heating their homes to combat the frigid weather placed an unmanageable demand for power on an electrical grid that was not designed to withstand such extreme loads or weather conditions. The system operator executed controlled, rolling blackouts, narrowly preventing a total, state-wide grid collapse. As a result of the strained infrastructure, millions of residents and businesses were left without power. Electric and natural gas heaters failed, the water supply faltered, water treatment backed up, and food spoiled, leading to billions of dollars in impacts. More than 200 casualties were attributed to the effects of the weather event.

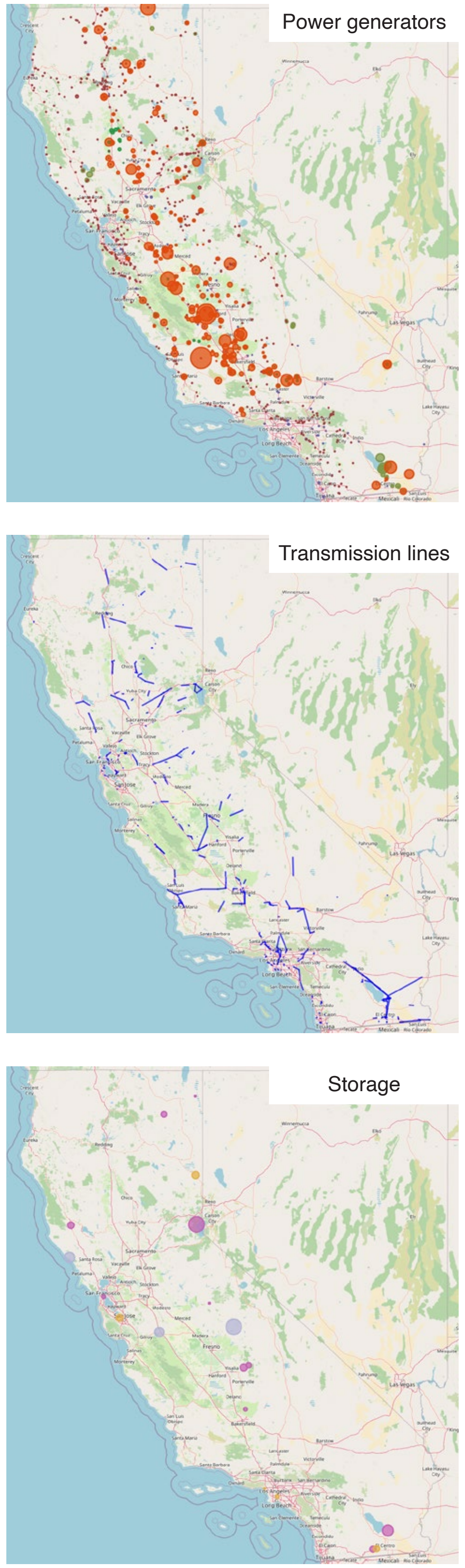
Inclement weather is the leading cause of power outages in the United States, and the consequences of power loss—as shown by the February 2021 event in Texas—can be severe. In the interest of bolstering national energy security, a Lawrence Livermore research team led by Philip Cameron-Smith and Jean-Paul Watson completed a Laboratory Directed Research and Development (LDRD) Strategic Initiative (SI) aimed at strengthening the nation's electrical grid. "We need investments to ensure that the U.S. power infrastructure remains reliable and resilient even as future energy needs and sources, as well as the threat landscape with respect to energy security, continue to evolve," says Cameron-Smith.

SI projects, focused on long-term solutions to mission-critical challenges, are the largest in scope within the Laboratory's LDRD Program. As part of this project, the team developed data-integration methods and computational models necessary to find the most cost-effective and resilient routes to expand the power grid, using a realistic version of California's grid as a test case. California's diversity of energy resources and geophysical features, differences in weather patterns, and changing energy needs highlight the importance of modeling resource availability and demand variability. With additional research talent from university partners—San José State University, the University of California (UC) at Davis, and UC Berkeley—the multidisciplinary and multidirectorate endeavor united Lawrence Livermore's deep expertise in energy security, machine learning, high-performance computing, and Earth system models, including wildfire and hydrological modeling.

## Optimizing Investments

Strengthening the power grid entails increasing both its reliability—the ability to regularly meet demand—and its resilience—the ability to withstand extreme threats in a cost-effective manner. Simultaneously expanding and hardening the power grid necessitates strategic investments in each class of electrical infrastructure: generation, transmission, and storage. Given the breadth of possible investment avenues for each infrastructure class, governments and private utilities alike need a way to judiciously determine the most effective capacity expansion projects, while also weighing economic and legal considerations of each option. While many such projects might seem far off in the future, investment decisions are already having major effects on the power grid. For instance, Diablo Canyon, California's only operational nuclear power plant, which recently received extensive state financial support to postpone its scheduled shutdown to 2030, will continue providing electricity for approximately 3 million Californians, and bolster grid reliability.

The SI project team focused on identifying and integrating diverse data sources on the weather and the electrical grid and developing a computational model, optimized using Pyomo (a



The power grid capacity expansion and optimization model yielded a set of infrastructure investments to maximize the grid's reliability while minimizing cost. Depicted are the model's determinations of new California generators (top), transmission lines (middle), and storage options (bottom), optimized for a 2045 scenario. In the top map, colored dots represent different fuel sources, such as natural gas or geothermal energy, for power generation. In the middle map, purple lines represent new transmission lines. In the bottom map, colored dots represent different energy storage options, such as batteries and hydroelectric pumped storage.

software package of which Watson is a lead developer), to identify the most cost-effective set of power grid infrastructure investments that will meet California state requirements and future power demands for a range of possible weather conditions. A grid that is cost efficient 99 percent of the time, but plunges users into darkness in the evenings of long, hot, windless summer days is not acceptable. "I encourage people to think of this work as developing an exploratory tool. The optimized investment plan depends on what assumptions are provided to it," says Tomas Valencia Zuluaga, a postdoctoral researcher in the Laboratory's Center for Applied Scientific Computing. Ultimately, the model can be adapted to any region's unique needs by adjusting data related to local patterns of energy consumption, weather risks, transmission lines, and energy technologies (available and emerging).

The model's proposed investment plans draw from a portfolio of options for power generation, transmission, and storage infrastructure. "On the generation side, we consider solar power and wind facilities, and in certain areas, we could also place natural gas units, biomass, hydropower, geothermal, and other facilities," explains Watson. The model can even accommodate not-yet-realized technologies such as fusion energy plants.

In the nearer future, however, users can investigate the wide deployment of small modular reactors, which are miniaturized nuclear fission reactors whose small footprint and affordability are attractive to technology companies looking to satisfy the demands of new data centers.

Generating energy is not helpful, however, if it cannot be either immediately supplied to consumers or stored for future use. Therefore, the team next looked downstream from power generation to transmission lines and substations, where high-voltage electricity is converted to lower voltage for safe distribution to consumers. Due to permitting and right-of-way considerations, Watson explains that the most feasible transmission upgrades involve either building additional lines within corridors already in use or modifying existing transmission lines to make them more efficient and operate at higher capacity. Finally, the team considered energy storage options, including large-scale lithium-ion batteries. In general, battery systems stand to become even more efficient and store greater amounts of power given ongoing materials science developments. Other viable storage system alternatives include pumped storage hydropower, which leverages the potential energy of water pumped to a higher elevation.

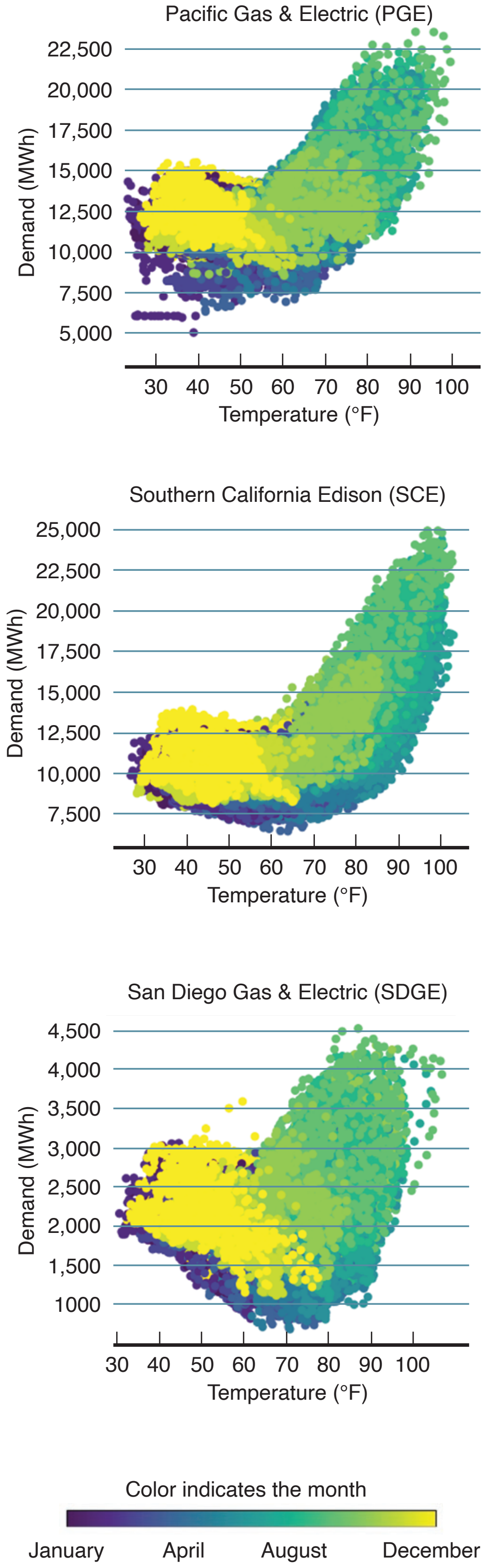
## High-Power Computing Approach

The researchers' approach to narrowing down grid configurations involves two coupled optimization stages. In the first stage, they determine a set of infrastructure investments that meets projected electricity demand at minimum cost. Then, in the second stage, they subject this grid model configuration to different weather scenarios and assess how well the proposed grid fares in demanding conditions.

Optimization is much easier said than done, however. "In our California test case, the grid contains roughly 9,000 buses (nodes where multiple circuits converge) and 11,000 transmission lines, offering many possible decisions from all the combinations of infrastructure locations and their operations," says Elizabeth Glista, an operations research engineer in the Laboratory's Computational Engineering Division. Valencia explains how these many elements complicate the task of optimization. "Our representation of the power grid uses a combination of binary, integer, and continuous variables," he says. "For example, we model transmission lines as binary variables—they are either built or not built. The number of power production units built and their capacities, however, are integer values. Certain types of energy generation cannot be fractional. We can't build half of a combustion turbine, but we can scale a solar farm by almost any amount."

The presence of binary and integer variables coupled with complex constraints makes their optimization task an NP-hard computing problem. (NP-hard problems are a class of computing problems whose solutions are simple to verify yet extraordinarily difficult—sometimes impossible—to obtain unless the problem is simplified, or "decomposed," to some degree.) "We spent a great deal of time considering how to decompose the associated problems and utilize our computational resources in clever ways to obtain results in a reasonable timeframe," says Valencia. The team considered a range of optimization scenarios that differ in how patterns of energy generation and consumption are projected to evolve over coming decades. Then, rather than simply determining investments for one demand scenario at a time, team members applied a stochastic programming methodology to simultaneously minimize investment cost across this range of future scenarios. This approach to computational problem-solving accounts for the intrinsic uncertainty that comes with forecasting future conditions—uncertainty introduced by possible technology improvements or policy changes, for example—and it encourages the grid solutions to feature realistically achievable modifications.

Heating and cooling buildings represent a significant portion of the nation's electricity demand. Therefore, understanding the effects of weather on energy demand is necessary to assess the reliability and resilience of future power grid configurations. When severe weather and extreme temperatures occur, providing power to people becomes all the more critical. Moreover, weather also impacts the ability of many types of power plants to provide electricity in the first place—and the ability of transmission lines to transmit power to users—making a case for new power generation and delivery infrastructure, too. Obtaining accurate, high-resolution simulations of possible future weather scenarios is, therefore, vital for making informed decisions about

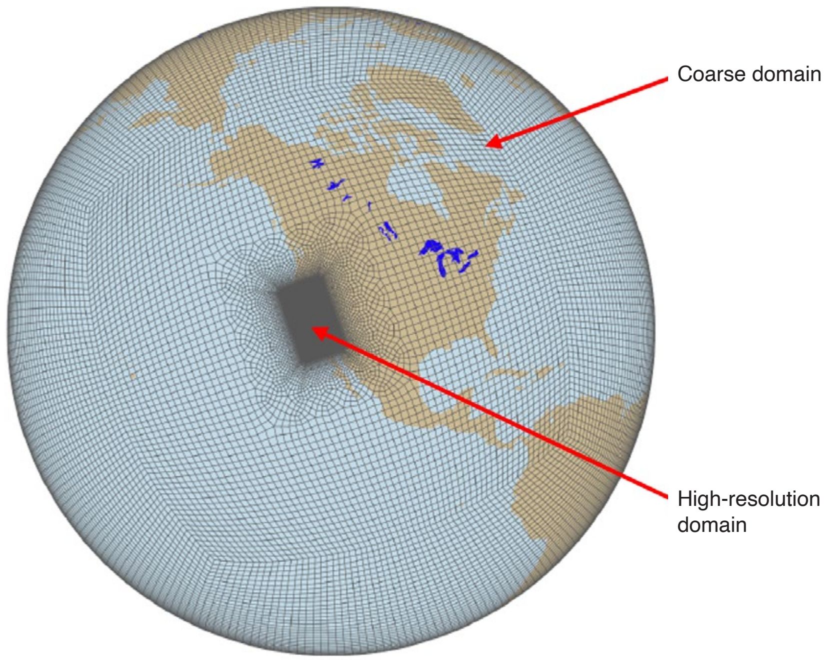


Weather conditions influence demand for energy. (right) Plots reveal the nonlinear relationship between temperature (in Fahrenheit) and electricity demand (in megawatt-hours) throughout a calendar year across three California utility regions. Demand values are sourced from utility provider reports from July 2018 to December 2022. (above) A California map indicates the geographical area represented by each of the three utilities.

whether, where, and how much to build, modify, or expand energy infrastructure, as well as what type of infrastructure to build, especially as the United States is poised for a rapid increase in demand due to increased manufacturing, additional computing resources for AI, and expanding electricity service to new areas. High-resolution Earth system simulations—about 3-kilometer (km) grid spacing—are required to provide a spatial resolution that resolves mountain passes funneling wind for wind turbines, and output is needed hourly to test whether power generation can meet demand throughout each day.

To enable the optimization model to incorporate the link between weather and its induced patterns on electricity demand, postdoctoral researcher Minda Monteagudo developed an electrical load model that enables the team to input any temperature time series—past, present, or possible future—and predict the associated electricity demand with hourly temporal resolution. Trained by regressing historical weather data on utility-reported demand, the load model predicts time- and temperature-dependent power demand throughout California while accounting for calendar effects such as time of day, season, and day of the week.

Equipped with an understanding of demand as a function of temperature and time, the Lawrence Livermore team can project future demand using representative days of weather—archetypes of daily weather conditions from scenarios simulated by Earth system models that mathematically integrate the planet’s physical, chemical, and biological processes. Each representative day has distinct influences on the expected patterns of energy production and consumption. “For example, on a specific simulated day in 2045—what we refer to as the ‘target horizon’—a location may experience more wind and less sun than usual. In this scenario, if only solar installations exist nearby, the grid would draw on electricity stored in batteries or other systems to satisfy demand not immediately met by solar power,” says Valencia. “The driving question is, how many representative days must we account for to capture sufficient weather variability at the target horizon?” Using fewer representative days simplifies calculations for the capacity expansion problem, but at the cost of limiting how much weather variability can be captured.



The Energy Exascale Earth System Model (E3SM) was used to develop a regionally refined model (RRM) and to simulate atmospheric phenomena at 3-kilometer (km) resolution over California, far exceeding E3SM’s standard 100-km resolution. Higher spatial resolution helps to provide better predictions of atmospheric phenomena, such as the winter precipitation pictured on p. 9.

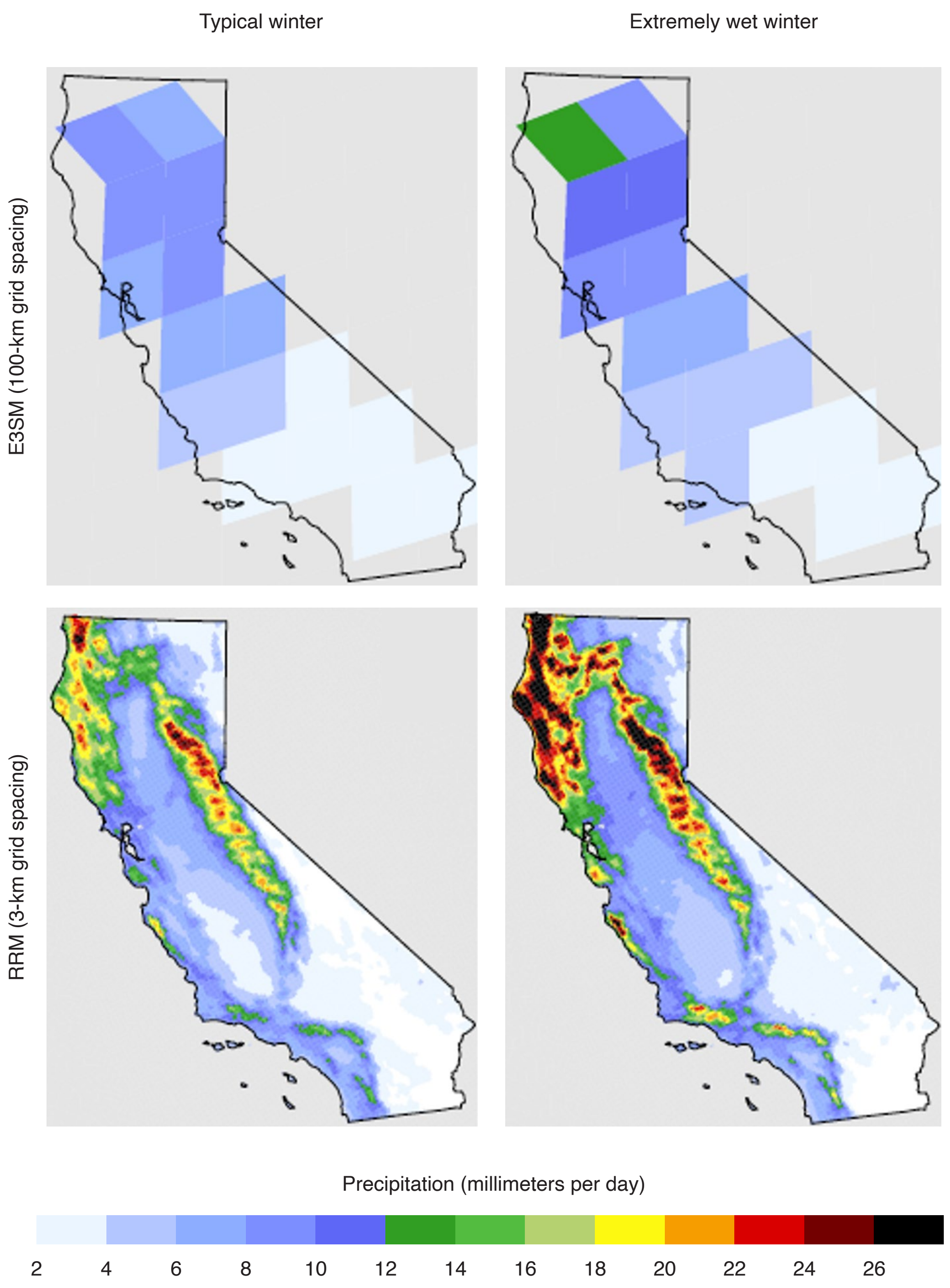
Without sufficient weather examples, the optimizer may provide a design for the grid that will fail if a weather event occurs that had not been considered, which carries direct, downstream impacts for the reliability and resilience of the realized grid. Thus, investigating numerous representative days covering the breadth of weather scenarios is desirable to address the intrinsic weather variability, as simulated by the Earth system models. Hourly time-series data for individual representative days in the target horizon is distributed to different computers within a parallel computer cluster; each computer then returns a power grid investment plan optimized for the weather time series provided to it. Solutions among computers will likely differ at first. “If one computer were to see a particularly cloudy day, it might determine that more hydropower is ideal overall. Likewise, if another computer sees a particularly sunny day, then it would recommend solar power investments because that is the most available resource. We are seeking a single investment plan, so the solutions must match,” says Valencia. Using the Laboratory’s Quartz computing cluster, the team could optimize grid investment plans across hundreds of weather scenarios at once. By strategically penalizing mismatched optimization solutions produced by different computers within the cluster, their algorithm can quickly converge on a single solution.

## Tracing Data Streams to the Source

The overarching grid optimization model comprises a constellation of computer scripts that ingest Earth system modeling data alongside infrastructure-focused technoeconomic considerations such as the locations of sited infrastructure, new infrastructure costs, generator and storage capacity, and many other factors. Constructing a software pipeline to join process data from these different sources into the form required to optimize the electrical grid required painstaking effort.

The team used the Department of Energy’s (DOE’s) well-established Energy Exascale Earth System Model (E3SM) to generate weather patterns for future scenarios of interest. With submodels capturing land, sea, rivers, ice, and the atmosphere, E3SM was built with DOE supercomputers in mind. However, properly integrating the E3SM data with other data streams in the pipeline calls for extensive conversions, corrections, and restructuring of data. “An enormous amount of work goes into turning existing Earth system data into the forms necessary for our purposes,” says Monteagudo. She explains that many of her efforts relate to assessing potential data sources for quality, relevance, and compatibility. “Does the data source support the variables that we need? Does it have the necessary resolution? Does it contain underlying statistical biases? We have to ask many questions to ensure that a particular data source will help us answer the questions we are interested in,” she says.

For instance, the team drew upon the Systems Advisor Model (SAM), a technoeconomic analysis tool developed by DOE’s National Renewable Energy Laboratory (NREL), to estimate the output of wind and solar power facilities for a



Higher quality weather predictions obtained with RRM are critical to power infrastructure decision-making. (top row) E3SM predictions show average winter precipitation for a typical year and an extremely wet year at E3SM’s standard 100-km resolution. (bottom row) The higher spatial resolution provided by RRM shows significantly more precision to better inform the efficacy of hydropower facilities, which rely on rainfall and snowmelt.

given weather scenario. "We found that the wind and solar output data produced by E3SM are not always a one-to-one match for what NREL's SAM would like to work with," says Monteagudo. For example, E3SM produced solar irradiance measurements from the perspective of planes parallel to Earth's surface. SAM, instead, utilizes measurements taken from planes perpendicular to incoming solar radiation. Other data preprocessing checks are similarly meticulous, such as choosing the appropriate brightness measurements for the Sun and deciding if hourly time-series data is collected at the beginning, middle, or end of the hour. "These are very in-the-weeds sorts of tasks, but if we didn't perform them—and if we didn't have the in-house expertise to know they were necessary—then we would obtain inaccurate power estimates without knowing the underlying reasons," says Monteagudo.

Although data preprocessing ensures the data pipeline draws on compatible data sources, the team still had to contend with intrinsic statistical factors—referred to as biases—that affect the predictions of these models. One source of such biases can arise from natural fluctuations such as El Niño and the Pacific Decadal Oscillation, which take place over longer periods of time than are normally simulated by weather models. Given the complexity of these phenomena, there is no one-size-fits-all approach to adjusting these factors. "Biases are hardly ever so simple as values being one degree too warm or cold across the board. They depend on one's location, weather patterns, and many other considerations," says Cameron-Smith.

Researchers must take these factors into account because they have direct ramifications for infrastructure decisions. For example, many power plants—regardless of whether they use coal, biomass, natural gas, or nuclear fuel for energy—rely on river water for cooling, which is returned at a higher temperature to the river source. However, high water temperature can cause die-off of aquatic life that people depend on for their livelihoods, so there are limits on the temperature of water that can be released by such a power plant back into the river. Hence, if the river's water temperature rises at the power plant's inlet, less heat can be absorbed by the water before it is discharged back to the river, and energy production must be reduced. If the water exceeds a threshold temperature, the plant may need to be turned off entirely. Cameron-Smith explains the impact of temperature biases when simulating such systems: "If our predicted values for river temperature are consistently too high, then we would wrongly reason that the power plant could never run, so we should invest elsewhere. On the other hand, if the readings are consistently too low, we would incorrectly predict that the plant could function without issue."

## Seeking High Resolution

High-resolution data directly impacts the optimization model's determinations for infrastructure investments. Cameron-Smith explains, "Wind turbines are, of course, placed where it's windy. These conditions often occur near mountain passes because the topography acts as a funnel for air currents. At 100-kilometer resolution, standard atmospheric models can hardly resolve mountain ranges, let alone individual mountain passes. Even at 25 kilometers, which many modelers would consider high resolution, we found that the implied power generation was still not accurate enough."

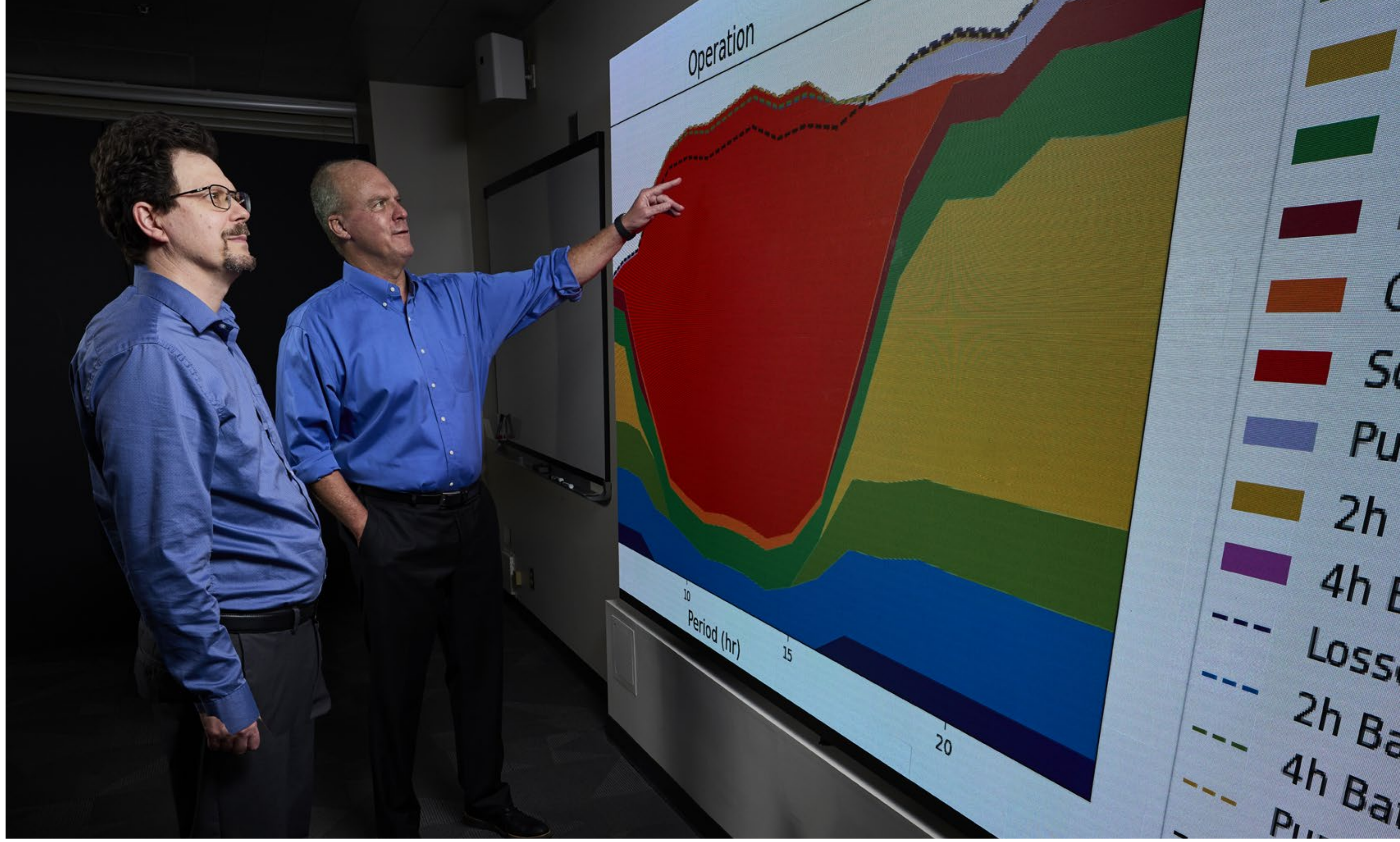
Fortunately, an extremely high-resolution version of E3SM's atmospheric model known as Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM) has recently been developed to operate with a grid spacing of just 3 km. (See *S&TR*, June 2024, pp. 16–19.) However, simulating the entire globe at this resolution is so computationally slow and expensive that not enough weather events could be simulated for the electrical grid optimization, and outputting the weather variables every hour would produce too much data to handle. Therefore, the SI team developed and tested a regionally refined model (RRM) version of SCREAM that used a stretched grid so that only the atmosphere over the region of interest—in this case, California—needed to be simulated with 3-km grid spacing, while the standard 100-km spacing applied elsewhere. RRM satisfied the tradeoff between simulation resolution and its associated compute time and storage requirements. Cameron-Smith explains that the team used California as a test case for developing their methodology because, apart from being home to Lawrence Livermore, the state's power grid is an exciting challenge to model. "California is large and geographically diverse, and it experiences significant variations in meteorological conditions. We experience a range of weather-related events, including atmospheric rivers, wildfires, and fog, that impact energy production and consumption." Using this RRM configuration, the team produced four individual 5-year simulations of weather through the end of the 21st century with the hourly output needed for the models that relate weather conditions to electrical generation and consumer demand.

In addition to the impact of daily weather on the electrical grid, extreme events can also provide shocks to the system that test the resilience of the grid. Two such low-frequency, high-impact threats are wildfires and floods. Few threats are as palpable among California residents as wildfires, which in recent years have led to unanticipated power loss and rising home insurance costs—let alone imminent threats to human life. Unusually high temperatures, dry vegetation, and strong winds create the greatest opportunities for fire to ignite and to spread, and this precise combination of factors led to the outbreak of devastating wildfires in Los Angeles in January 2025. At the other end of the scale, floods can damage power lines, substations, and transmission equipment, leading to outages and safety risks. For both wildfires and floods, a longer-term view of weather history is required, since the conditions for fires and floods usually take weeks, months, or years to develop. To better inform both fire and flood risks, the team developed machine-learning systems that leverage historical observations to forecast dead fuel moisture and river flow across California. For wildfire prediction, the fuel moisture model is critical to the flammability of dead vegetative fuels, such as fallen sticks and branches, driving fire behavior. In parallel, river flow forecasts support early warnings for flooding by capturing hydrologic responses to precipitation and snowmelt. This will facilitate inclusion of such extreme events stochastically into the grid optimization system in the future to make sure the recommended grid will also be resilient to such catastrophic events.

Although the LDRD project has concluded, the effort yielded new computational capabilities that enable additional research efforts—for instance, finding grid solutions that incorporate distributed energy resources (DERs). DERs—a class of small-scale, consumer-operated generation and storage devices that include rooftop solar panels and associated battery storage—are being installed at increasing rates. Further areas of interest include studying new regions, tackling challenges related to new energy sources, such as small modular reactors, and exploring rapid technological developments in energy storage, including new chemical battery technologies—gravity batteries that lift heavy weights and flywheels.

Cameron-Smith says a fundamental goal of LDRD SI research projects is to facilitate exchanges and collaborations across directorates, which is evidenced by this team's combination of subject-matter experts from Livermore's Physical and Life Sciences, Global Security, Computing, and Engineering principal directorates as well as university partners. "Of course, we have excellent codes and powerful computers, but what I argue proved even more critical is the domain expertise provided by our research team to bridge the gap between environmental science and infrastructure," he says. "The nature of these projects is to get scientists reaching across directorates and talking to each other. I believe Lawrence Livermore does this particularly well. Even if the collaboration requires extra effort, that effort lets us get to the science and develop impactful capabilities."

*—Elliot Jaffe*



Philip Cameron-Smith (left) and Jean-Paul Watson led the Strategic Initiative to develop a computational model relating weather events with choices for optimizing power grid infrastructure investments. Shown here, Cameron-Smith and Watson refer to a model of different power-generation and energy storage options optimized over a 24-hour period.

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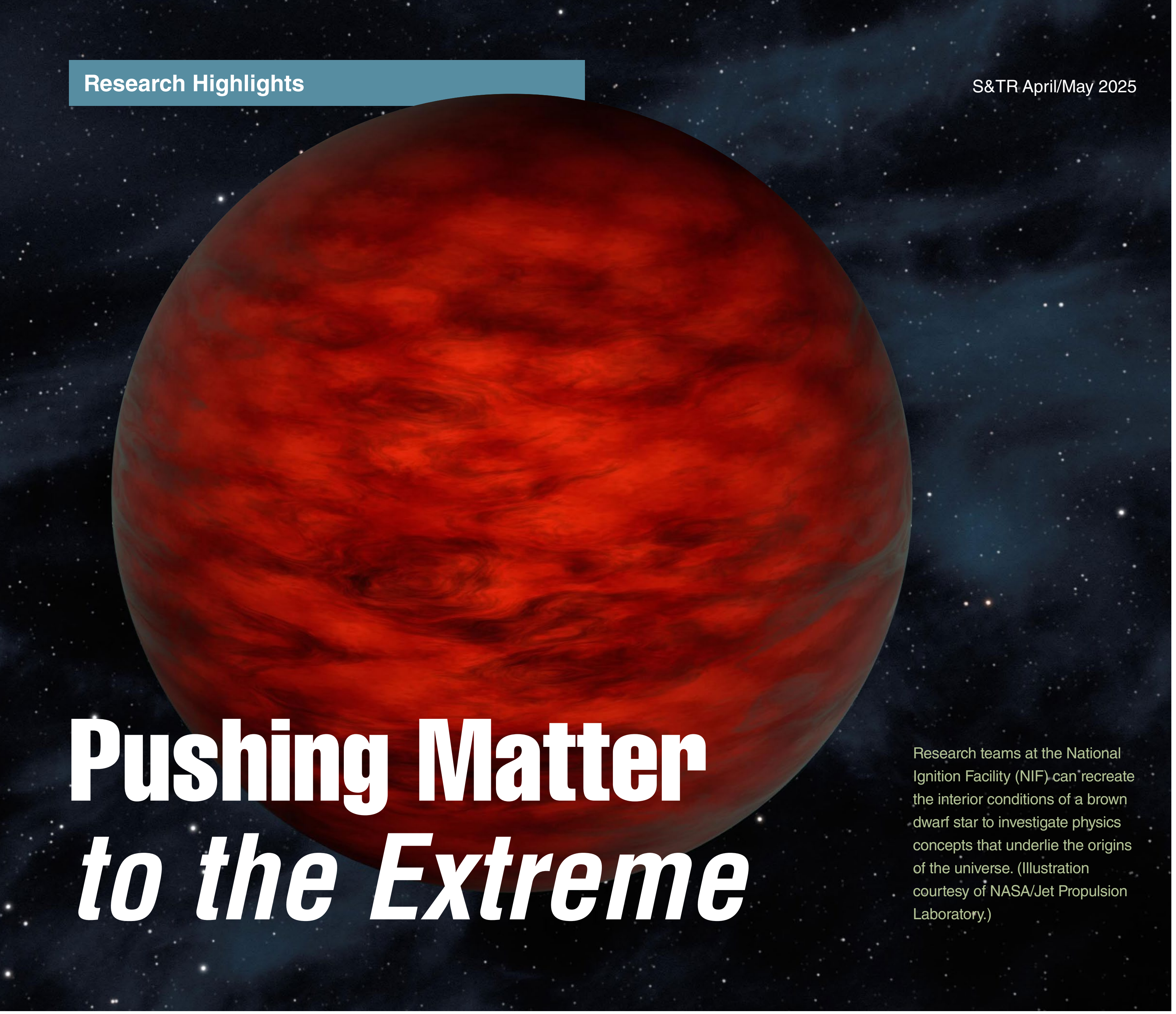


# Pushing Matter *to the Extreme*

Research teams at the National Ignition Facility (NIF) can recreate the interior conditions of a brown dwarf star to investigate physics concepts that underlie the origins of the universe. (Illustration courtesy of NASA/Jet Propulsion Laboratory.)

By creating plasmas—mixtures of ions and free electrons—under extreme conditions, the National Ignition Facility (NIF) becomes a terrestrial test bed for extraterrestrial conditions. In these environments, NIF provides an Earth-based laboratory for understanding the cosmos, providing insight into questions about how stars and planets begin and end their lives. Researchers in the Discovery Science Program at Lawrence Livermore are particularly interested in understanding the mechanism by which atoms gain or lose electrons (ionization) at high pressures and densities.

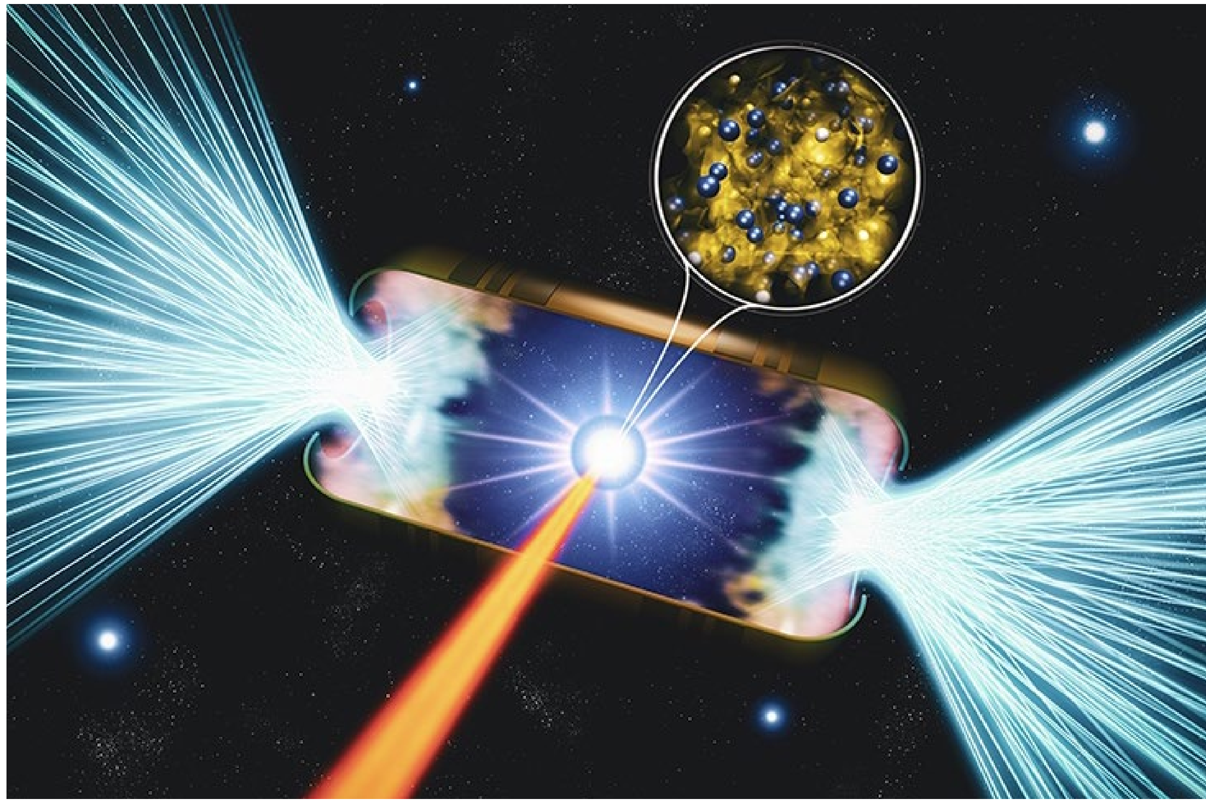
The extent of ionization in stars and giant planets determines their material properties, such as their thermodynamic behavior and electrical conductivity, and whether they have a surrounding magnetic field. Understanding the ionization process is, therefore, crucial to accurately modeling these objects. Ionization is conventionally driven by high temperatures such as those found in burning stars. Cooler astrophysical objects, however, can be ionized by a different mechanism: pressure-driven ionization, in which the object's outer layers compress the matter in its interior. This effect is felt even at the atomic level, where extreme pressure squeezes atoms together so intensely that the atoms' nuclei approach their neighbors' K-shell, the innermost and most tightly bound shell of electrons around the nucleus. This proximity leads nearby particles to interact and modify one another's electron structure, causing the atoms to become ionized. As the ions are forced closer together under pressure, electrons are released into the surrounding plasma, further ionizing it. However, despite its importance, many parameters in this process remain unknown.

## Coming Out of the K-Shell

Since electrons in the K-shell are the most strongly bound in an atom, they require the most energy to unbind. As a result, these K-shell electrons are the dominant factor in determining the radiation transport—the process of energy transfer through radiation. "Radiation transport is very important in stars, for example, because it determines their structure, how energy flows from the center of a star to the outside, and vice versa," explains NIF experimentalist Tilo Doeppner. Understanding how K-shell electrons behave and survive at the extreme temperatures and densities in stars is a significant step toward improving understanding of radiation transport as a whole.

In a yearslong collaborative campaign, Doeppner and his research team used NIF to generate the extreme conditions necessary to achieve pressure-driven ionization and study its effects on K-shell electrons. NIF's 192 lasers heated up the inside of a hollow cavity, called a hohlraum, and a beryllium shell placed at its center. Upon heating the hohlraum with lasers, the outside of the shell rapidly expands while its inner surface accelerates toward the center at pressures exceeding 3 billion atmospheres and temperatures of around 2 million Kelvin. For just a few nanoseconds, this process creates a tiny piece of matter analogous to a dwarf star. "Right now, NIF is the only experimental facility where we can create and study these states under controlled conditions," says Doeppner.

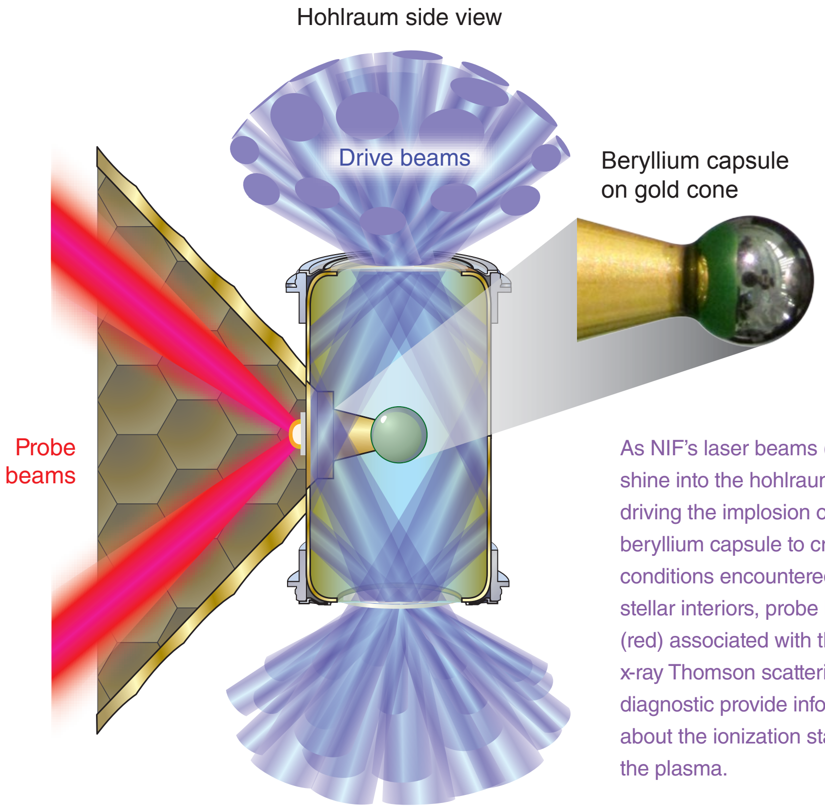
Using a technique called x-ray Thomson scattering (XRTS), Doeppner and his collaborators worked to determine how many electrons remain in a bound state during pressure-driven ionization—that is, remaining part of an ionized atom—versus how many would release into the surrounding plasma. A major benefit of XRTS is its simplicity; the technique depends purely on the analytical relationships among quantities. Lawrence Fellow Max Boehme says physicists can define and solve these relationships without complex computational techniques. "There's a sophisticated quantum mechanical theory behind XRTS, and it gives us a lot of information," he says. "This is one of the most promising methods to directly probe the microphysics of these dense plasmas."



A capsule implosion experiment at NIF creates starlike conditions inside a hohlraum. Plasma ionization (inset) occurs near maximum compression of the imploding shell. (Illustration by Greg Stewart, SLAC National Accelerator Laboratory. Inset illustration by Jan Vorberger, Helmholtz-Zentrum Dresden-Rossendorf.)

To carry out an XRTS measurement experimentally, the researchers shine x-rays into a plasma. The x-ray photons scatter off electrons in the plasma, which can be either free, loosely bound, or tightly bound to the ionic cores of atoms. XRTS measures the intensity and spectral distribution of these photon scattering events under a certain deflection angle. In each scattering scenario, photons emerge with an identifiable energy spectrum that reflects the type of interactions that occurred with the electrons in the plasma. "I describe this as a relativistic billiard ball problem," says Alison Saunders, a Livermore experimental physicist working at NIF. "If someone were to roll one ball—representing the x-ray photon—on a billiards table so that it impacts a second ball—representing an electron—the first ball would bounce differently off the second one depending on whether the second ball was stationary or already in motion. The mechanics of interpreting XRTS is conceptually similar. If we know the momentum of the ball going in and the momentum of the ball going out, we can say something about what it must have scattered off of."

If an x-ray intercepts a free electron, energy transfers from the photon to the electron, and the photon emerges with slightly less energy than when it entered. Intercepting a loosely bound electron also reduces a photon's energy, but the amount of energy transferred is distinct from the first case, resulting in a unique energy spectrum that allows researchers to differentiate between the scattering events. Finally, a photon scattering off a tightly bound electron, such as the ones in the K-shell, rebounds as if off a mirror—known as elastic scattering—and retains its initial energy. "Scattering a lot of photons off the plasma, we can begin to understand how many electrons were free, loosely bound, or tightly bound from the distributions in the resulting scattering spectra, thereby providing a constraint on the plasma's overall ionization state," says Saunders.



As NIF's laser beams (blue) shine into the hohlraum, driving the implosion of the beryllium capsule to create conditions encountered in stellar interiors, probe beams (red) associated with the x-ray Thomson scattering diagnostic provide information about the ionization state of the plasma.

### Testing the Models

Doeppner, Saunders, Boehme, and their team used XRTS measurements to observe the onset of pressure-driven ionization in beryllium. The researchers found at least three of beryllium's four electrons were removed during compression. At the highest levels of compression, they found a reduction in elastic scattering, which is related to tightly bound electrons, thus confirming the tendency of the single remaining K-shell electron to delocalize.

This information about pressure-induced ionization can be used to predict the extreme temperature and pressure conditions needed to accurately model the inner workings of stars, planets, and even inertial confinement fusion (ICF) experiments. Doeppner says, "A lot of similarities exist between these astrophysical questions and the ICF experiments that we do at Lawrence Livermore." However, because the reduction in elastic scattering that the team observed with XRTS is often overlooked, most of the widely used ionization models for ICF might underestimate the degree of ionization and the effects it can have on experiments.

Incorrect ionization models have long-ranging effects as they determine how easily x-rays can pass through a plasma and, hence, determine the radiational energy transport in stars and in ICF experiments. With XRTS studies, scientists can now confirm the validity of their ICF models for the first time—and NIF is the only place where that can be done. "We find that electrons can be in a weird state between bound and free, which is challenging for simulations to describe," says Doeppner.

Highlighting the importance of new experiments that create conditions matching those at cores of planets, exoplanets, and some stars, Boehme adds, "NIF has the ability to reach conditions at which today's models haven't been tested before—a unique situation." The ability to field experiments that test such extreme conditions is central to NIF's core function of supporting stockpile stewardship.

### Exemplar for Discovery Science

A portion of NIF's approximately 400 annual experiments are set aside for basic science campaigns through NIF's Discovery Science Program, with the bulk supporting NIF's primary application in support of the National Nuclear Security Administration's science-based Stockpile Stewardship Program. The Discovery Science Program provides opportunities for external users to take advantage of NIF's unique facilities and capabilities and to perform laboratory experiments in high-energy-density regimes. As both a recruiting tool and a scientific success story, XRTS measurements are exemplary of the Discovery Science Program and its mission. To date, more than 100 such experiments have been conducted or are planned. (See box above.)

## Other NIF Discovery Science Projects

NIF's Discovery Science Program offers opportunities for external facility users and Lawrence Livermore scientists to perform research in high-energy-density science. As part of the Discovery Science Program, researchers have:

- Recreated the conditions inside Jupiter, Saturn, and other planets by compressing a diamond sample to a record 50 million megabars—50 million times the pressure of Earth's atmosphere.
- Brought new insights into fluid hydrogen transformations, providing key information about how giant planets and solar systems form.
- Recreated conditions similar to the inside of stars.
- Used collisionless shocks to study exotic astrophysical phenomena, including supernova remnants and cosmic magnetic fields.

"Alison Saunders and Max Boehme were early career scientists when this project started. They exemplify how NIF's Discovery Science Program provides opportunities for young scientists to participate in the work done at NIF and how that can serve as a hiring pipeline for the Laboratory," says Doeppner. Now a staff scientist and group leader, Saunders began work on this project as a postdoctoral researcher. Boehme first came to the Laboratory as a summer intern analyzing XRTS spectra for this project. As a Lawrence Fellow, he runs quantum simulations bridging the gap between theory and experiment.

The cycle between theory and newly gathered data creates a test bed for advancing science with new, testable ideas. "I have a high-quality data set of conditions that have never been created in any experiment before. We're literally the first ones to probe this data, and that's exciting to me," says Boehme.

The collaborative nature of Discovery Science projects attracts researchers from prestigious universities, national laboratories, and others from around the world, creating new research opportunities for the future. "Putting words to the level of exhilaration we feel is difficult," says Doeppner. "Perhaps the best comparison is that of children exploring the world by playing in a sandbox. In our case, we get to explore the principles of the universe with the biggest laser in the world."

*—Anashe Bandari*

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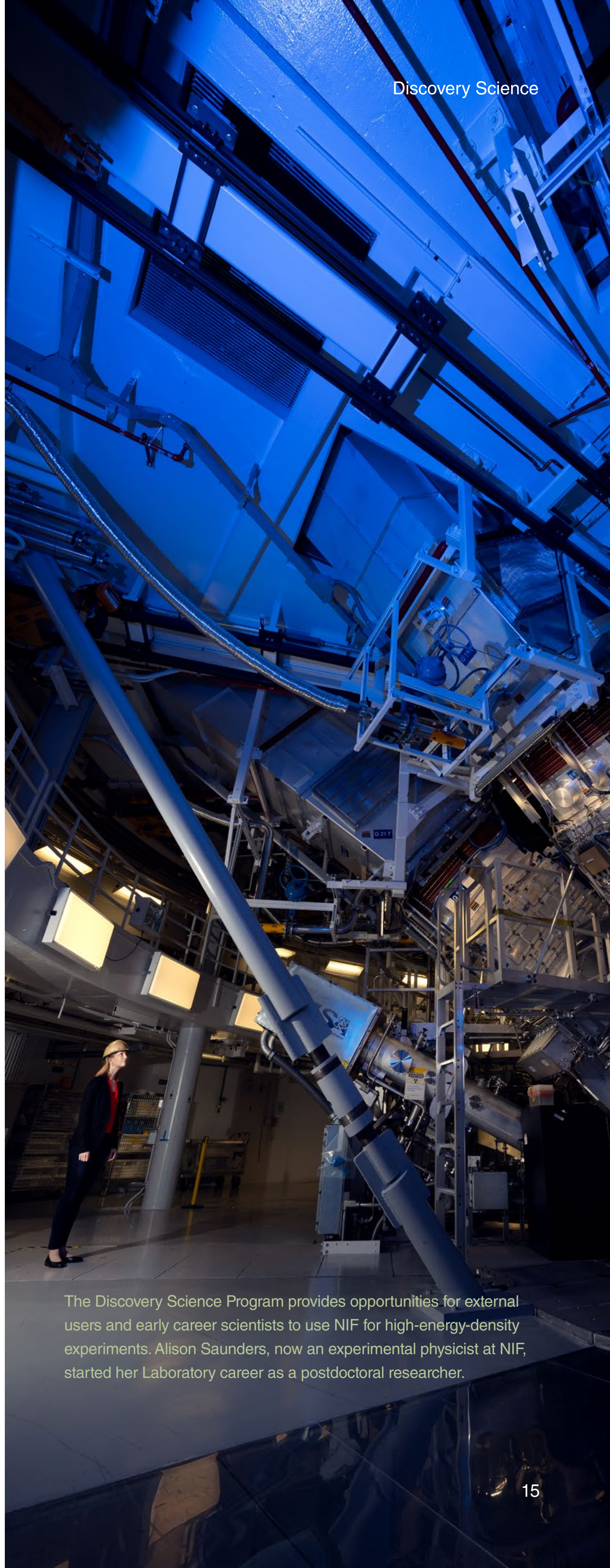


The Discovery Science Program provides opportunities for external users and early career scientists to use NIF for high-energy-density experiments. Alison Saunders, now an experimental physicist at NIF, started her Laboratory career as a postdoctoral researcher.

# Printing the Future of Fusion Targets

Postdoctoral researcher Widi Moestopo observes a 3D-printed, direct-drive inertial confinement fusion (ICF) target capsule connected to a fill tube, which injects ignition fuel. The target is printed with an ultrahigh-resolution technique called two-photon polymerization (2PP).

Inertial confinement fusion (ICF) target capsules are a key enabling component for the future of fusion energy. Energy gain through ICF requires target capsules with unimaginably smooth surfaces and ignition fuel suspended uniformly inside, making current target capsules at Lawrence Livermore National Laboratory's National Ignition Facility (NIF) an engineering miracle. However, fabricating and fielding these capsules is currently too difficult, costly, and time-consuming to advance future fusion technology such as an inertial fusion energy (IFE) power plant, which would require an estimated 800,000 capsules per day produced at less than $0.50 each.

Lawrence Livermore has begun exploring additive manufacturing (AM) as a potential path for mass producing ICF capsules faster, cheaper, and with previously impossible designs. A team of engineers, chemists, physicists, and technicians demonstrated the technology's potential by conducting the first four NIF experiments with fully 3D-printed ICF capsules. The capsules feature leak-tight walls just a few micrometers thick and an internal lining of extremely low-density foam that wicks up and suspends liquid fuel for ignition—all made possible through the flexibility and ultrahigh resolution of two-photon polymerization (2PP) printing. "For a power plant or a facility with a high-repetition shot rate, the traditional capsule fabrication approach probably isn't going to work," says staff scientist James Oakdale. "Although the 2PP materials aren't as perfect, our approach is potentially much faster because we can change parts on the fly, and we're not locked into a specific manufacturing process or design."

## Foams and Flexibility

The 2PP technique uses light to print features as small as 100 nanometers (nm)—1,000 times thinner than a human hair. The printer shines a laser on a liquid resin. Once the irradiated energy is high enough, the resin absorbs photons and its monomer molecules link together to "cure" into a solid polymer.

Other light-based AM techniques print by curing at the energy of one ultraviolet photon (wherever the light hits). 2PP cures at the energy of two infrared photons, which, statistically, can only happen over a small volume within a tightly focused beam, enabling high-resolution printing. "The beam is like a tiny laser pointer. Wherever it moves, the resin only polymerizes within that approximately 100-nanometer space," says Oakdale.

Capsules printed using 2PP can be ready in 24 hours and filled within minutes, making them potentially much easier to fabricate and field than traditional targets. The process may enable rapid prototyping as well. "This is an exciting new territory," says physicist Elijah Kemp, principal investigator on the first four experiments. "Having this level of control over properties is unheard of for capsule manufacturing."

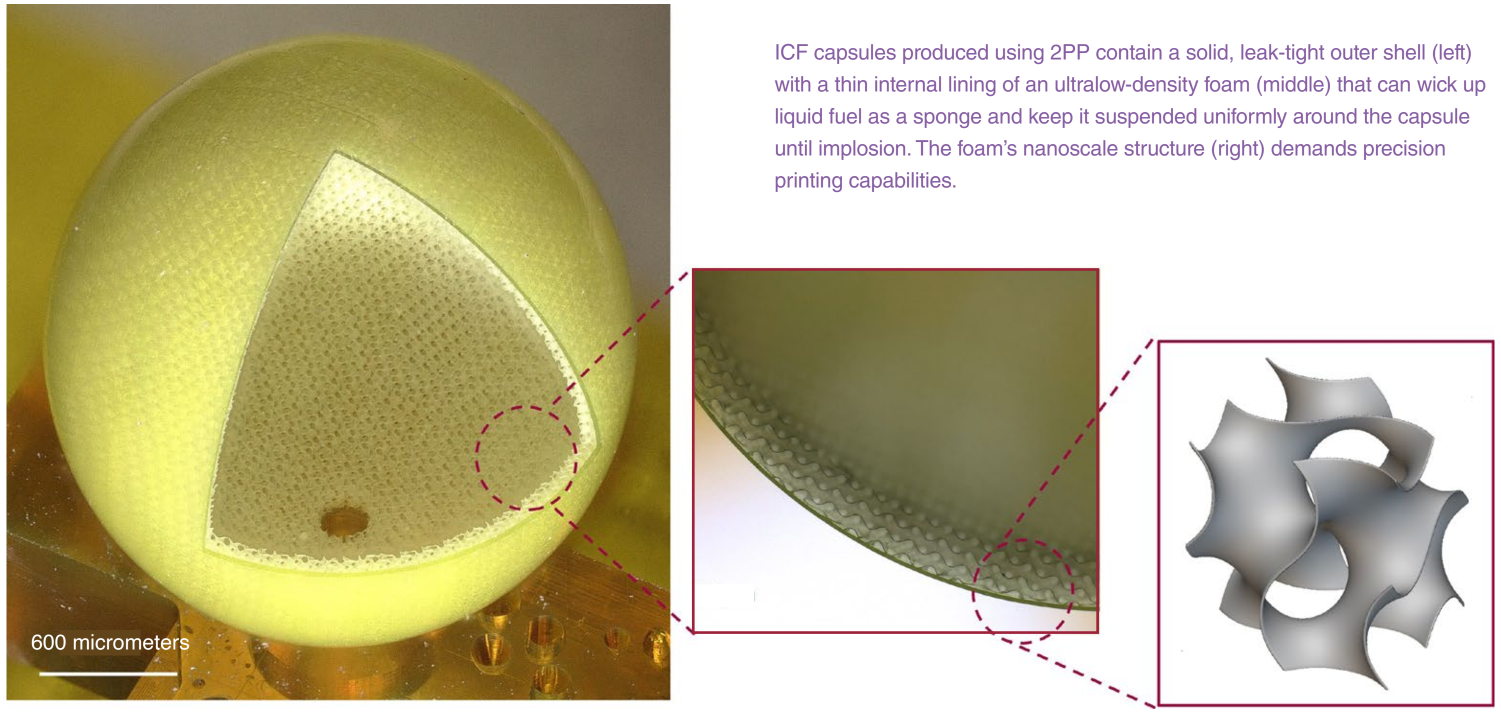
Kemp was an early champion of 2PP for printing ICF target capsules for direct-drive experiments, in which lasers hit targets directly (in contrast to indirect drive, with a hohlraum surrounding the target capsule). 2PP makes it possible to fabricate direct-drive concepts, which have unique design requirements that make them delicate and difficult to manufacture. "If we print a very thin shell with very low-density foam on the inside, these features support each other throughout the printing process so we can make the shell thinner and the density lower," says staff scientist Xiaoxing Xia. "ICF targets are the perfect application for 2PP because these small, intricate parts need the precision only this technology can provide."

The concept combines Oakdale's work printing 2PP capsules for non-ICF experiments at NIF with precisely placed features, such as voids or doped elements, with wetted foam capsule design. (See *S&TR*, October 2017, pp. 16–19.) Current high-yield ICF targets contain deuterium-tritium (DT) fuel vapor and a thin layer of solid DT ice that uniformly coats the inside surface, which is frozen manually in an arduous process that can take up to a week. Liquid fuel is just as effective and much easier to work with, but it needs to be uniformly suspended with a foam or other porous material.

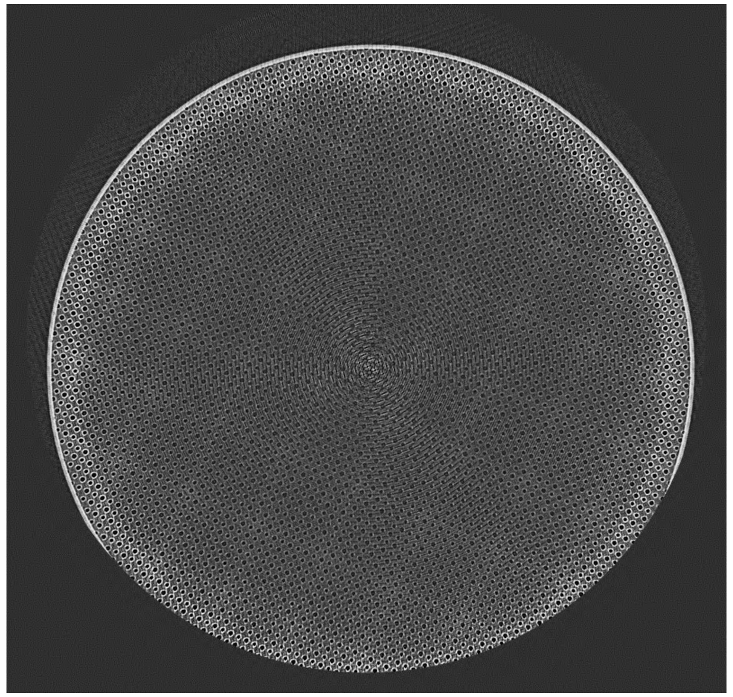
Since 2016, the Laboratory has made wetted foam capsules by chemically growing aerogels—ultralow-density foams with nm-sized pores—to address this challenge, as the lower the foam density, the less detrimental it will be to the implosion. "Simply reducing the amount of foam mass is probably the most important lever to improve fusion performance," says physicist Steve MacLaren. (See *S&TR*, January 2016, pp. 4–11.)

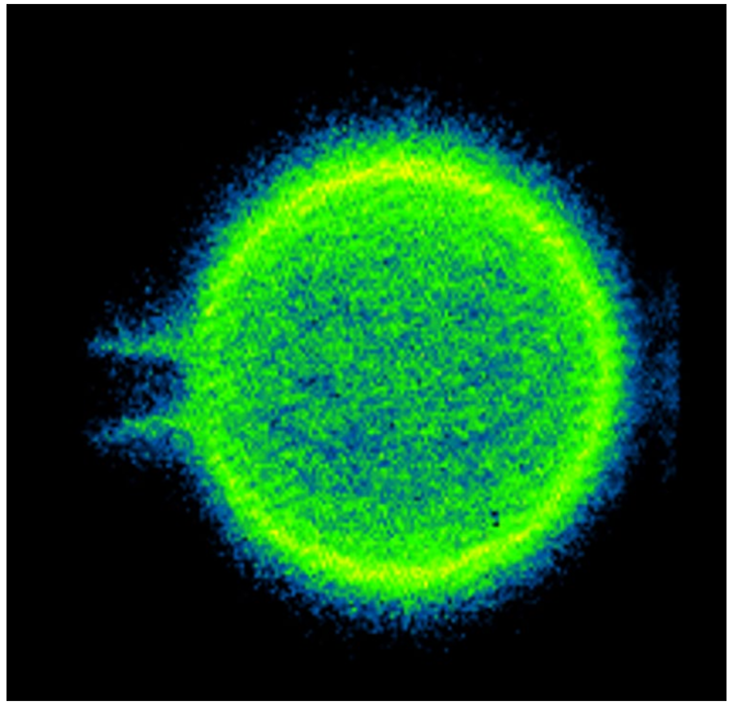
## Navigating a New Technology

The first 2PP target capsules fielded on NIF were both foam-lined capsules on direct-drive experiments performed in March and May 2024. The first target contained only fuel vapor, and the second contained only suspended liquid fuel. While the experiments were successful, fielding the unfamiliar target technology proved challenging and prompted innovation among the researchers, Livermore's Target Fabrication team (TFab) and



ICF capsules produced using 2PP contain a solid, leak-tight outer shell (left) with a thin internal lining of an ultralow-density foam (middle) that can wick up liquid fuel as a sponge and keep it suspended uniformly around the capsule until implosion. The foam's nanoscale structure (right) demands precision printing capabilities.





A commercial 2PP printer prints in small, square sections, shown at the micrometer scale, that are stiched together like patches of a quilt (top). This stitching is one of the major sources of defects in a 2PP capsule, and its artifacts can be seen on x-rays from a March 2024 shot (bottom).

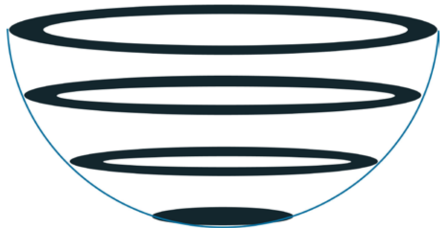
industry partner General Atomics. “Individually, 2PP and the printed wetted foam are different technology from other targets we’ve fielded at NIF, so using them both on the same experiment created novel situations for us,” says cryogenic process engineer Travis Briggs.

Commercial 2PP printers, such as TFab’s, print in small, square sections that are stitched together similar to patches of a quilt to form structures, but the stitching was a major source of capsule defects. “Stitching that is too big can cause instability and impact implosion,” says Abbas Nikroo, NIF’s deputy director for physics integration. Xia and Oakdale sought to improve capsule quality by designing a custom, dual-wavelength 2PP printer optimized for capsule fabrication. The printer’s motion stage—the path of the print head—moves in a ring shape, and a galvo scanner directs the beams in three dimensions so the stitching better complements the spherical shape of the capsules.

The printer also seeks to improve precision and design flexibility with a dual-wavelength printing (two-color) configuration. Oakdale says this configuration eases simultaneous printing of different features and compositions, such as using one color of light to print porous foam and another to print a solid shell, or adding doping elements to improve performance. “The two wavelengths give us spatial control over density of the material and chemical composition, which gives us more tools to respond to designs that physicists dream up,” he says. To complement the printer, Oakdale and colleagues Magi Yassa and Johanna Schwartz are developing a dual-wavelength photo resin. “We’re targeting a single formulation where we can turn on one wavelength and the material comes out nanoporous, and we can turn on the other wavelength and the material comes out solid,” says Oakdale. “That way, we could print the shell and inner foam all at once by turning the lasers on and off or choosing one laser over the other.”

TFab is instrumental in every NIF shot, but the team has been especially crucial for fielding 2PP target capsules. “One of the biggest challenges was delivering a leak-tight capsule that would retain the fuel,” said TFab engineer Montu Sharma, whose team solved the problem by improving the printed shell quality and adding a new target coating. Another obstacle was the “ice plug”—a tiny piece of ice that seals the fill tube to keep liquid fuel inside the capsule and prevent the foam layer from overfilling. The team addressed this challenge by developing a dual-heat switch target assembly that controls the temperatures of the capsule and fill tube independently so the ice plug forms farther away from the capsule.

TFab achieved a leak-tight, liquid-filled capsule in November 2024, giving the team the confidence to perform the first layered (with both a central $D_2$ vapor region and a liquid-wetted foam layer) direct-drive experiment in March 2025. “I’m proud of our flexibility and the work we’ve done so far to develop a process to fill the capsule and maintain that fill,” says Briggs.



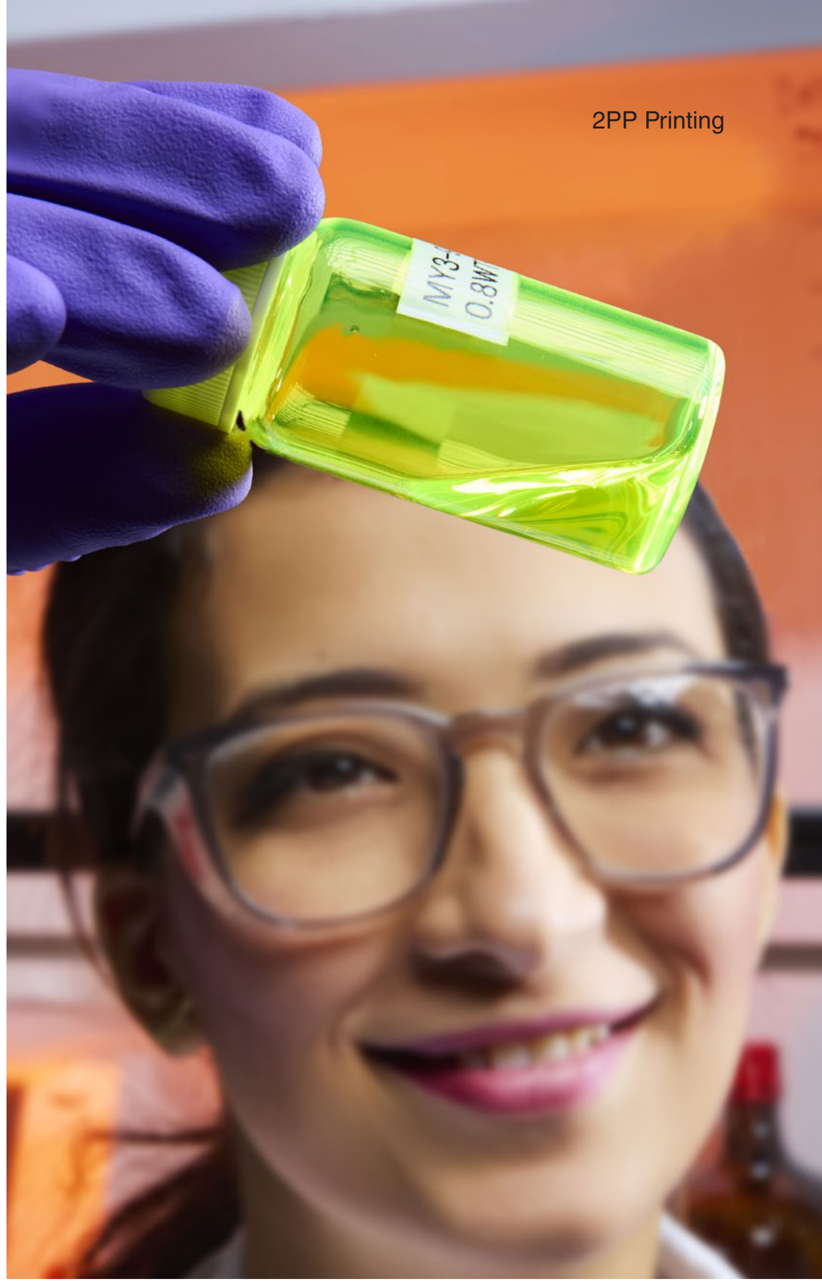
The team’s custom 2PP printer, optimized for capsule production, prints in circles to reduce the amount of stitching by better conforming to the capsule’s shape.

## Beginning a Journey

Targets printed with 2PP are promising, but they face a long road toward viability. Even the best printers cannot yet match the quality of traditional capsules or achieve the fabrication speed needed for an IFE plant. Xia’s team is working to improve production speed through parallelization—essentially an assembly line of print heads working simultaneously. One method they explored uses metalenses, a microfabricated chip with tiny nanostructured pillars that focus an ultrafast laser to create 100,000 focal spots in parallel. (See *S&TR*, April/May 2024, pp. 12–15.) With a metalens array, the team’s 2PP printer could print sample structures across a 3-centimeter wafer 1,000 times faster while retaining 100-nm resolution. Another project, inspired by colleagues from the Laboratory’s IFE STARFIRE initiative, explores scrolling lightsheet AM in which a photo resin moves past a series of parallel print heads on a conveyer belt.

Other potential options for rapid target fabrication at Livermore include microfluidics and volumetric AM, which prints objects all at once instead of layer by layer. With every approach, the challenge is finding the right balance of speed and precision. “This could be the way of the future, but we have to be conscious of the fact that ICF needs perfection, and we need time to achieve our goals for printed ICF targets,” says Nikroo.

All experimental data for ICF is difficult to come by, given the demands for shot time at NIF, but the team aims to use every chance it gets to learn as much as possible about the 2PP targets. MacLaren is leading a series of tests with 2PP wetted foam intended for capsules for indirect-drive ICF to measure the impact of four distinct foam geometries on implosion performance as his team prepares for proposed shots on NIF in 2026. “Our goal is to field an implosion with wetted foam that is nearly identical to ice-layered implosions except for the fuel layer,” says MacLaren. “This test gives us the chance to benchmark our models of a liquid layered indirect-drive implosion.”



Research scientist Magi Yassa holds a sample of the team’s dual-wavelength photo resin. The liquid monomer resin is being developed to solidify, or “cure,” in different ways when it absorbs different colors of light, enabling researchers to print both solid and porous features using the same material.

Accurate models can help researchers design around 2PP’s limitations or leverage its capabilities to design future targets with unprecedented performance. “In theory, 3D printing has the capability to optimize designs, so I’m interested in finding out how, given any configuration constraints, we can find a design solution that gives us the best result,” says Xia. He acknowledges that the team is on a long journey, but he remains optimistic. Says Xia, “A dedicated team required decades to even get close to fusion ignition, and going from ignition to an IFE power plant is another decades-long effort that will require a lot of work. But I feel good about Livermore’s team, and I’m very excited to be a part of it.”

—*Noah Pflueger-Peters*

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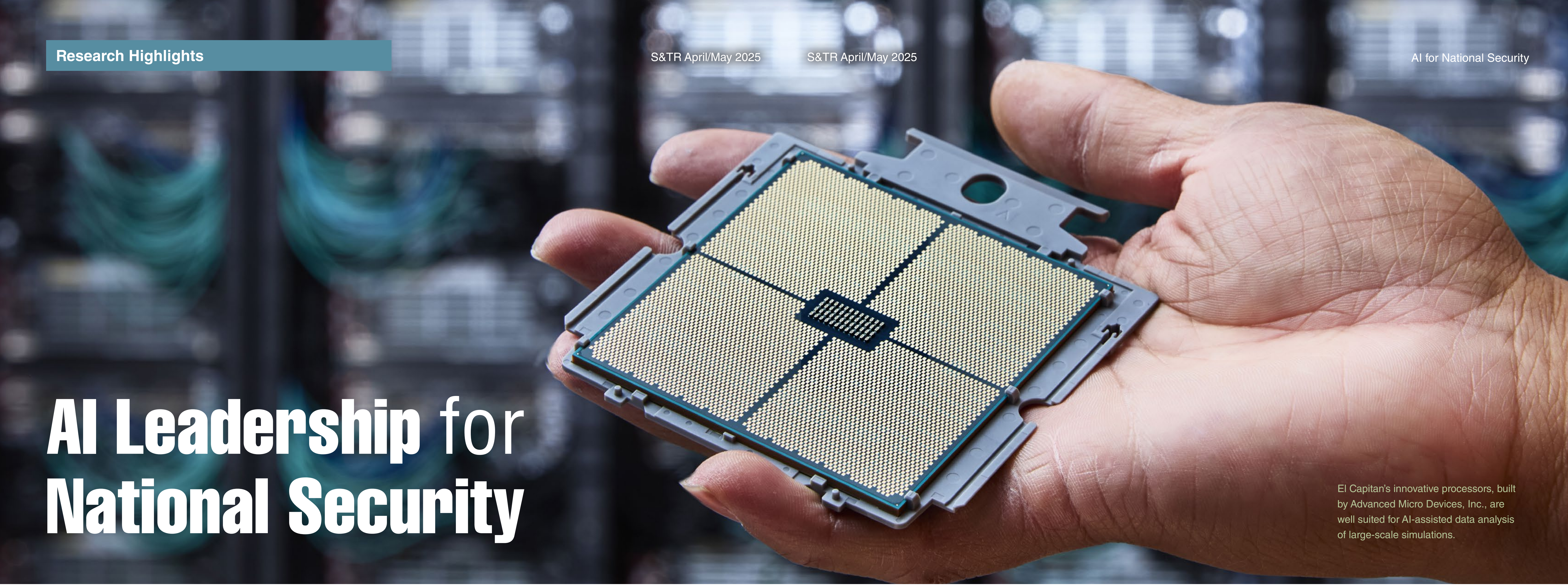


# AI Leadership for National Security

El Capitan's innovative processors, built by Advanced Micro Devices, Inc., are well suited for AI-assisted data analysis of large-scale simulations.

AI has become a turning point in the current technological era, a force not only transforming humans' daily lives but revolutionizing entire sectors. As the application of AI across industries accelerates the pace of development, so too must national security remain at the cutting edge, a task requiring extensive collaboration to deploy the nation's most critical resources.

"We're seeing AI penetrate all aspects of modern life—science, mathematics, literature, media—and the national security space is no exception," says Brian Giera, the director of Livermore's Data Science Institute (DSI). "Understanding the gap between what the rest of the world is working on informs the refinements we need to deploy in our space." Adds Brian Spears, the director of Livermore's AI Innovation Incubator (AI3) and Cognitive Simulation Institutional Initiative, "AI tools have become so powerful that they're transforming and accelerating the way science itself is done, and the entity that succeeds in capturing these technologies for scientific innovation first is likely to gain advantage for itself in a way that will not be overcome short of another scientific revolution." In pursuit of this advantage, Lawrence Livermore leads efforts to leverage AI through varied scientific research, diligent work with external stakeholders, and internal knowledge base development.

## Poised for Leadership

The national advancement of AI at a competitive pace requires strength in data, modeling, computational capabilities, and applications—the four pillars of AI for science. The Department of Energy (DOE) provides this strength through existing infrastructure and expertise, with Lawrence Livermore playing a critical role. "We already have diverse AI research and a portfolio in AI with many programmatic hooks. Some projects have used AI for over a decade," says Giera. "People at the Laboratory can definitely claim they worked on AI before AI was cool."

Livermore is a significant supporter of the first pillar: data. The Laboratory possesses around 1,000 trillion tokens of scientific data, approximately 100 times the amount of data that OpenAI used to train the GPT-4 large language model. According to Spears, no models in the world can understand such a high volume of data, making that data a key asset. Livermore stands as a leader in the second pillar—modeling—not only using million-line simulation codes to verify the predictions of AI models but also possessing an institutional understanding of scalable machine learning (ML) to take models to the large scales necessary for solving ever-complex national security problems. To manage and make sense of this data and to train and then run such resource-intensive models requires computational capabilities—the third pillar—on an even grander scale. In addition to El Capitan, the world's fastest supercomputer and the National Nuclear Security Administration's (NNSA's) first exascale computer, Livermore brings its entire computing enterprise to bear on national security missions. (See *S&TR*, December 2024, pp. 4–11.)

This core combination of data, modeling, and computational capabilities comes together in pursuit of applications, the fourth pillar of AI for science. According to Spears, national security efforts such as strategic deterrence, biodefense, manufacturing, and fusion science provide AI models with some of the most complicated reasoning tasks imaginable—tasks that enable models' continuous improvement. Cindy Gonzales, DSI's deputy director, says, "The computational heft that Livermore brings to the table is that we work in a context to support national security missions. We're generating models of the highest consequence alongside leading experts with the knowledge and expertise needed to create an effective system to defend our country." Adds Spears, "Offering this expertise to ourselves and to our private partners for a strategic U.S. ecosystem sets the north star toward which we build out all our capabilities."

## Discover, Design, Manufacture, Deploy

The complexity of high-consequence national security missions means that efforts to generate technological solutions for the nation's pertinent problems often unfold in stages. Aligning all its capabilities, Livermore applies AI for groundbreaking projects in every stage of the "Discover, Design, Manufacture, and Deploy" (DDMD) framework for national security science.

“Modern AI solutions are a way to accelerate the path from concept to solution in our strategic space,” says Spears.

For example, in the realm of discovery, the Laboratory’s Generative Unconstrained Intelligent Drug Engineering (GUIDE) program harnesses ML in its process for therapeutic development. Through AI-assisted supercomputing, the GUIDE platform narrows down vast amounts of antibody candidates to those most viable as defenses against an antigen. This approach significantly decreases the amount of experimental testing required and the time to discover a successful therapeutic. (See *S&TR*, September 2024, pp. 4–11.) The program has been applied in the fight against the spread of COVID-19 and offers potential for defense against other emerging biological threats.

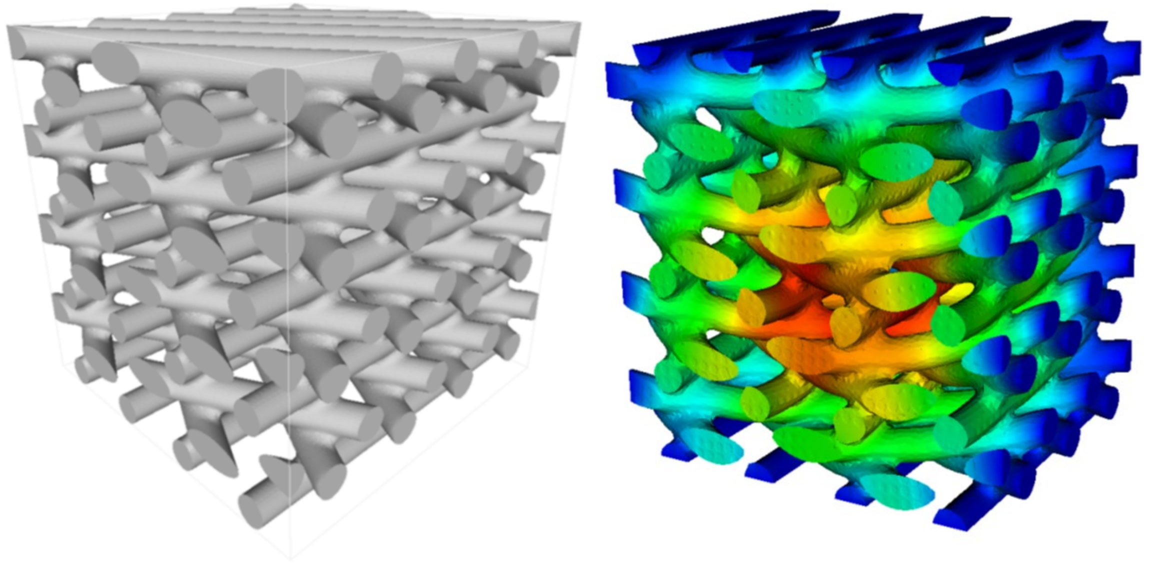
AI poses huge benefits to engineering and design, as evidenced by the Laboratory’s DarkStar Strategic Initiative. DarkStar investigates applications of AI in scientific problems of complex hydrodynamics, shockwave physics, and energetic materials. (See *S&TR*, October/November 2024, pp. 4–11.) A notable result was the creation of the AI-aided inverse design approach, which points researchers to the best engineering-based design solutions by working backward from the desired result: specifically controlled material dynamics. “Demonstrating that complex systems can be developed directly from a final state and the initial design resolved by satisfying several constraints simultaneously via AI and machine learning allowed us to make groundbreaking discoveries in the area of hydrodynamic instability,” says Jon Belof, DarkStar project lead.

AI can improve manufacturing efficiency and quality for national security-relevant projects. For example, the Scorpius accelerator, to be installed at the Nevada National Security Site, will enable the radiographic imaging of dynamic subcritical experiments with plutonium, simulating late stages of a nuclear implosion and providing data about the effects of aging and manufacturing methods on nuclear weapons. (See *S&TR*, April 2021, pp. 16–19, and March 2025, pp. 16–19.) AI and ML ensure high-quality images are produced as Livermore manufactures the accelerator’s eventual 984 pulsed-power cells, called line replaceable units (LRUs). The team uses AI to model the environment of the pulsers and optimize them to create clean waveforms on every pulse, despite differing conditions. Working in tandem with hardware testing, this model improves the manufacturing process and ensures that the hundreds of LRUs will work together to generate images effectively.

The centerpiece of the deployment stage at Livermore is its work on stockpile material aging and compatibility to certify the safety of assets deployed in the nuclear stockpile. Although “deploy” is the most recently applied capability at the Laboratory, future AI projects will capitalize on existing aging data and build better predictive models to identify the need for new materials, mitigate aging conditions, and more. In addition, digital twins—exact digital versions of physical parts with part-specific understanding—assist with deployment by tracing part behavior over time and providing further aging data.

## Wide-Reaching Efforts

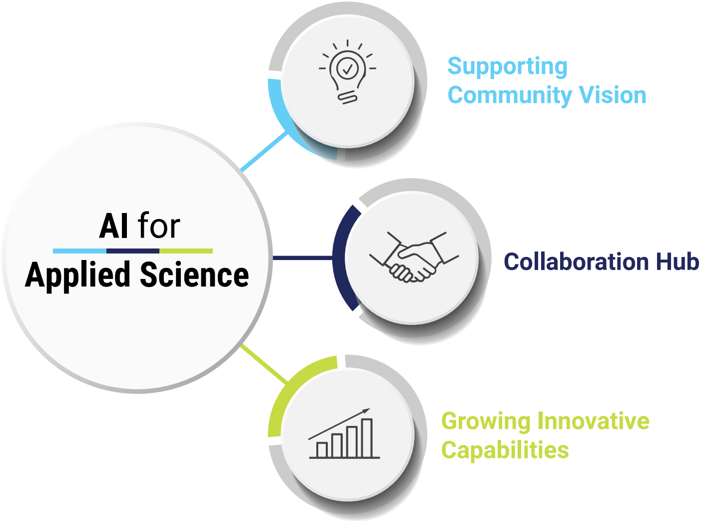
In addition to Livermore’s existing scientific applications of AI, external and internal efforts include engaging with partners and building a national AI program. DOE is working to secure funding for a nationwide AI initiative intended to accelerate national security missions and keep the U.S. competitive in the race to capture AI tools for science. With the potential for a multibillion-dollar investment in the three NNSA laboratories, the initiative would expand Livermore’s computing and personnel capabilities significantly in pursuit of this goal. “Sandia, Lawrence Livermore, and Los Alamos national laboratories have had a fantastic partnership over the last couple of years, and we’re all on the same page trying to advance a national AI initiative,” says Jason Pruet, the director of the AI Office Council at Los Alamos. “One dimension of AI’s importance in the national security space is its potential for enabling us to solve challenges we had not expected to be able to solve for generations.”



A digital twin can be compared to its physical counterpart, then the resulting data can be fed back into the manufacturing pipeline. In addition, digital twins can be used to simulate a part under different conditions. For example, a digital mesh of a woodpile structure printed by a direct-ink-writing machine (left) was simulated (right) when uncured and subjected to self-weight, providing a representation of its deformation and range of stresses (represented by different colors) under these conditions.

AI3 is another external vehicle for partnerships and conversations surrounding AI. Through relationships with companies providing each component of AI infrastructure—OpenAI for large models, Microsoft for applications of models to Laboratory-relevant workflows, NVIDIA as a producer of computing hardware, and Hewlett Packard Enterprise as an integrator for computers, for example—Livermore supports the scale-up of AI technologies that would not otherwise be possible. Such relationships provide value in both directions; the Laboratory remains in touch with future technologies that might help advance the national security mission, and other companies gain an understanding of the problems existing in the national security space that can make models better. “A transformational science technology is being driven at enormous scale outside the Laboratory,” says Spears. “Public–private partnerships are the central focus of AI3. We must understand and steer what’s going on outside Lawrence Livermore. We also must be able to pick up those capabilities and pull them inside for our Laboratory missions.”

Complementary to AI3, DSI contributes to both internal and external efforts surrounding AI. Externally, DSI fosters partnerships with academic institutions through programs such as the Data Science Summer Institute and, for the University of California system specifically, the Data Science Challenge, each designed to engage students in solving challenging, real-world data science and AI problems and to build an informed workforce pipeline. Livermore and DSI also have a rich partnership with Case Western Reserve University through an NNSA-funded Center of Excellence. “The Center is a type of academic open space to which we bring partners from all over the NNSA complex and help them learn materials data science,” says Giera. “They’re experts at looking at materials data, the nuances associated with that, and deploying AI or machine learning in those spaces.” Internally, DSI contributes to Livermore’s workforce development and AI Community of Practice—an umbrella organization encompassing AI at the Laboratory—through its consulting service, seminar series, staff training program, and variety of workshops.



Public–private partnerships are a key element of the Laboratory’s AI Innovation Incubator, which communicates a vision for activities to grow external collaboration and internal AI capabilities.

Other internal efforts aligned with the AI Community of Practice are designed to prepare the entire Laboratory workforce to use AI for the benefit of national security. aiEDGE (AI Education for Development, Growth, and Excellence) encourages Laboratory staff to use AI tools, lowering the barrier to entry through accessible training modules, seminars, sample prompts, and shared success stories. LivChat, an internal AI tool similar to ChatGPT, further encourages employee participation. Greg Herweg, chief technology officer for the LivIT (Livermore Information Technology) program, says, “We have high hopes that, from a day-to-day productivity perspective, AI will help employees deliver more, whether they have a scientific role or an operational role. If we’re more productive, then we’re going to be more competitive with other enterprises.”

In a near future in which AI is an inevitable element of emerging technologies for national security, Livermore’s efforts position the Laboratory, DOE, and the nation at the leading edge. “AI is proliferating more rapidly than anything we’ve seen previously, and we’re at an inflection point as a global society in how we embrace or don’t embrace it,” says Gonzales. “Being in the AI and machine-learning fields and tackling some of the nation’s and the world’s hardest problems is exciting.” Adds Spears, “I’ve used these models, and I’ve seen what we can achieve that we’ve not been able to do before. That level of capability in the hands of a hundred or a thousand people, or shared with 20 or 30 thousand DOE scientists, means that we’re going to do transformational things.”

*—Lilly Ackerman*

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## Patents

*In this section, we list recent patents issued to 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 eight-digit number in the search box at the U.S. Patent and Trademark Office's website (uspto.gov).*

**System and Method for Multi-Channel Pyrometer Allowing Non-Contact Temperature Measurements Down to 800K on the Microsecond Scale**
**Jeffrey Montgomery, Magnus Lipp**
U.S. Patent 11,933,675 B2
March 19, 2024

**System with Liquid and Solid Media for Target Binding**
**Jane P. Bearinger**
U.S. Patent 11,933,782 B2
March 19, 2024

**Ultralight Conductive Metallic Aerogels**
**Fang Qian, Thomas Han, Marcus Worsley**
U.S. Patent 11,938,545 B2
March 26, 2024

**Separation and Conversion of Carbon Dioxide to Syngas Using a Porous Ceramic Dual Membrane in a Thermo-Electrochemical Reactor**
**Patrick Campbell, Maira Ceron Hernandez, Jeremy Taylor Feaster, Sneha Anil Akhade**
U.S. Patent 11,939,686 B2
March 26, 2024

**Engineered Current-Density Profile Diode Laser**
**Paul O. Leisher, Robert J. Deri, Susant K. Patra**
U.S. Patent 11,942,759 B2
March 26, 2024

**High-Power Electrically Tunable Switch**
**Lars F. Voss, Adam M. Conway, John E. Heebner**
U.S. Patent 11,942,760 B2
March 26, 2024

**Additively Manufacturing Bio-Based Conductive Shape Memory Polymer Macrostructure Parts with Highly Ordered Microstructures**
**Jennifer Nicole Rodriguez, Eric B. Duoss, James Lewicki, Christopher Spadaccini, Thomas S. Wilson, Cheng Zhu**
U.S. Patent 11,945,151 B2
April 2, 2024

**Massively Parallel Hierarchical Control System and Method**
**Robert Matthew Panas**
U.S. Patent 11,947,470 B2
April 2, 2024

**Event Detection Unit**
**James Vincent Candy, Karl Albert Fisher, Christopher Roland Candy**
U.S. Patent 11,948,438 B2
April 2, 2024

**Mechanical Reticulation of Polymeric-Based Closed Cell Foams**
**Jennifer N. Rodriguez, Duncan J. Maitland, Thomas S. Wilson**
U.S. Patent 11,958,220 B2
April 16, 2024

**Post Polymerization Cure Shape Memory Polymers**
**Thomas S. Wilson, Michael Keith Hearon, Jane P. Bearinger**
U.S. Patent 11,958,932 B2
April 16, 2024

**Dilute Alloy Catalysts for Electrochemical $CO_2$ Reduction**
**Juergen Biener, Sneha Akhade, Monika Biener, Zhen Qi, Joel Varley, Stephen Weitzner, Vedasri Vedharathinam**
U.S. Patent 11,959,183 B2
April 26, 2024

**System and Method for Thermal Emission Control Using Segmented Array**
**Robert Matthew Panas, Cynthia Dawn Walker Panas, Robert McHenry**
U.S. Patent 11,971,225 B2
April 30, 2024

**Multi-Channel Optical Detection System and Method for Multi-Chamber Assays**
**Lawrence C. Dugan, William J. Benett, Elizabeth K. Wheeler**
U.S. Patent 11,975,321 B2
May 7, 2024

**Products Having Sheets of 2D Materials and Related Inks for Direct Ink Writing**
**Swetha Chandrasekaran, Marcus A. Worsley**
U.S. Patent 11,976,200 B2
May 7, 2024

**Methods of Detecting Predators in Algal Cultures**
**Carolyn Laura Fisher, Todd Lane, Kristen Leigh Reese, Matthias Frank**
U.S. Patent 11,977,060 B2
May 7, 2024

**Aluminum-Cerium-Nickel Alloys for Additive Manufacturing**
**Ryan R. Dehoff, Hunter B. Henderson, Scott McCall, Richard Michi, Peeyush Nandwana, Ryan Ott, Alexander J. Plotkowski, Orlando Rios, Amit Shyam, Zachary C. Sims, Kevin D. Sisco, David Weiss, Ying Yang**
U.S. Patent 11,986,904 B2
May 21, 2024

**Cell-Free Protein Synthesis Systems**
**Nicholas N. Watkins, Neil Reginald Beer, Kenneth W. Turteltaub**
U.S. Patent 11,987,830 B2
May 21, 2024

**System and Method for Adaptable LIDAR Imaging**
**Robert Matthew Panas, Phillip Harris Paul**
U.S. Patent 11,988,748 B2
May 21, 2024

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## Abstract

### Strengthening the Power Grid to Weather the Elements

A Strategic Initiative completed through Lawrence Livermore's Laboratory Directed Research and Development Program aimed to inform a more reliable and resilient national power grid. Using California as its test case, due to the state's range of energy resources, geophysical features, weather patterns, and evolving energy needs, the project team identified and integrated data sources to develop and optimize a model that identifies the most cost-effective set of power grid infrastructure investments to meet current and future power requirements given likely weather conditions. Ultimately, the model may be adapted to any region by adjusting data related to energy consumption, weather risks, available transmission infrastructure, and emerging energy technologies.

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# R&D 100 Award Winners

Lawrence Livermore's three 2024 R&D 100 Award–winning technologies offer paths to greater innovation and commercialization in laser optics and computing applications.

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- *New advances in laser pulse shaping technology enable Livermore to better understand high-energy-density experimental regimes.*
- *Livermore researchers are 3D printing liquid crystal elastomers that change shape and respond to external stimuli such as temperature, light, and electrical fields.*
- *The Laboratory celebrates 30 years of* Science & Technology Review.

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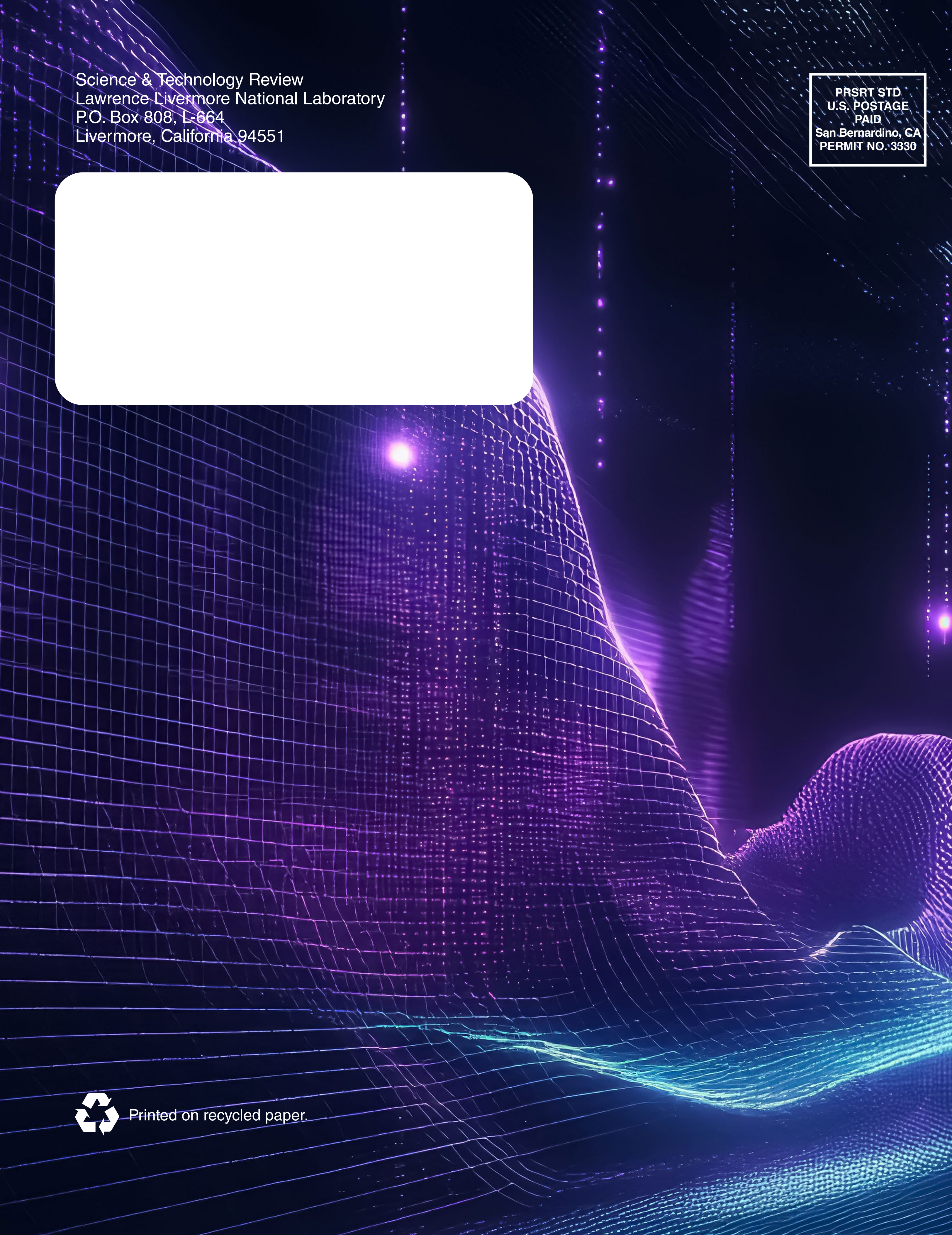

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