

# SCIENCE AND TECHNOLOGY

Expanding the boundaries of scientific knowledge and advancing the technological state of the art to solve problems of national and global importance

**THROUGH** its science and technology capabilities, Livermore makes fundamental discoveries about nature, develops innovative technologies that improve life and drive the economy, and carries out its mission to improve national security.

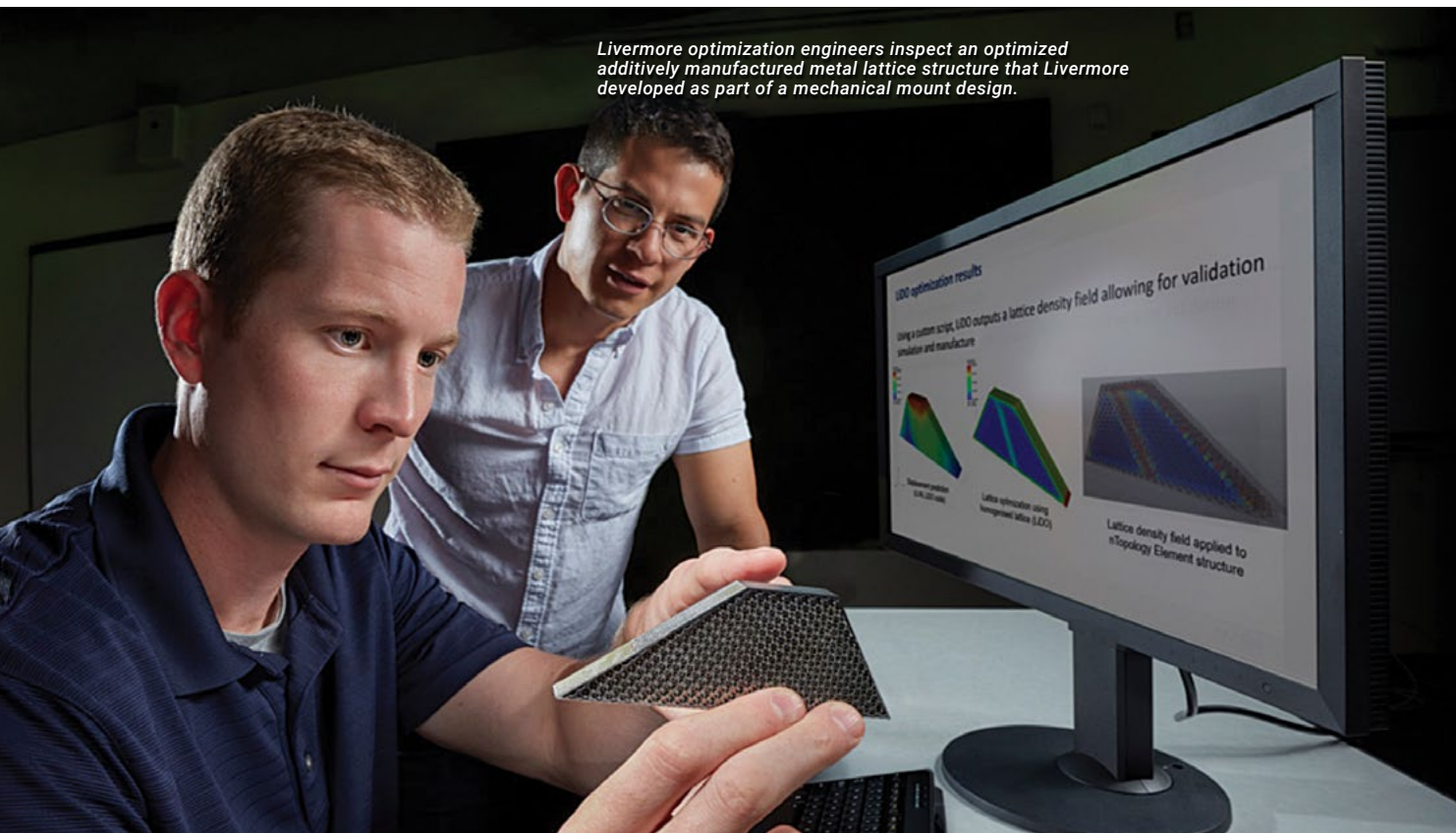
## HARNESSING THE POWER OF AI

On December 5, 2025, DOE formally announced the launch of the Genesis Mission, a national initiative led by the Department and its 17 national laboratories to accelerate discovery, strengthen national security, and drive energy innovation. The mission is led by the Office of Science in partnership with NNSA. LLNL has much to contribute, as it has been exploring use of generative AI and advanced machine learning (ML) to make transformative breakthroughs with mission-critical applications. The overarching goals of expedited scientific discovery and rapid design-to-product-delivery to meet mission needs have resulted in key advances, some of which are described throughout the *Annual*

*Report*. Two particularly important mission applications for NNSA and LLNL are rapid, optimized design for product manufacturing and discovery of next-generation materials.

Additive manufacturing (AM) offers researchers unprecedented flexibility to print structures with shapes and properties that do not readily exist in nature and with previously impossible microscopic features (see pp. 16-17). Simultaneously, AM poses a design challenge because the many available material layouts necessitate considering billions of design possibilities. Computational design optimization can resolve extremely large and complex design problems that cannot be solved by intuition or trial and error. Two complementary codes—Livermore Design Optimization (LiDO) and Smith—automate the most challenging parts of the design process. Using LiDO, researchers can directly pose optimization problems and automatically generate designs that might not be intuitive. Smith can examine the design

Livermore optimization engineers inspect an optimized additively manufactured metal lattice structure that Livermore developed as part of a mechanical mount design.



An engineering intern monitors the Autonomous Alloy Prediction and Experimentation platform, which was developed to accelerate the alloy-discovery process by leveraging robotics and machine learning to design, build, and test samples without human intervention.

and determine performance gradients with respect to the design variables, which enables researchers to evaluate how changes affect performance and iterate LiDO for further improvement.

As for the discovery of new materials, a Livermore research team developed the Materials Acceleration Platform (MAP), a design framework to computationally determine optimal alloy compositions and associated AM process parameters to meet material performance targets. Specially tuned materials are needed for applications such as hypersonics, nuclear weapons, and fusion energy. Ensuring that a brand-new alloy exhibits desired properties is a challenge that was addressed through ML. For example, when designing a new alloy, selecting 10 elements from the periodic table to serve as the materials palette yields 1,023 possible systems with different combinations of those elements. As the team identified promising alloy candidates using MAP, it produced them in the laboratory and used a host of characterization instruments to evaluate material properties. Other Laboratory researchers have developed the Autonomous Alloy Prediction and Experimentation platform, which uses MAP to accelerate the alloy-discovery process by leveraging robotics and ML to design, build, and test samples without human intervention.

## RUBIN OBSERVATORY FIRST IMAGES

On June 23, 2025, Laboratory scientists celebrated the release of the first images taken at the Vera C. Rubin Observatory in northern Chile. Funded by DOE and the National Science Foundation, the

observatory features an 8.4-meter diameter three-mirror telescope and a 3.2-billion pixel camera that gathers 15 terabytes of data each night. LLNL has been involved in the design and development of the telescope and camera system from the earliest stages of the project, at first making pivotal contributions to the design of the telescope. LLNL researchers designed the major optical assemblies and built large lenses for the telescope's Legacy Survey of Space and Time (LSST) camera system, which weighs more than 3 tons. LSST will photograph the entire visible sky frame-by-frame every few nights, creating a time-lapse "movie" of the sky at unprecedented resolution. For Laboratory researchers and colleagues,

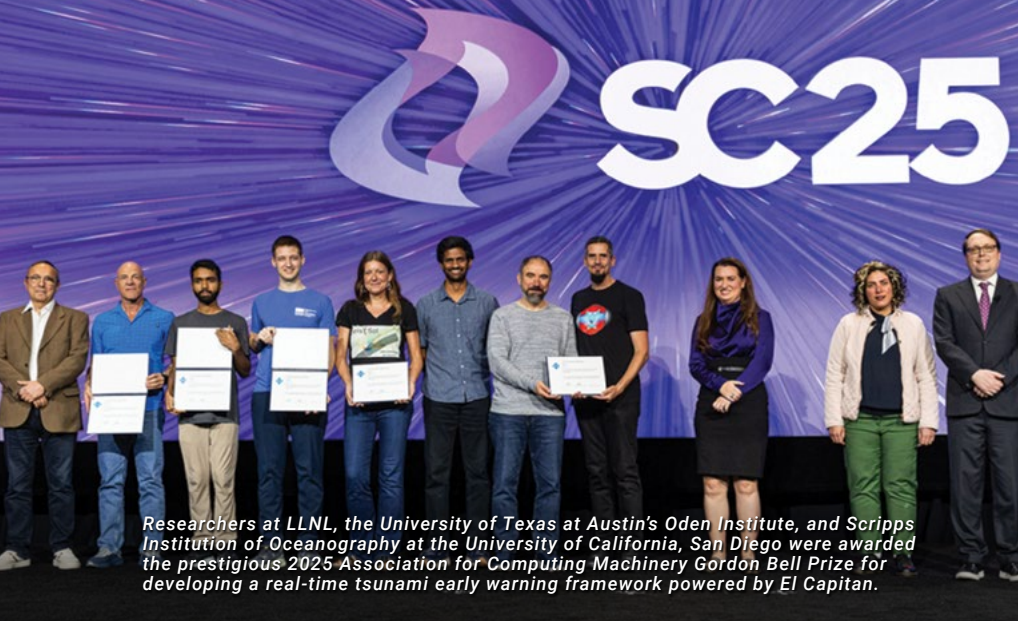


LLNL optical engineers work on an LSST camera lens. The Laboratory designed three lenses and six filters for the world's largest camera.

data analyses are beginning. They are challenged to discover the nature of dark matter and dark energy by sifting through the 60 petabytes ( $10^{15}$  bytes) of data that will be collected over the planned 10-year survey.

## DENOVO AND ANTIBODY DESIGN

LLNL is working to transform medical countermeasure development and biologics discovery through pioneering work aimed at revolutionizing the design of antibodies through the power of AI. The project is part of an interagency agreement between the Advanced Research Projects Agency for Health and DOE. Under the three-year DeNOVO project, LLNL and partnering institutions will apply high-performance computing and AI to overcome significant challenges in antibody design, including the sparseness of publicly available datasets and the substantial computing resources required for training predictive models. DeNOVO will develop experimental methods for ultrahigh-throughput antibody characterization to enable computational prediction and, ultimately, generative design of antibody-antigen interactions. The initiative leverages LLNL's exceptional computational capabilities and interdisciplinary collaboration with world-class research partners. The team, including the University of California, San Francisco; the Institute for Protein Design at the



Researchers at LLNL, the University of Texas at Austin's Oden Institute, and Scripps Institution of Oceanography at the University of California, San Diego were awarded the prestigious 2025 Association for Computing Machinery Gordon Bell Prize for developing a real-time tsunami early warning framework powered by El Capitan.

tsunami forecasting. El Capitan solved a billion-parameter Bayesian inverse problem in less than 0.2 seconds, accurately predicting tsunami wave heights at an astounding 10-billion-fold speedup over existing methods. The forecasting tool can be run on much smaller systems for early warning and emergency response.

Another Gordon Bell Prize finalist team used El Capitan to perform the largest fluid dynamics simulation ever—surpassing one quadrillion degrees of freedom in a single fluid dynamics problem. The simulation modeled the turbulent exhaust flow generated by many rocket engines fired simultaneously. Space launch vehicles are being designed to rely on arrays of compact, high-thrust engines, and designers need to understand the flow of the hot gases. Yet another team of researchers produced high-quality 3D structure predictions for more than 41 million proteins at a scale and speed previously thought impossible. For unclassified research projects, Tuolumne, which shares the same system architecture as El Capitan at one-tenth the scale, is helping NNSA scientists make inroads in broad research areas from energy security to particle physics. For example, researchers involved in the Laboratory's highly successful Computing Grand Challenge Program, which celebrated its twentieth year in FY 2025, will have a factor ten more capability in FY 2026 to solve higher fidelity, higher resolution simulations much faster than previously achievable.

### DESIGNER MATERIALS WITH POTENTIAL

The accelerated pace of innovation in materials science and use of AM are leading to breakthroughs in materials design, fabrication, and utility. Livermore researchers and their collaborators have

microbial vitality or mortality and affect carbon and nutrient transport. To further these studies of the soil microbiome and other related projects, LLNL is constructing a new Organic Matter Research Laboratory.

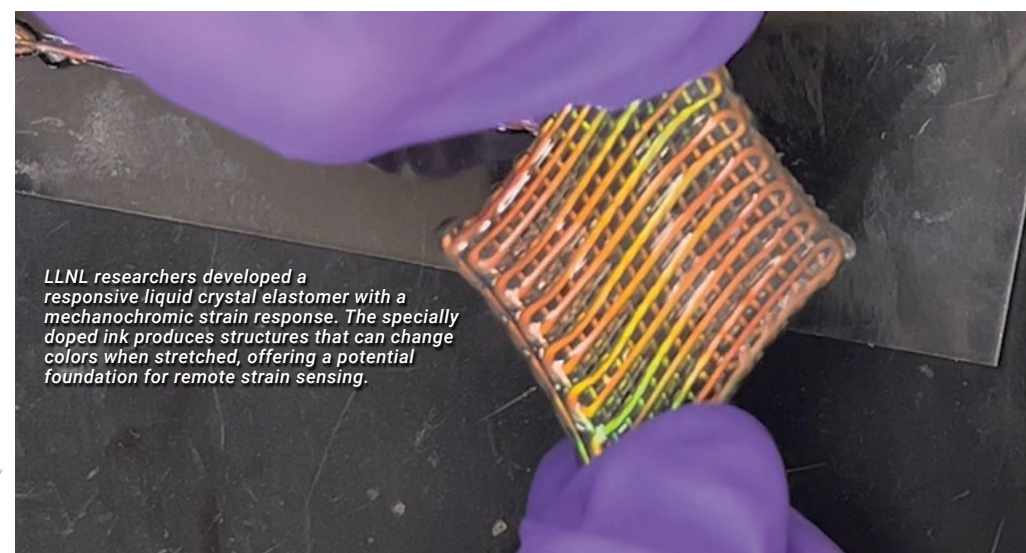
### TRANSFORMATIVE SIMULATION CAPABILITY

Livermore's El Capitan supercomputer demonstrated its versatility and unprecedented capability before transitioning to classified work in March 2024 (see p. 6). Researchers challenged the machine with outsized unclassified scientific problems. A tsunami forecasting demonstration won the coveted Association for Computing Machinery's 2025 Gordon Bell Prize. Livermore researchers and collaborators leveraged the system's full computing power to run physics-based simulations of extreme-scale, acoustic-gravity wave propagation in the ocean. This one-time, offline precomputation produced an extensive dataset—mapping ocean-floor motion and seafloor sensor data to resulting tsunami waves. The dataset underpins the team's newly developed "digital twin" framework for real-time

University of Washington; Los Alamos National Laboratory; and A-Alpha Bio, will collect training data, validate model predictions, and develop new methods for data generation.

### UNDERSTANDING THE SOIL MICROBIOME

Soils, which hold more organic carbon than the atmosphere and terrestrial biosphere combined, comprise the most biologically complex systems on Earth. Agriculture depends on their health, yet soil systems are poorly understood. As part of a multi-institutional effort funded by the DOE Biological and Environmental Research Genomic Science program, LLNL researchers are studying how microbial ecophysiology, population dynamics, and microbe–mineral–organic matter interactions regulate the persistence of microbial residues in soil as moisture levels fluctuate. This year, the team was awarded additional DOE funding to continue this important work through 2029. They are using isotopic tracing and imaging techniques, such as quantitative stable isotope probing and secondary ion mass spectrometry, along with multivariate 'omics data (DNA, RNA, proteins, and metabolites) to build a detailed picture of how plant carbon moves through soil microbes during life, growth, and death under different moisture conditions. Through such analyses, combined with computational models, the team aims to determine which microbial traits and functions, influenced by environment, are most responsible for carbon persistence and release. Results have already provided insight into the role of viruses in soil carbon and nutrient cycling, showing how viral infections strongly influence



LLNL researchers developed a responsive liquid crystal elastomer with a mechanochromic strain response. The specially doped ink produces structures that can change colors when stretched, offering a potential foundation for remote strain sensing.



LLNL researchers perform analyses in the laboratory where samples retrieved from the asteroid Benu were prepared and analyzed. A suite of mass spectrometers provided the concentrations of most elements in the periodic table. From there, the team has been separating the sample by element and analyzing isotope ratios of selected elements.

created a new class of programmable soft materials using a special extrusion-based 3D printing process that carefully aligns the molecular structure of liquid crystal elastomers (LCEs) into lattice structures with customizable properties. Remarkably, these structures can be designed to stiffen, soften, or deform, depending on their architecture and external stimuli. In tests, the shape-shifting structures exhibited the desired performance. They were soft and flexible under slow compression, but when impacted at high velocities, they absorbed up to 18 times more energy than similar silicone-based lattices yet remained intact. Computer simulations also helped optimize specially-designed LCE lattice structures that are able to directionally shrink and expand when temperatures rise, and to bend and rebound rather than fracture when impacted forcefully. The adaptability of LCE lattices makes them uniquely suited for demanding environments, including in applications such as protective gear, aerospace, and shape-morphing robotic systems. Previously, team members also demonstrated the ability to 3D print cholesteric LCEs, which change color in response to stress, to produce a strain-stimulated material for remote detection sensors.

In other work, LLNL researchers are developing new formulations for 3D printing, including a two-part "fast cure" silicone-based ink for building larger, taller, thinner, and more porous silicone structures than were previously possible. The method uses a process called inline

mixing, wherein the ink catalyst and crosslinker (a substance that chemically joins molecules together) are kept separated until just before extrusion, after which the ink sets rapidly at room temperature. This innovation allows for longer print times and the fabrication of intricate designs, such as tall overhangs and highly porous lattices, which were unattainable with conventional methods.

### JUPITER LASER FACILITY

Since the grand reopening of Livermore's Jupiter Laser Facility (JLF) in 2024, research teams have been busily engaged in exploring challenges and advancing key objectives in high-energy-density, fusion energy, and laser science. As an intermediate-scale, institutional laser facility and one of the founding members of LaserNetUS—a network of high-intensity laser systems at national laboratories and universities across the United States—JLF is providing the greater scientific community with a remarkable capability for testing new technical and experimental platforms, such as Livermore's Big Aperture Thulium laser (see p. 19) and STILETTO (Space-Time Induced Linearly Encoded Transcription for Temporal Optimization) optical device. STILETTO is a time-resolved, x-ray imaging and spectroscopy diagnostic designed to capture x-ray images or spectra with very fine time resolution. JLF is serving as a test bed for the device, which can fine-tune laser pulse profiles relevant to the experimental regimes of inertial confinement fusion and

high-energy-density physics discovery. STILETTO is primarily fielded on JLF's Janus and Titan systems, which provide the laser conditions and experimental geometries needed to generate and diagnose the relevant x-ray sources. Work at JLF is key to optimizing the device for future development at larger facilities, such as the National Ignition Facility.

### REVEALING SECRETS OF THE SOLAR SYSTEM

As one of a select group of institutions capable of housing, handling, and analyzing extraterrestrial materials, Livermore cosmochemists had the unique opportunity to characterize pristine samples from the Benu asteroid. The material was extracted directly from the massive object by NASA's Origins, Spectral Interpretation, Resource Identification, and Security—Regolith Explorer (OSIRIS-Rex) spacecraft in 2023. The team carefully prepared the sample for testing and used a suite of mass spectrometers to precisely determine its elemental composition and the isotopic ratios of several identified elements. The sample's confirmed composition—a combination of water, ammonia, and other volatile compounds—indicates that the asteroid is likely a remnant of a body that formed in the outer solar system. Isotopic data also provided evidence for a third possible primordial reservoir from which meteorites may originate. Research in this area is key to understanding the early solar system, its evolution, and planetary formation.