## LAB AT A GLANCE

# LAWRENCE LIVERMORE NATIONAL LABORATORY

Science and technology on a mission is the hallmark of Lawrence Livermore National Laboratory (LLNL). In service to the Department of Energy/National Nuclear Security Administration and other federal agencies, LLNL develops and applies world-class science and technology (S&T) to ensure the safety, security, and reliability of the nation's nuclear deterrent. LLNL also applies S&T to confront dangers ranging from nuclear proliferation and terrorism to energy shortages and climate change that threaten national security and global stability.

As a national security laboratory, LLNL harnesses operational excellence and strategic partnerships to meet its mission and applies the talents of our multidisciplinary staff, premier facilities, and core competencies to the nation's pressing issues. Through strategic support of S&T, LLNL translates innovations into national security and global stability.

#### **FACTS**

■ Location: Livermore, California

■ Type: Multidisciplinary national security laboratory

■ Year Founded: 1952

■ Director: Kimberly S. Budil

■ Contractor: Lawrence Livermore National Security, LLC (LLNS)

■ Responsible Site Office: Livermore Field Office

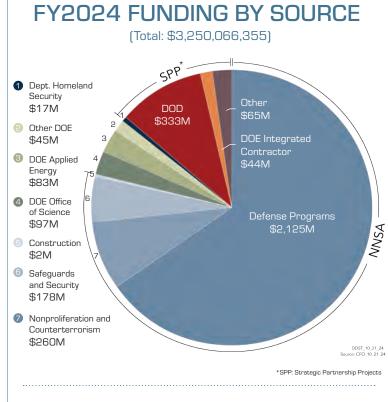
■ Website: www.llnl.gov

#### **CORE COMPETENCIES**

- Advanced Materials and Manufacturing
- Bioscience and Bioengineering
- Earth and Atmospheric Sciences
- High-Energy-Density Science
- High-Performance Computing, Simulation, and Data Science
- Lasers and Optical Science and Technology
- Nuclear, Chemical, and Isotopic Science and Technology

#### MISSION-SPECIFIC FACILITIES

- Advanced Manufacturing Laboratory
- Center for Micro-and Nanotechnology
- Center for Accelerator Mass Spectrometry
- Contained Firing Facility
- Electron Beam Ion Trap
- Forensic Science Center
- High Explosives Applications Facility
- Livermore Computing
- Polymer Enclave
- National Atmospheric Release Advisory Center
- National Ignition Facility
- Select Agent Center



### FY2024 COSTS

- FY24 LLNL operating costs: \$3.52 billion
- FY24 DOE/NNSA costs (includes DOE/IC): \$3.1 billion
- FY24 SPP costs (excludes DHS and DOE/IC): \$442 million
- FY24 SPP as a % of operating costs: 12.6%
- FY24 DHS costs: \$24 million

## PHYSICAL ASSETS (FY24)

- 7,617 acres (DOE owned) and 511 buildings/trailers
- 6.7 million GSF\* in operational buildings
- 52 non-operational buildings/trailers with 0.59 million GSF
- 45,706 GSF leased
- Replacement plant value: \$32.8 billion

## **HUMAN CAPITAL (FY24)**

- 9,563 LLNL employees, including:
  - 11 joint faculty
  - 311 postdoctoral researchers
  - 133 undergraduate interns
  - 172 graduate students
- 473 contractors (non-LLNS employees)



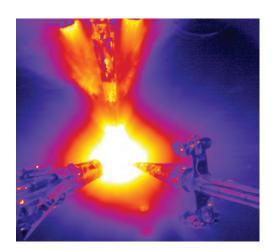
## LABORATORY HIGHLIGHTS



#### **UNIQUE FACILITIES**

#### One of the World's Premier High-Performance Computing Facilities

Lawrence Livermore is home to Livermore Computing (LC), a premier high-performance computing facility. LC boasts more than 3.28 exaflops of peak computing power and numerous TOP500 systems, including the #1-ranked, 2.79-exaflop El Capitan system, the 294+-petaflop Tuolumne system, and the 125-petaflop Sierra system. These flagship supercomputers are GPU-enabled and produce multiphysics simulations in 3D at never-before-seen resolutions for a variety of mission-critical needs. LLNL is also working with industry partners, including Cerebras Systems and SambaNova, to integrate cutting-edge artificial intelligence hardware with top-tier high-performance computers to improve the fidelity of models and manage the growing volumes of data for speed, performance, and productivity gains. LC platforms are supported by our LEED-certified, innovative facilities for infrastructure, power, and cooling; a storage infrastructure including three varieties of file systems and the world's largest TFinity tape archive; and highest-quality customer service. Our software ecosystem showcases our leadership of many large open source efforts, from TOSS with Lustre and ZFS to the R&D 100 Award-winning Flux, SCR, and Spack.



#### **CUTTING-EDGE RESEARCH**

#### **Achieving Fusion Ignition**

LLNL is home to the National Ignition Facility (NIF), the world's highest-energy laser system. NIF's 192 lasers can fire 2.2 megajoules (MJ) of ultraviolet energy into a hohlraum—a cylinder the size of a pencil eraser—compressing and heating a tiny hydrogen-filled capsule suspended in the hohlraum until the hydrogen atoms fuse and release an immense amount of energy. As the premier facility creating conditions relevant to understanding the operation of modern nuclear weapons, NIF is a crucial element of the United States Stockpile Stewardship Program, producing experimental data that validates 3D weapon simulation codes, improving understanding of important weapon physics, and investigating questions remaining from underground nuclear tests. On Dec. 5, 2022, NIF made scientific history with an experiment that achieved fusion ignition in a laboratory for the first time. The shot generated 3.15 MJ of fusion energy from an input of 2.05 MJ of laser energy. This feat has been repeated four times, most recently setting a record fusion yield of 5.2 MJ. Fusion ignition provides new opportunities for stockpile stewardship applications and lays the groundwork for laser fusion energy. LLNL scientists and engineers are pushing on all fronts to increase NIF's capabilities to address challenges, including higher energy and power limits, next-generation optics, improved targets with tighter specifications, and better diagnostics.



#### **TECHNOLOGY TO MARKET**

#### **EVOQ and LLNL: Innovating Autoimmune Disease Treatment**

EVOQ Therapeutics has harnessed advanced biomedical technology developed at LLNL to create innovative treatments and vaccines for autoimmune diseases. Their work focuses on using nanolipoprotein particles (NLPs) technology and has been shown to be 30 times more effective at delivering antigens to the lymph nodes. This technology has garnered industry recognition, with LLNL researchers receiving multiple awards for their contributions to technology transfer and collaboration.

EVOQ's partnerships with major pharmaceutical companies highlight the importance of innovation in healthcare, demonstrating how cutting-edge research can lead to real-world applications. By leveraging LLNL's expertise, EVOQ is not only advancing medical treatments but also setting a precedent for successful collaborations between research institutions and the biotech industry. This partnership is crucial for accelerating the development of new therapies, ultimately improving patient outcomes and showcasing the vital role of technology in addressing complex health challenges.



## Science-Based Stockpile Stewardship

Lawrence Livermore National Laboratory (LLNL) plays a key role in the nation's strategic deterrent, acting as a nuclear weapon design laboratory responsible for the safety, security, and effectiveness of the U.S. nuclear stockpile. This core responsibility includes annual assessment of the active stockpile, culminating in a quantification of confidence that the weapon systems still meet military requirements, as well as leading the modernization of systems that are approaching the end of their useful service life. LLNL is partnering through these stockpile modernization programs to modernize the nuclear weapon enterprise, ensuring resiliency in an uncertain global future.

LLNL executes this mission through development and application of world-class scientific and engineering tools, enabling the development of modern designs that ease manufacture and the assessment and certification of systems without conducting nuclear tests. These scientific capabilities include world-class computing and experimental facilities, such as El Capitan, the first exascale supercomputer, and the National Ignition Facility, the world's most energetic laser system. These capabilities inform the judgement of weapon experts, underpinning the nation's confidence in its strategic deterrent.

## **Applications**

LLNL is the lead design agency for the nuclear explosive package in two separate modernization programs: the W80-4 Life Extension Program (LEP) and the W87-1 Modification Program (Mod). LLNL is also responsible for assessing and sustaining three systems in the active stockpile—the W80-1, B83, and W87-0 warheads—establishing scientific confidence in the systems.

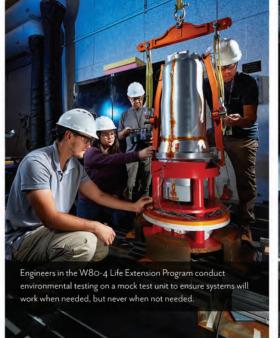
More than 5,000 LLNL team members contribute to these annual assessments, stockpile modernization programs, and the scientific capabilities that underpin this work. These employees partner closely with production agencies, NNSA, and the U.S. Air Force to design and test hardware, transfer technology, address manufacturing issues, assess material compatibility, execute vital system assessments, and ultimately deliver a deterrent the nation will rely on for decades.

The W80-4 is replacing the W80-1 warhead and will be employed in the U. S. Air Force's new Long Range Standoff (LRSO) missile. The W80-4 will be the first warhead designed for use with a new missile since nuclear testing ended in 1992. The W87-1 Modification Program will replace the W78 warhead and will sit atop the Air Force's new Sentinel Intercontinental Ballistic Missile (ICBM). The W87-1 is the first warhead to have all components newly manufactured since testing ended, unlike prior life extension programs that relied heavily on component reuse. These systems are based on tested nuclear designs and will not require new nuclear tests. Certification will rely on improved understanding and the highly capable toolset developed by the science-based Stockpile Stewardship Program.

In 2023, the W87-1 Mod entered the development engineering phase of the program (Phase 6.3), and the W80-4 LEP entered the production engineering phase (Phase 6.4). Both programs are working hand-in-hand with production agencies to ensure successful delivery of parts and systems that meet requirements. Simultaneously, researchers at LLNL are conducting an extensive range of full-system tests and hundreds of small-scale tests to validate computational models and the scientific basis for certifying the systems.









LLNL has come a long way in its ability to develop, assess, and certify warheads since the end of nuclear testing in 1992. Researchers today synthesize historic nuclear test data with computational simulations and a suite of modern experiments and tests to inform their expert judgement. Scientific advancements through decades of stockpile stewardship are now enabling certification of modernized systems in both normal and abnormal environments, without new nuclear testing. Recent accomplishments include:

- LLNL researchers have followed the fusion ignition achievement at NIF with repeated increases in yield. Experiments at NIF continue to play key roles in advancing weapon physics understanding and lend confidence to today's stockpile assessments, including leveraging ignition for weapon survivability certification experiments.
- High-performance computing advances are making possible regular use of high-fidelity, 3D simulations. These advancements are being furthered by the El Capitan supercomputer, the first exascale machine in the U.S. dedicated to national security, and through application of machine learning and artificial intelligence.
- The LLNL team successfully executed the NIMBLE subcritical experiment at existing facilities, providing data in support of certification. A next generation accelerator, Scorpius, is being built that will provide the nation's first capability to capture multiple late time radiographic images of subcritical experiments.
- The Nuclear Security Enterprise, with LLNL as the Design Agency, is on track to achieve the first production unit (FPU) of plutonium pits for the W87-1 by the end of 2024. Development of this key component will revitalize the national production enterprise.
- LLNL is driving the introduction of innovative technologies through collaboration between design and production agencies at the Polymer Enclave and the Energetic Materials Development Enclave Campus (EMDEC). These enclaves are creating a new paradigm for partnering to accelerate delivery of innovative solutions.

These accomplishments all have roots in the stockpile stewardship era and are being leveraged to expand the envelope of the types of systems that can be certified as safe, secure, and effective without nuclear testing. Elements of each advancement were initially developed through Laboratory Research and Development (LDRD) funding. When they showed promise, they were further matured with program funding to the point where they could make a difference for the nation's strategic deterrent.

## The Future

The past decade has seen the emergence of two nuclear adversaries aggressively modernizing their nuclear capabilities. Meanwhile, the 10- to 15-year timeline to field a life-extended warhead in the U.S. highlights a significant risk to the nation's ability to respond in relevant timeframes, should a new threat arise. LLNL and its partners are revitalizing the enterprise to improve responsiveness and resilience. Key prongs to the strategy include:

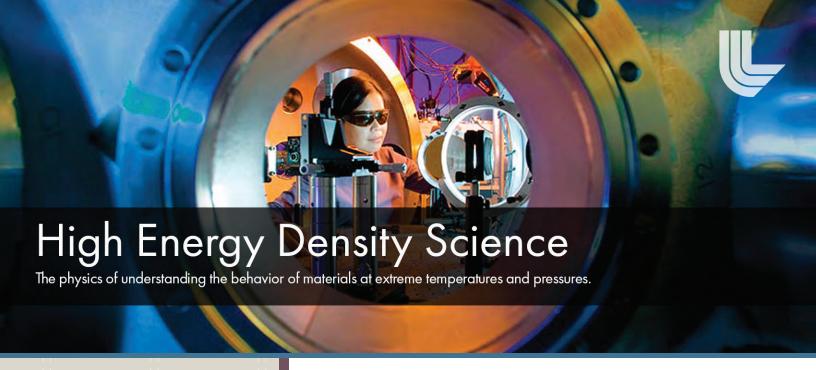
- Partnering with the Department of Defense to deliver options ensuring the long-term effectiveness of our nuclear deterrent.
- Conducting pilots focused on realizing efficiencies and prototyping aimed at accelerating maturation of technologies.
- Advancing the science, technology, and engineering required to certify novel systems with confidence.
- Developing the next generation of experts responsible for future systems.
- Modernizing the vital infrastructure that has deteriorated in the absence of new weapon development activities.

LLNL is acting in earnest on these strategies, all while delivering on the W80-4 and W87-1.

LLNL-MI-2001118

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

December 4, 2024



# Exploring Matter under Extreme Conditions

High energy density (HED) science, exemplified by the National Ignition Facility (NIF), explores matter under extreme conditions, generating temperatures higher than 180 million degrees Fahrenheit and pressures of more than 500 billion Earth atmospheres—conditions more extreme than the center of the sun. This combination of increased temperature and pressure results in matter where energy has been concentrated in space and time. Currently, LLNL is the only place on Earth studying thermonuclear ignition and some of the most extreme conditions possible in a laboratory setting, opening new frontiers in materials science.

HED experiments yield essential data for understanding nuclear weapons' conditions, validating weapon simulation codes, advancing inertial confinement fusion, and exploring related areas of national security. By replicating celestial objects' properties in the laboratory, NIF helps researchers understand how the energy mechanisms of stars are important to astrophysics.

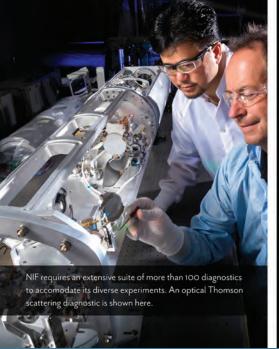
HED research explores unique states of matter and their applications. LLNL uses world-class facilities to understand HED physics while developing leading diagnostics, new platforms, and new theoretical and computational capabilities.

## **Applications**

The Laboratory's heritage of expertise in HED science is world-renowned and a jewel in the national science-based Stockpile Stewardship Program. HED science at LLNL informs annual assessments of the active stockpile, warhead modernization design decisions, and expert certification judgements about modernized warheads without nuclear testing.

HED research provides experimental data and important insights about the materials used in nuclear weapons as they age or are subjected to the immense pressures and temperatures of a thermonuclear explosion. These experiments provide experimental design opportunities, illuminate weapons-relevant phenomena, and supply data for code validation. Further applications of HED expertise at the Laboratory include:

- Setting the standard in inertial confinement fusion research, including design and analysis of igniting inertial confinement fusion experiments, design and planning for future high-yield capabilities, and understanding closely related areas of astrophysics, such as stellar structure and supernovae.
- Offering opportunities for scientists and engineers to access world-class experimental
  facilities and collaboratively explore matter and energy under extreme conditions
  at the High Energy Density Science (HEDS) Center. The HEDS Center engages
  a growing HED research community through outreach activities, including guest
  researchers, named fellowships, and HED programs at universities.
- Delivering leading-edge science and supporting the high energy density science research community with access to high-energy and high-power laser platforms at the Jupiter Laser Facility (JLF).
- Generating ultra-short, intense x-ray and neutron sources, including robustly igniting plasmas, which are routinely used to understand weapons survivability conditions.
- Measuring the strength of materials at extreme temperatures and pressures on ultrashort time scales, including turbulent mixing of materials at high compression rates.
- Determining structural phase changes of materials, such as melting and recrystallization, or transitions between crystal lattice structures.







For more than 60 years, LLNL researchers and colleagues worked to achieve fusion ignition, one of science's most challenging goals. After improvements to the design, target precision, and laser performance, an experiment on Dec. 5, 2022, passed this historic milestone, opening new vistas of HED science and enabling access to new regimes relevant for future stockpile stewardship. LLNL researchers have achieved fusion ignition multiple times since that landmark experiment, resulting in even higher yields. These ignition experiments were leveraged to establish a new experimental platform to test the survivability of materials.

In support of HED science, LLNL has developed multiple diagnostics to measure material properties on short time scales and at high densities and temperatures. LLNL researchers developed high-speed cameras to create "movie frames" of experiments with time resolution better than 1/10th of a nano-second using x-rays capable of probing ultra-dense materials. Instruments capable of measuring changes in material structures using x-ray scattering from crystals have allowed scientists to update models of solid transformations. Livermore researchers have also harnessed the emerging scientific areas of machine learning and artificial intelligence to advance HED simulation capabilities. Further accomplishments from the HED team include:

- Experiments to understand the physics within planets, including the Earth's core, inside our solar system's gas giants, and in exoplanets.
- Experiments to explore astrophysics, such as the interactions of supernova explosions with surrounding interstellar gas.
- Study of the interaction of magnetic fields and turbulence as supernova shock waves propagate through space.
- Development of x-ray imaging diagnostics capable of resolving features 1/10th the size of a human hair in billionths of a second.
- Measurements of velocities and temperatures of materials and shock fronts with time-resolved x-ray spectroscopy measurements at extremes.
- Quantification of energy transfer rates through materials and plasmas.
- Development of the "OPAL" radiation opacity code—part of the "Standard Solar Model."
- Development of novel machine learning algorithms for predicting the probability of achieving ignition in ICF experiments.

LLNL-MI-2001238

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#### The Future

The HED field continues to advance to even higher temperatures and pressures. Addressing NIF's mid-life deferred maintenance and obsolescence issues and maximizing its full potential with the NIF Enhanced Yield Capability will expand the application suite for stockpile science and inform requirements for a future high-yield capability.

Achieving high yields will enable LLNL researchers to experimentally replicate a larger range of extreme conditions that exist during a thermonuclear detonation and to probe weapon physics phenomena in ways that have never been possible, even during the era of nuclear testing.

HED research is also opening new frontiers in materials science research. Researchers have developed new capabilities to measure the basic properties of matter, including the equation of state at the highest pressures ever achieved in a controlled laboratory experiment. LLNL researchers are also poised to leverage the robust ignition platform at NIF to execute high-Z nuclear survivability experiments.

Future improvements in measurement techniques will allow scientists to study nature in more extreme conditions, including more energetic astrophysical explosions and during more energetic phases of nuclear explosions.



# Transforming Theories and Data for Mission Needs

The goal of high-performance computing (HPC), simulation, and data science at Lawrence Livermore National Laboratory (LLNL) is to transform theories and data that explain physical phenomena into models that can reliably predict outcomes.

State-of-the-art simulations running efficiently on the world's most advanced computers are the integrating element of science-based stockpile stewardship and are critical to other national security needs. Our scientists use HPC to simulate the behavior of matter under extreme temperature and pressure conditions, which are characteristic of nuclear detonations.

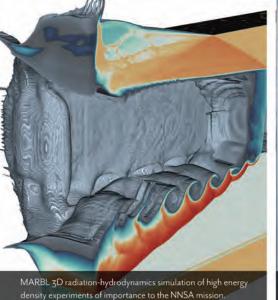
The expanding scale and complexity of the Laboratory's mission requires new data-driven and artificial intelligence (AI)-augmented approaches to scientific discovery and engineering design. These techniques applied to massive datasets—in conjunction with simulations—can help Livermore researchers better understand and predict the behavior of complex systems.

## **Applications**

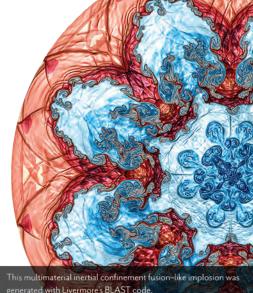
HPC at Livermore has a long history of success in close association with the Laboratory's nuclear deterrence mission. Computational scientists, computer scientists, data scientists, software engineers, statisticians, and mathematicians develop and use HPC to support nuclear deterrence, national security, and basic scientific research. HPC capabilities remain critical to the Laboratory's science-based stockpile stewardship work, ensuring the nation's existing nuclear weapons systems are safe and reliable. LLNL also uses HPC to continuously improve the scientific underpinnings of this deterrent, such as studying the effects of material aging. Likewise, HPC facilitates stockpile modernization with newly designed and manufactured systems—like the W80-4 life extension and the W87-1 modernization programs, representing the first significantly redesigned systems to enter the stockpile since the cessation of underground nuclear testing.

LLNL's national security mission relies on simulation codes that investigate a range of physical processes. These highly specialized codes must be able to run on a variety of advanced HPC architectures to incorporate efficient solvers and numerical algorithms and to enhance researchers' predictive capabilities. Further illustrations of HPC expertise at LLNL include:

- Livermore Computing houses some of the world's most powerful computers, which
  use tens of thousands of processors (both CPUs and GPUs) running cooperatively
  and concurrently.
- El Capitan, NNSA's first exascale computing system—with peak performance of more than 2.7 quintillion (10<sup>18</sup>) calculations per second—will aid the nation's effort in a significant, time-critical weapons modernization project.
- Advances in HPC enable the use of 3D modeling in design and uncertainty quantification ensembles, which improves the accuracy of our predictions beyond outdated approximations developed during the nuclear test era.
- Innovative HPC systems, simulation codes, and complex workflows improve
  predictive understanding in complex application areas such as advanced
  manufacturing, climate change, bioscience and biotechnology, energy security,
  nuclear science, and emerging national security threats.







generated with Livermore's BLAST code

Livermore is a leader in developing and using HPC, simulation, and data science to carry out mission-driven work in strategic deterrence, national security, and fundamental scientific research. Incredible computational capabilities make LLNL a premier destination for HPC researchers, whether their expertise is in numerical algorithms and simulation, machine learning and AI, or parallel systems and performance. LLNL scientists, researchers, and technicians collaborate with government, academic, and industry colleagues to tackle pressing challenges using Livermore's formidable HPC resources. Some of the Laboratory's significant recent accomplishments include:

- Developing exascale-ready simulation tools that continue to assure the safety, security, and reliability of the nation's enduring nuclear deterrent during NNSA's annual stockpile assessment process and allow for new designs to enter the stockpile through multiple modernization programs, both in-progress and planned.
- Extending Flux—Livermore's scalable, flexible next-generation workload management framework—to enable converged computing, an environment that allows scientific workflows to run faster and more efficiently by combining the power of HPC with the portability and automation of cloud.
- Integrating machine learning and other AI methods into the feedback cycle of experimentation and simulation to accelerate scientific discovery. These "cognitive simulation" tools helped LLNL scientists achieve fusion ignition by providing new insights into inertial confinement fusion implosions as well as more accurate predictions through the merging of experimental and simulation data.
- Combining Al techniques with supercomputing to develop a novel antibody design platform comprising experimental data, structural biology, bioinformatic modeling, and molecular simulations. This program addresses the urgent need for a rapid, agile approach for biological threat response.
- Using numerical simulations, powerful supercomputers, and new techniques to understand the life and death of a neutron, providing scientists a window into the subatomic world and insight into how the universe has evolved.

## The Future

As LLNL's mission continues to expand in scale and complexity, so too must our computational and predictive capabilities. A computational ecosystem capable of exascale—and beyond—performance will enable new data-driven and Al-augmented approaches to national security mission applications, scientific discovery, and engineering design.

We continue to build our expertise in computing hardware, software, algorithms, data workflows, and the physical sciences to simulate and understand application phenomena with higher fidelity, more realism, and greater insights.

Livermore is also pushing the frontiers of:

- Computing beyond exascale: heterogeneous, neural, and quantum architectures.
- Novel paradigms for science enabled by large-scale data analytics, machine learning, and cognitive simulation.
- New simulation technologies and algorithms, specifically in design optimization and decision support.
- The interplay between HPC and cloud computing paradigms.

LLNL-MI-2001167
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December 4, 2024



# Innovative Solutions for Complex Problems

Lawrence Livermore National Laboratory (LLNL) brings a multidisciplinary approach to address our nation's need for rapid development of advanced materials and manufacturing (AMM) processes. Laboratory scientists and engineers develop innovative materials with tailored properties that can be used for energy absorption, dissipation, generation, or storage; bioinspired structures for use in drug delivery; advanced optics used in satellites, telescopes, and enabling high energy density experiments on highpowered lasers; quantum materials; and components that can function effectively in extreme environments.

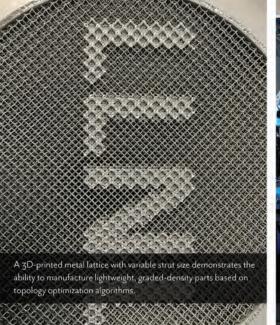
Livermore advances manufacturing technology through the development of customized feedstocks and invention of unique fabrication techniques. Diagnostic methods are developed and implemented to test components during manufacturing, which accelerates LLNL's ability to deliver timely solutions.

AMM uses an agile material development and manufacturing ecosystem to meet stakeholders' needs. The team enhances performance of materials and components, cuts manufacturing costs, minimizes supply chain vulnerabilities, recycles and reuses material, reduces waste, and accelerates discovery, development, scalability, and deployment timelines.

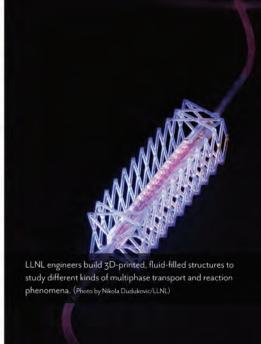
## **Applications**

LLNL's research leverages decades of experience studying materials, manufacturing technologies, and mission-relevant applications. Livermore's expertise spans the design—development—deployment cycle, including materials that can meet emerging mission needs, capabilities to produce materials at scale, advanced manufacturing methods, and structures tailored to meet specific performance requirements. AMM expertise is evident across the Laboratory:

- LLNL's high-performance computing (HPC) resources and artificial intelligence (AI)
  expertise accelerates multiscale, high-fidelity modeling of material synthesis and
  manufacturing processes, enabling scientists to design new materials and feedstocks.
- The Advanced Manufacturing Laboratory (AML) facilitates industrial and academic partnerships to address challenges across commercial and government projects.
- The Polymer Enclave enables rapid development of polymer parts for stockpile modernization programs.
- The Laboratory for Energy Applications for the Future (LEAF) fosters research that
  accelerates scalable structures for energy production, storage, and transmission, such
  as batteries, supercapacitors, energy systems, desalination, and carbon capture.
- Advanced, in-situ diagnostics and non-destructive characterization tools, including quantum 3D imaging, spectroscopy, x-ray computed tomography, and high-resolution electron microscopy lets researchers assess a material's properties and identify defects.
- The Materials Characterization Center (MCC) is designed to handle a wide range of material classes from energetics to advanced radiological materials to establish processstructure-property relationships for mission-critical applications.
- The Center for Engineered Materials and Manufacturing (CEMM) develops advanced and additive manufacturing techniques, new feedstock materials, multi-material and multiscale structures, and applies these advances to LLNL's mission-critical work.
- The Center for Design and Optimization applies computational methods to optimize systems governed by nonlinear, dynamic, multiphysics, or multi-scale phenomena.
- Organ-on-a-chip systems and 3D-printed biological cells and matrices greatly accelerate testing of medical countermeasures.
- Surfaces and interfaces are designed to mitigate corrosion and increase component lifetimes







LLNL integrates expertise in engineering, materials science, physics, chemistry, data science, modeling and simulation, and manufacturing to co-design innovative solutions. For example, material scientists study the chemical, electronic, structural, and kinetic properties of materials—including polymers, alloys, ceramics, foams, and biomimetic materials. Researchers also explore ways to enhance feedstock development, fabrication techniques, and characterization methods, while studying material aging and degradation that can impact long-term performance. Livermore experts leverage the power of artificial intelligence (AI) and data science to optimize designs and achieve rapid advances in materials science. A broad suite of LLNL resources contribute to these accomplishments, such as:

- Microcapsules containing carbon-trapping sorbents that can rapidly absorb chemicals
  and make them available for reuse in a range of applications, such as capturing carbon
  dioxide or biogas to be removed and reused or compressed and stored underground.
- A method to 3D print microbes in controlled patterns, expanding the potential for using engineered bacteria to recover rare-earth metals, clean wastewater, and detect actinides.
- Al-driven discovery of interatomic potentials to rapidly discover new materials for applications in solid-state batteries, hydrogen storage, and CO<sub>2</sub> electrolysis.
- Invention of a Volumetric Additive Manufacturing (VAM) technique, which can fabricate complex 3D objects in seconds to minutes by projecting a combination of tomographic images into a photosensitive resin.
- A commercially available materials modeling platform, The Alloy Optimization Software (TAOS), that enables computational design of optimal alloys with targeted properties.
- Additively manufactured transparent glass with customized composition and structure to create a gradient index of refraction optical components.
- Customized metal alloys with thermally stable microstructures that are lightweight, corrosion-resistant, and radiation tolerant, and use of predictive models to identify ageresistant designs with applications in hypersonic vehicles, space science, high-power lasers, and nuclear reactors.
- A groundbreaking method for fluid transport using 3D-printed open-cell lattice structures using capillary action could impact fields from CO<sub>2</sub> conversion to solar desalination.
- Advancing additive manufacturing by constructing a workflow to design, fabricate, characterize, and field fully 3D-printed fuel capsules for use in ignition experiments at NIF.

#### The Future

The long-term vision of the AMM team involves leveraging LLNL's newest resources to expand the collaborative research space. AMM staff will explore new partnerships with industry and other research institutions, both domestically and internationally, to boost the Laboratory's ability to deliver cutting-edge solutions.

LLNL will continue to take a leadership role in Department of Energy (DOE)-sponsored research activities involving clean energy technologies such as hydrogen, including developing new materials to enable compact and efficient storage and delivery of hydrogen. LLNL experts will also continue participating in the DOE Energy Materials Network and the DOE Critical Materials Institute Hub.

Additionally, the team will explore ways to adapt innovative solutions for new environments, including biosecurity, water security, space science and security, and materials for environmental remediation. LLNL will support efforts to ensure the long-term performance of our energy production and delivery infrastructure as they face risks to material used in pipelines, turbines, and nuclear power plants. At the same time, the Laboratory will continue to focus on accelerating delivery of solutions supporting the reliability of the nation's nuclear deterrent.

LLNL-MI-2001473
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-ACS2-07NA27344. December 9, 2024



# Bioscience and Bioengineering

Protecting the nation by countering current and future biological and environmental threats.

# Health, Environment, and Energy Security

Bioscience and bioengineering research at Lawrence Livermore National Laboratory (LLNL) delivers transformative biological solutions for national health, environment, and energy security needs. This research capitalizes on LLNL's capabilities in high-performance computing, experimental biology, and automation platforms. Research is guided by multidisciplinary innovation and collaboration with academia, industry partners, and government agencies.

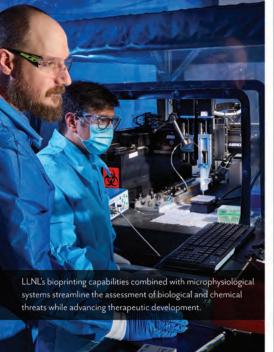
By combining capabilities and forging partnerships in quantitative biology, computing, engineering, and precision measurement, LLNL assesses, designs, and tests medical countermeasures against biological and chemical threats while finding new approaches for low-carbon materials. By expanding biological models, researchers are pioneering solutions for biofuels, carbon sequestration in soils, and eco-friendly extraction of critical minerals.

Bioengineering advances include implementating the polymerase chain reaction (PCR) technique on new platforms. By integrating analytical tools, systems biology techniques, human-on-a-chip models, and high-performance computing, staff explore the mechanisms of disease, develop novel diagnostics and therapeutics, and engineer microbial communities to counter emerging threats in biosecurity, health, and the environment.

## **Applications**

Teams of scientists and engineers converge their expertise in biological science, high-performance computing, precision measurement, and engineering to understand, predict, and engineer the behaviors of complex biological systems. By coupling world-class computational resources with targeted experiments, LLNL teams apply the design—build—test—learn cycle to tailor biological molecules and systems to achieve new functionalities. Applications of cutting-edge capabilities in bioscience and bioengineering include:

- High-performance computing to simulate biological systems across scales, including atomistic and coarse-grained molecular dynamics, quantum simulations, constraintbased genome-scale simulations, reaction-transport dynamic simulations, as well as agent-based, whole-organ, and pharmacokinetic and pharmacodynamic models.
- The National User Resource for Biological Accelerator Mass Spectrometry, the only U.S. facility that offers ultra-high-sensitive isotopic analysis for biomedical researchers measuring extremely low radioisotope concentrations.
- A Biomedical Foundry within our microfabrication facility (ISO 13485 compliant) for manufacturing medical prototypes and developing human-on-a-chip models.
- A Rapid Response Laboratory (RRL) with a high-throughput automated pipeline to rapidly produce and evaluate computationally designed antibodies.
- Experimental multiphysiological systems and computational platforms for biological and chemical threat analysis and therapeutic evaluation.
- A combination of stable isotope probing, advanced imaging, genomic profiling, and computational modeling to investigate microbial communities within ecological frameworks.
- Synthetic biology techniques and secure biosystems design for engineering safe and
  effective microorganisms and microbial communities for environmental applications
  and medical countermeasures.
- A BSL-3 Select Agent Center and Animal Care Facility; additive manufacturing with a focus on bioprinting and biomaterials; and bio-forensic science capabilities at the Laboratory's Forensic Science Center.
- LLNL's Bio Resilience Mission Focus Area integrates biology with high-performance computing to enable innovative threat analysis and therapeutic development.







LLNL brings together multidisciplinary biological expertise with world-class resources in high-performance computing and unique experimental facilities to tackle pressing national health and environmental challenges. LLNL's expanding areas of research include early biological and chemical threat detection, assessment, and impact predictions, accelerated development of therapeutics and countermeasures, and engineering of microbiomes for health, energy, and environmental sustainability. Furthermore, the Laboratory is at the forefront of developing innovative diagnostics and treatment approaches for cognitive impairment. Examples of LLNL bioscience and bioengineering accomplishments include:

- Development of miniaturized fieldable PCR and droplet PCR. These inventions have led to multiple FDA-approved commercial medical diagnostic products for detecting diseases such as tuberculosis, AIDS, and COVID-19.
- Development of the Lawrence Livermore Microbial Detection Array, a pangenomic platform capable of rapid detection of over 12,000 microorganisms within a single day. This platform is now used for applications in diverse fields such as biodefense, drug and food safety, and space biology.
- LLNL played a critical role in developing the world's first artificial retina. The invention led to high-density, microfabricated, and fully implantable neural prosthetics. Implantable/wearable interfaces now expand beyond the brain including spinal cord electrode arrays.
- Microphysiological systems including an instrumental 3D brain model and neurovascular unit provide understanding to mitigate neurological threats.
- High-performance computing enabled development of the LLNL therapeutic antibody design platform, capable of designing antibodies in weeks compared to months-to-years using conventional methods.
- Novel nanoparticle-based vaccine delivery formulations are undergoing animal testing to evaluate efficacy against infections caused by chlamydia and other pathogens.
- Identification of wound microbial signatures that inform the treatment of soldiers' combat-related injuries using microbial metagenomic DNA sequencing and advanced machine learning (ML) techniques.
- Acceleration of drug discovery by coupling physics-based modeling with ML algorithms.
   A first-in-class medication targeting cancer-related genetic mutations is in clinical trials.

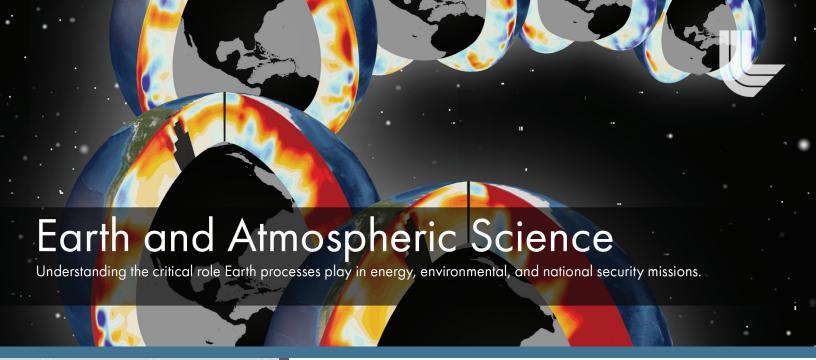
The Future

Laboratory bioresearchers integrate experimental and computational models with unique laboratory capabilities to accelerate diagnostics, therapeutics, and sustainable biomanufacturing. A multifaceted approach includes early biological threat assessment, broadtarget antibodies, and novel therapeutics and vaccines. Additionally, there is a strong commitment to bioeconomy and sustainability, driving advancement in biomanufacturing, biofuels, and ecosystem management.

Integration of big-data analytics and computational and biological modeling enhances genotype-to-phenotype predictions, improving our understanding of pathogens, host factors, and infectious disease outcomes. This involves a meticulous dissection of the intricate relationship between pathogen genotype, exposure conditions, and host fitness, offering revolutionary insights for disease anticipation and management.

Predictive design via computational and experimental integration focuses on engineering of microbial systems and biomolecules—from proteins to small molecules—with applications in healthcare, energy, climate solutions, and supply chain resiliency. Through innovation and collaboration, the future holds proactive solutions to national security challenges.

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December 4, 2024



## Science at a Global Scale

Earth and atmospheric sciences play a central role in Lawrence Livermore National Laboratory's (LLNL's) mission-driven work. LLNL scientists bring unique expertise and capabilities to advance engineering applications above, on, and below the Earth's surface. From refining space-based observations to analyzing seismic signals under the Earth's crust, LLNL's research teams use their expertise to help build a safer and more resilient future.

For decades, LLNL scientists have been at the leading edge of climate science, forecasting the likely impacts of future emissions scenarios and supporting resilience planning. In parallel, Laboratory staff develop sustainable energy technologies and carbon management techniques to support a netzero greenhouse gas future.

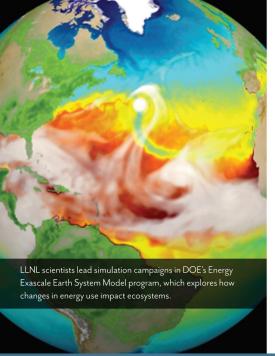
In the national security arena, Lawrence Livermore advances global-scale monitoring techniques for detecting, locating, and characterizing underground nuclear testing. LLNL's decades of innovations have strengthened response efforts for nuclear emergencies and hazardous material releases.

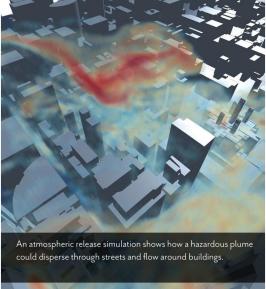
In these efforts, LLNL leverages state-of-theart computational methods, validated with unique laboratory capabilities and large-scale field experiments.

## **Applications**

Researchers in the Earth and atmospheric sciences continually innovate to make the world safer, the environment cleaner, and our energy resources more sustainable. Our key areas of research include seismology, geophysics, geomechanics, geochemistry, hydrology, atmospheric turbulence and dispersion, climate modeling and model intercomparison, climate change detection and attribution, climate sensitivity and feedback, energy systems, and carbon cycles. We maintain advanced experimental and computational capabilities to better understand the complex processes at the core of our mission applications. Select applications of LLNL's expertise in Earth and atmospheric science are noted below:

- LLNL leads the development of DOE's Energy Exascale Earth System Model (E3SM) Project. E3SM leverages capabilities at eight DOE National Laboratories and academic partners to harness the world's largest supercomputers to model and understand anthropogenic impacts on our ecosystem.
- Climate Resilience has been identified as a Mission Focus Area for LLNL and includes efforts in greenhouse gas mitigation to limit climate change, climate simulation to predict climate change on spatial and temporal scales required by decision-makers, and analysis of climate change impacts on the various systems and operations that influence national security (e.g., the electrical grid, military installations, and supply chains).
- Atmospheric researchers develop high-fidelity atmospheric fluid dynamics, turbulence, and aerosol dispersion codes. These models are used to study nuclear weapons effects, atmospheric contaminant releases, wind and solar energy systems, and high-altitude flight environments.
- The Center for Accelerator Mass Spectrometry (CAMS) is a signature user facility providing ultra-sensitive isotope ratio measurements and ion-beam analytical techniques. CAMS conducts up to 25,000 measurements per year to support a wide array of scientific studies.
- LLNL maintains one of the most complete geomaterial modeling libraries available for national security applications. The library incorporates complex phenomena related to impact and explosions in hard rock and similar materials.
- LLNL leads development of GEOS, an open-source reservoir simulator for subsurface energy systems. This exascale capability, developed by a community of industrial and academic partners, has been used in numerous studies to support geologic carbon storage, geothermal energy, and hydrogen storage projects.







an operational wind farm.

LLNL has been leading climate science research since the Laboratory developed the world's first atmospheric general circulation model in the 1960s. In Earth science, LLNL scientific advancements have informed state- and federal-level policy for managing subsurface resources in technology areas such as geologic carbon storage and geothermal energy. In the national security arena, LLNL researchers are key enablers in national and international agency cooperation regarding treaty verification, nuclear non-proliferation, and nuclear emergency response. Key accomplishments include:

- LLNL scientists participate in assessments conducted by the Intergovernmental Panel on Climate Change, a Nobel Prize-winning institution established in 1988 to provide the scientific basis for understanding climate change.
- The inaugural Gordon Bell Prize for Climate Modeling was awarded to LLNL researchers in 2023 for their work on an exascale-capable atmospheric modeling code that is paving the way towards unprecedented resolutions in climate simulations.
- Since 1979, the National Atmospheric Release Advisory Center (NARAC) has been on call 24/7 to respond to hazardous release emergencies around the world. NARAC monitored data from radiation detection sensors in Ukraine (2022), responded to nuclear power plant failures at Chernobyl (1986) and Fukushima (2011), and assessed airborne hazards in the wake of Hurricane Katrina (2005), the Deepwater Horizon oil spill (2010), and the spread of ruthenium across central Europe (2017).
- The Stellar Occultation Hypertemporal Imaging Payload (SOHIP) prototype telescope, recently installed on the International Space Station, uses LLNL-patented technology to detect and characterize atmospheric waves and high-altitude properties such as temperature, pressure, and density at altitudes up to 50 kilometers.
- The Geophysical Monitoring Program at LLNL generates global-scale tomographic images of the Earth's interior to improve seismic and nuclear event monitoring. This work has led to fundamental discoveries, such as identifying the previously unknown southeast Indian Ocean slab.
- LLNL led state-wide and national studies outlining feasible strategies to achieve netnegative greenhouse gas emissions. "Roads to Removal" is a national scale analysis of carbon dioxide removal required to achieve a net-zero greenhouse gas economy in the United States by 2050. "Getting to Neutral: Options for Negative Carbon Emissions in California" assesses the technologies and tradeoffs necessary to reach the state's decarbonization goal and received the 2021 Secretary of Energy Achievement Award.

## The Future

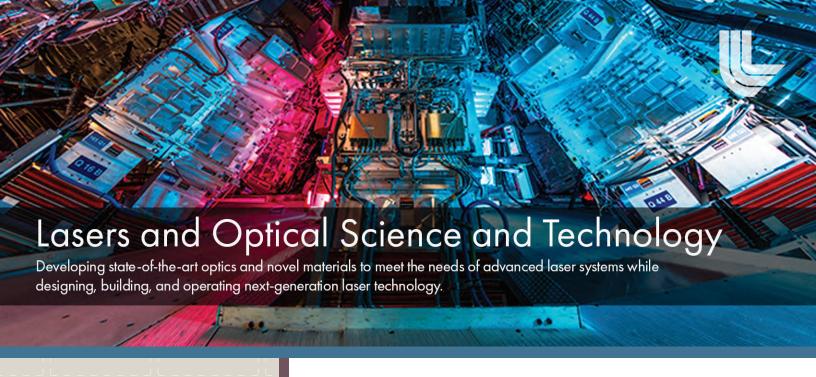
Over the next few years, LLNL is prioritizing several Earth and atmospheric sciences investment areas to prepare for future challenges. These include:

- Enhancing regional-to-local seismic and nuclear event characterization through investments in novel methods that leverage machine learning and artificial intelligence, data fusion, big-data analysis, and exascale computing.
- Expanding research on the low carbon energy transition in emerging technologies like hydrogen storage and direct air capture of carbon dioxide, and eliminating bottlenecks on the path to large-scale deployment.
- Providing decision-makers, including U.S. agencies tasked with ensuring our national security, with actionable data to foster climate resilience. LLNL scientists are tackling several remaining challenges in using climate modeling data effectively for resilience planning.

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December 4, 2024



# Lasers and Optics for Basic and Applied Science

Lawrence Livermore National Laboratory (LLNL) designs, builds, and operates a series of large and complex laser facilities for basic and applied science, driven by national security needs. These lasers have set world records in laser energy, power, and brightness. This singular capability enables groundbreaking science, including the first-ever achievement of fusion ignition in a laboratory on December 5, 2022.

The National Ignition Facility (NIF) is a valuable tool in pursuing LLNL's core mission of safeguarding America's nuclear weapon stockpile while exploring high energy density (HED) regimes that cannot be replicated at other facilities. NIF provides key insights and data for simulation codes used in weapon performance assessments and certification. It is also an important resource for weapons effects studies and nuclear forensics analysis.

Fusion ignition was made possible by long-term investments in laser systems and optical science and technology. Future advances in this space can help bring about a high-yield fusion facility for broader stockpile stewardship applications while laying the groundwork for inertial fusion energy (IFE) and delivering directed energy capabilities for national security missions.

## **Applications**

The Laboratory's leadership in lasers and optical science and technology reflects longstanding expertise in systems engineering, laser construction and operation, and collaboration with commercial partners. This is complemented by leadership in photonics, HED science, optical materials, the physics of laser–material interaction, and modeling and simulation capabilities. The following areas of expertise exemplify LLNL's leadership:

- Advanced Laser Architectures and Technologies: LLNL develops and deploys high energy, high peak power, and high average power laser technology.
- Advancing the State of the Art: LLNL is continually seeking to improve capabilities in pulse energy, wavelength, repetition rate, peak power, efficiency, beam quality, laser precision, and cost-per-delivered-energy in high energy laser systems.
- Laser System Engineering and Performance Modeling Codes: LLNL leverages physics-based models run on high-performance supercomputers for systems design and optimization. These tools enable innovative architectures with a shorter development cycle, reduced risks and costs, and safe operations.
- Laser-Material Interaction Science: The Laboratory's expertise in matter-light interactions extends beyond conditions associated with HED science to include optical material damage and the fundamental science of laser-based material processing.
- Optical Diagnostics and Photonics Technologies: This area of expertise supports LLNL experimental science platforms by delivering data to the Stockpile Stewardship Program, measuring inertial confinement fusion (ICF) target performance, and certifying precision laser pulse shaping at NIF.
- Optics and Optics Manufacturing Technologies: LLNL researchers are developing novel designs and processes, including coatings, materials, and methods to extend the lifetime of optics.
- Pumping Technologies: Diodes, Pulsed Power, and Energy Storage: LLNL
  is advancing pump diode technologies to enable compact and efficient laser
  architectures. This is driving the need for energy storage and delivery technologies
  to power high-efficiency pump diodes, including new pulsed power technologies.
- Adaptive Optics and Beam- and Pulse-Shaping Technologies: The Laboratory
  is advancing mission-critical technologies for the precision adjustment of laser beam
  profiles, wavefronts, waveforms, spectra, and polarization, resulting in reliable
  operation of experimental facilities and optimized laser-target interactions.







Over the last decades, LLNL has been a world-renowned center of excellence in the field of lasers and optical science and technology. The Laboratory's Laser Program has delivered major breakthroughs in ICF and other capabilities that support Department of Energy (DOE) and Department of Defense (DOD) missions. Recent accomplishments include:

- On December 5, 2022, the NIF laser precisely delivered 2.05 megajoules (MJ) of energy and 440 terawatts (TW) of peak power to the target, enabling the first demonstration of fusion ignition in a laboratory setting. This achievement, which generated 3.15 MJ of fusion energy, has since been repeated at even higher levels, with a record high yield of 5.2 MJ achieved in 2024.
- Optical component resilience to laser damage has been increased by four orders of magnitude since 1997, enabling higher energy densities in laser architectures, including NIF, and more sustained and economically viable operations.
- Recent debris-induced laser damage mitigations on optics have enabled NIF to operate at 2.2 MJ (>20% above initial facility requirements) and 440 TW in FY24.
- Dramatic enhancements of multi-physics laser modeling capabilities on high performance computing platforms with an increase in fidelity of 2–5× and spatial resolution by three orders of magnitude.
- Modernizing NIF pulse-shaping technology has improved the precision for power balance and accuracy on target by 2–5×; new advances in technology promise future shaping with sub-picosecond resolution over nanosecond record length.
- Designing, constructing, and operating state-of-the-art high energy and/or short pulse laser systems for the National Nuclear Security Administration, DOE, DOD, and scientific user facilities.
- Collaborating with the University of California in pioneering adaptive optics to compensate atmospheric turbulence for ground-based observatories.
- Understanding failure modes of, and innovating new, thermal management schemes for laser diode stacks and arrays while deploying this technology for compact and efficient pumping for high power and high energy laser systems.
- Photonic analog-to-digital and digital-to-analog conversion systems operating at gigahertz (GHz) bandwidths have demonstrated improved dynamic range over conventional electronic counterparts by over an order of magnitude.

### The Future

The next generation of laser systems will continue to expand the envelope of capability in energy, pulse width, and repetition rate.

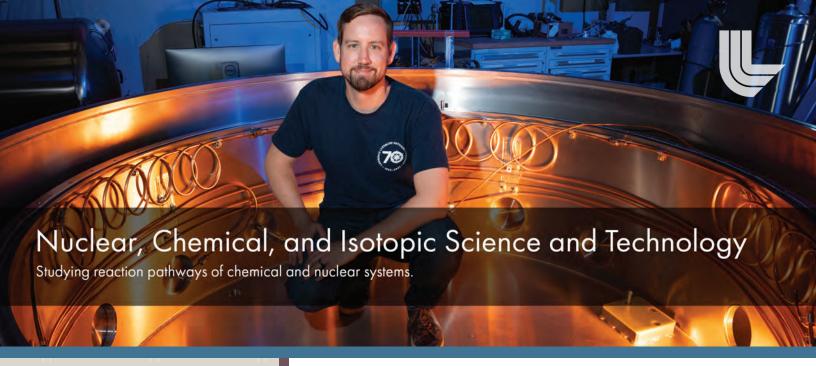
Optics mitigations will continue to increase functionality, lifetime, and yield to enable improved performance of high energy and high power lasers; there will be special focus on even higher energy and power at NIF after facility sustainment efforts are completed.

Improving precision and control over all laser properties, including time-dependent waveforms and spectra, beam intensity, and wavefront profiles, while tailoring polarization states to enable novel modalities for optimizing laser interactions with matter and mitigating instabilities.

The Laboratory will continue to advance the design, development, construction, and optimization of high energy laser systems for stockpile stewardship, DOD, IFE, and directed energy applications. The Laboratory is also building the next generation of ultrashort-pulse lasers, designed for DOE-relevant HED science applications as well as broader national security needs.

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December 4, 2024



# From the Evolution of our Planet to Nuclear Stability

Research at Lawrence Livermore National Laboratory (LLNL) in nuclear, chemical, and isotopic science addresses our strategic deterrence and global security missions and contributes to scientific advances in high explosives research, nuclear and particle physics, environmental radiochemistry, cosmochemistry, and forensic science.

Leveraging unique experimental and computational tools, researchers study nuclear reactions, the limits of nuclear stability, actinide behavior, chemical reactions of energetic compounds, and heavy-element chemistry. LLNL staff also explore the evolution of our planet, solar system, and universe, from the origin of matter to the formation of the nuclei in the periodic table.

The Laboratory's scientific research efforts provide the foundation to address these challenges. The team's overarching strategy is to position LLNL at the nexus between fundamental nuclear and chemical science research and nuclear security applications. This approach supports efforts to recruit, train, and retain top-flight scientists and engineers who are key to executing the Laboratory's core nuclear security missions, while also enhancing LLNL's reputation as a world-leading scientific research center.

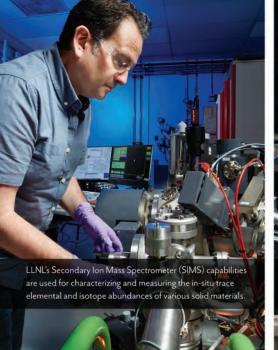
## **Applications**

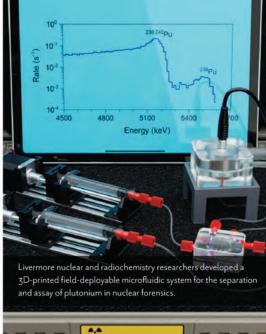
The Laboratory pursues a wide range of research that directly benefits LLNL's national security mission by improving the safety and reliability of the nuclear deterrent and enhancing detection and attribution capabilities for nuclear materials and detonations. These developments also help answer far-reaching questions in fundamental science. As part of these efforts, LLNL researchers are:

- Refining new isotopic markers to support carbon-neutral strategies and mitigate the impacts of climate change on water resources.
- Developing new approaches that bring together radioactive beams, radiochemistry techniques, and machine learning tools to improve our understanding of nucleosynthesis and reduce uncertainties in nuclear data cross-sections to support strategic deterrence and nonproliferation.
- Launching a major new effort that will unlock the mysteries of the elusive neutrino particle and help scientists better understand the evolution of our universe.
- Creating novel detectors to determine material composition and to detect threats from a distance.
- Developing a high intensity, tunable neutron source for neutron measurements that will better characterize a larger set of materials and help determine how neutrons interact with nuclei.

Examples of the specialized tools and facilities used to perform this work include:

- The Nuclear Counting Facility, which supports research in stockpile stewardship, nonproliferation, and counter-terrorism by providing high-sensitivity radiation measurements using gamma spectrometers, solid-state detectors, alpha and beta counting systems employing ionization gas chambers, and liquid scintillation techniques.
- The Center for Acceleratory Mass Spectrometry, a signature facility that uses diverse analytical techniques and state-of-the-art instrumentation to develop and apply unique, ultra-sensitive isotope ratio measurements and ion beam analytical techniques to address a broad spectrum of scientific needs.
- LLNL's microanalytical capability, which includes a one-of-a-kind imaging secondary
  ion mass spectrometry instrument with 10-nanometer spatial resolution. This capability
  is used to obtain trace element and isotopic information from solid samples in support
  of nuclear forensics, nonproliferation, cosmochemistry, and more.







The success of LLNL's nuclear, chemical, and isotopic research depends first and foremost on the capabilities of our scientific workforce, including staff, students, and postdoctoral researchers. At LLNL, researchers are able to take advantage of a wide array of state-of-the-art equipment and capabilities, from the mass spectrometry instruments used for isotopic analysis, to novel radiation detection systems for tracing radioactive signatures, to world-class high-performance computing capabilities needed for simulations with ever-increasing precision.

These unique tools enable our scientists to be at the forefront of a wide range of topics, including nuclear and particle physics, nuclear structure and reaction data, radiochemistry, nuclear detection technology and algorithms, nuclear and chemical forensic science, cosmochemistry, and environmental isotope systems. Recent accomplishments include:

- Analyzing asteroid and lunar samples to understand the evolution of the solar system and support future exploration of the Moon.
- Developing a novel microfluidic platform for rapid radiochemical separations and measurements in a laboratory or in the field.
- Leading an international effort to develop a modern toolkit for storing and using evaluated nuclear reaction data, enabling higher-fidelity nuclear physics simulations and faster adoption of new data and techniques into nuclear science applications.
- Performing the highest precision measurements of nuclear fission properties, ranging from cross-sections to fission-product yields and decay properties, with the Neutron Induced Fission Fragment Tracking Experiment (NIFFTE) experiment and specialized detection systems.
- Setting new limits for the axion dark matter candidate with ADMX and for sterile neutrinos with the BeEST and PROSPECT experiments.
- Using findings from Large Hadron Collider experiments to better study the interactions
  of quarks and gluons in conditions resembling the first microsecond after the Big Bang.
- Developing novel separation extraction schemes for actinide elements using ligands and proteins that enable study of their fundamental chemical properties.
- Producing realistic surrogate nuclear debris for testing rapid and sensitive analysis capabilities.

#### The Future

Scientists working in nuclear, chemical, and isotopic science and technology are addressing the next big challenges:

- Studying the origin of matter with the nEXO experiment, the nature of the proton at the Electron Ion Collider, and the origin of the elements at the Facility for Rare Isotope Beams.
- Expanding scientific understanding of exotic nuclei by leveraging artificial intelligence and machine learning techniques, the fastest highperformance computing architectures, and quantum computing platforms.
- Harnessing the unparalleled high energy neutron flux at the National Ignition
   Facility to determine stockpile-relevant nuclear reaction cross-sections.
- Employing LLNL's novel microfluidic chemistry and detection system to perform the first aqueous chemistry experiments with element 112.
- Resolving the building blocks of the solar system and the timescales of earliest planetary differentiation through nextgeneration sample analysis approaches.
- Inventing mass spectrometers
   to maximize isotope analyses in microscopic particles.

LLNL-MI-2001156

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December 4, 2024



# Countering Emerging Threats

Energetic materials (EM), such as explosives, thermites, propellants, and pyrotechnics, are central to Lawrence Livermore National Laboratory's (LLNL's) national security mission. EM are utilized throughout a nuclear weapon and also provide the energy source for most conventional munitions.

LLNL is a Department of Energy/National Nuclear Security Administration Center of Excellence for the research, development, synthesis, formulation, and characterization of explosives. The primary mission of LLNL's EM Enterprise is to ensure the safety, security, and effectiveness of the U.S. nuclear deterrent.

Researchers also apply their expertise to develop solutions for Department of Defense (DOD) conventional weapons, explore new ways to detect and defeat home-made explosives for the Department of Homeland Security (DHS), and develop strategies to counter the threat of improvised explosive devices for nuclear counterterrorism.

Experimental facilities at Livermore's main Site 200 and remote Site 300 enable research, that, when coupled with high-fidelity modeling and simulation, help advance scientific discovery in EM.

## **Applications**

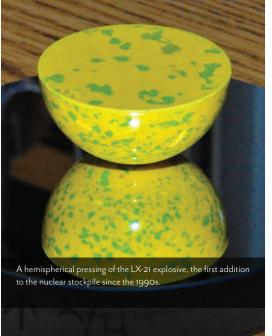
Ensuring and assessing the nation's nuclear deterrent, countering threats from adversaries, and supporting DOD conventional munitions research requires outstanding inquiry performed by exceptional scientists working at world-class facilities. EM scientists explore the energy released during energetic chemical reactions, the mechanical response, and long-term aging characteristics. Taking advantage of LLNL's family of supercomputers and advanced simulation codes, scientists continually improve EM performance and safety. Objectives for the next decade to more closely apply EM expertise across the Laboratory include:

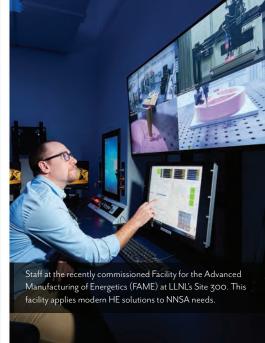
- Qualification Science: Continue evolving advanced certification and qualification of explosives with next-generation theory and modeling, coupled to quantification of uncertainties and state-of-the-art experiments using advanced diagnostics.
- **Safety:** Enabling rapid new explosive and process adoption through a science-informed safety basis.
- Material Aging and Compatibility: Integrating age-aware performance models incorporating the latest data science into LLNL's code framework.
- Manufacturing Modernization and Material Development: Transitioning novel components and manufacturing technologies for high explosives (HE) to production in response to new requirements.

#### World-Class Facilities:

- High Explosives Applications Facility extension: integrates new technologies.
- Site 300 Energetic Materials Development Enclave Campus: synthesizes, formulates, manufactures, tests, and transitions HE to production.
- Contained Firing Facility: houses hydrodynamic experiments up to 60 kg.
- Engineering Test Complex: ensures the lifetime of systems.
- Forensic Science Center: supports ultratrace chemical analysis of explosive materials and decomposition products for weapon and global security programs.







LLNL scientists have developed numerous new energetic materials (EM), especially high explosives (HE), experimental techniques for their characterization, and computational models (e.g., Cheetah and ALE3D) to predict their behavior. These advancements form much of the scientific basis for the modern EM research and devleopment (R&D) community. EM developed by LLNL are used by Livermore and Los Alamos nuclear weapon programs, and the DOD uses LLNL explosives, initiation systems, and models for their unique weapon designs. Accomplishments from the EM team include:

- Inventing and implementing the Mechanical Safing and Arming Device (MSAD) which prevents accidental or unintended detonation of a nuclear warhead.
- Developing LX-21, the first new explosive to enter the stockpile without underground testing. LX-21 is based on the LLM-105 explosive molecule, invented by LLNL.
- Using pioneering additive manufacturing for complex, multi-material, explosive components resulting in three LLNL patents on the technology.
- Leading the remanufacturing of critical IHEs for W80-4 and W87-1 LEPs. LLNL researchers identified key production parameters and LLNL's Forensic Science Center developed chemical analysis protocols.
- Mitigating the risk of high-consequence subsea drilling operations (i.e., Deepwater Horizon), LLNL designed a linear shaped charge array for Shell Oil Company to sever a drill collar on-command.
- Predicting effects of material aging on explosives' performance and improving assessments of weapon service life through groundbreaking capabilities.
- Obtaining never-before-captured high-resolution data in the reaction zone of a detonating HE through research at DOE user facilities.
- Identifying new explosive threats to Homeland Security by using advanced x-ray, dual-energy, and computed tomography processing.
- Developing the patented E.L.I.T.E.<sup>TM</sup> (Easy Livermore Inspection Test for Explosives) system for first responders' use of chemical reactions to quickly detect explosives.

## The Future

Looking ahead, LLNL will continue to support EM R&D for advanced conventional weapons, rocket and gun propellants, homeland security, demilitarization, and industrial applications of energetic materials.

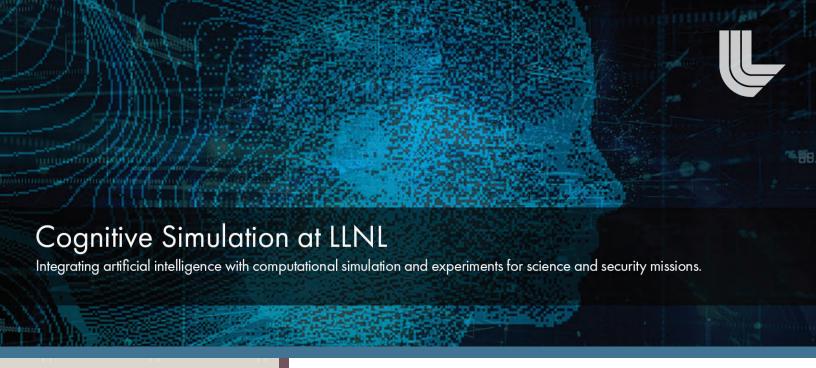
In direct support of the Laboratory's mission, the program will uphold high confidence in the safety, security, reliability, and effectiveness of EM used in our nation's nuclear deterrent.

Researchers will attain program goals, transform our enterprise, develop relevant capabilities, and advance the science, technology, and engineering of EM.

LLNL maintains a steadfast commitment to the Laboratory's national security partners. This includes addressing the needs of the Department of Homeland Security and its Transportation Security Administration while countering the threat of nuclear proliferation.

LLNL-MI-857181

This work performed under the auspices of the U.S. Department of Energy by—awrence Livermore National Laboratory under Contract DE-AC52-07NA27344, November 13, 2023



### Using Al Across LLNL's Mission Areas

Institutional Initiatives reflect Lawrence Livermore National Laboratory's (LLNL's) "team science" approach and support the Laboratory's institutional mission by anticipating issues of national importance.

LLNL's Cognitive Simulation (CogSim) Institutional Initiative aims to accelerate the integration of artificial intelligence (AI), computational simulation, and empirical experimental datasets for a range of scientific applications. For example, researchers focus on inertial confinement fusion (ICF) and high energy density (HED) projects crucial to stewardship of the nation's nuclear stockpile, then use these results to seed new opportunities across other mission areas, including climate studies, AI-driven manufacturing, and biosecurity projects modeling disease spread and drug design.

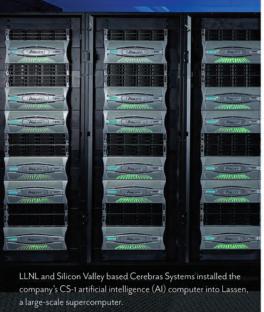
CogSim models improve scientific predictions by coupling large ensembles of simulations with limited quantities of experimental data—a process that enables Al to incorporate, adapt to, and guide experimental observations. These improved models deliver highly detailed uncertainty quantification and quantitative measures of the value of past and future experiments.

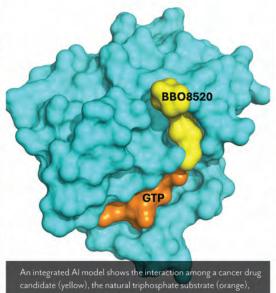
## **Applications**

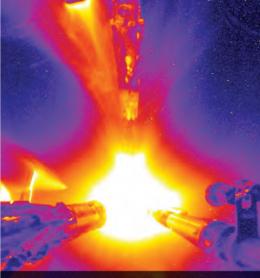
CogSim transforms the ways we apply computational capabilities to experiments and mission-driven science. LLNL's CogSim investments harness AI to accelerate scientific discovery and progress in strategic deterrence, bioresilience, space security, and other areas. Our innovative Discover, Design, Manufacture, Deploy (DDMD) strategy employs CogSim at key points throughout the scientific lifecycle to greatly shorten the time to innovation. Additionally, recognized leadership in high-performance computing, simulation, experimentation, and advanced manufacturing are foundational components of this strategy for revolutionizing mission solutions.

LLNL applies CogSim methods across mission-critical multidisciplinary programs:

- ICF: The ICF program in LLNL's Strategic Deterrence (SD) directorate uses Al surrogate models of advanced simulations to integrate exceptionally precise, yet sparse, experimental data. These models help us better predict fusion experiment performance and optimize shot design using the world's most capable supercomputers.
- **HED physics:** Teams from the SD and National Ignition Facility and Photon Science (NIF&PS) directorates couple edge computing (real-time computing in the experimental space itself) and Al algorithms that steer high-repetition-rate lasers (multiple experiments per second) to greatly accelerate data collection and discovery for national security missions as well as inertial fusion energy.
- **Material design:** SD and Physical and Life Sciences (PLS) teams use generative Al models to develop new molecular structures for critical nuclear weapons materials, such as high explosives and their polymeric binders.
- Advanced manufacturing: SD and Engineering directorate teams design digital twins of critical manufacturing and 3D printing processes to increase throughput and prevent defects in components for the nuclear stockpile.
- **Drug design:** Teams in the Global Security (GS) and PLS directorates use CogSim to develop novel therapies for emerging disease agents.
- Global security and space applications: Teams from across the Laboratory perform CogSim-accelerated verification, validation, and calibration of simulation models for orbital debris impacts as part of the U.S. Space Force's Digital Test Range.







This colorized image depicts an implosion at the NIF, the world's largest and most energetic laser. Laser systems with Al-powered controls can attain higher performance and efficiency.

CogSim provides solutions to key problems across LLNL's national security missions. While many techniques are pioneered entirely inside the Laboratory, several CogSim methods are expanded through public/private partnerships steered by the Al Innovation Incubator (AI3). This enables LLNL to share compelling interdisciplinary science challenges with AI, computing, and other technology industry leaders. Demand is high for engagement with LLNL's unique CogSim research ecosystem because of the possibilities for new techniques and approaches that benefit both national security and domestic economic competitiveness:

- ICF predictions for fusion ignition: CogSim techniques help predict shots at LLNL's National Ignition Facility (NIF) by measuring variability across multiple shots, updating the variability distribution for future shots, and propagating variations through ICF simulations to predict critical performance—such as the first-ever ignition of a laboratory fusion target.
- Generative molecular design for drug optimization: With the Accelerating Therapeutics for Opportunities in Medicine (ATOM) consortium, LLNL has developed a unique CogSim system that evaluates molecular structures for their potential as diseasefighting drugs. The system combines powerful supercomputers with AI techniques and a dataset of more than a billion molecules.
- Self-driving high-repetition-rate laser experiments: LLNL is working with computer
  chip manufacturer NVIDIA to develop a CogSim-based automated control system for
  high energy laser experiments, leveraging the latter's research on autonomous vehicles
  and graphics processing unit (GPU) hardware. Laser systems with Al-powered controls
  can attain higher performance and efficiency than traditional systems.
- Predictive tools for stockpile materials: CogSim techniques accelerate stockpile modernization by predicting physical properties of new materials and enabling the rapid discovery of high explosives, polymers, alloys, and more. These Al-driven tools provide predictive capabilities—such as the chemical structure of a new polymer—and shorten material development times compared with traditional optimization methods. Working together with IBM, these material discovery workflows are being joined with robotic chemistry to synthesize materials in record time.
- Digital twins for weapons manufacturing: Machine learning methods have accelerated the capture of important part metrology and digital representation for detailed simulation evaluation. In partnership with Aerotech, LLNL is developing these detailed models by combining software innovation with key hardware.

#### The Future

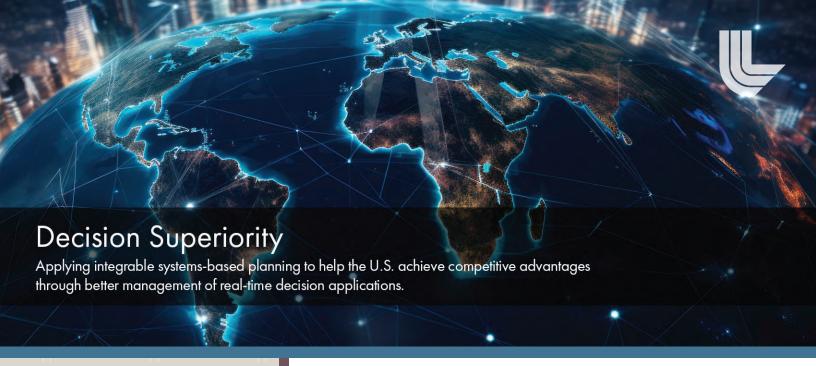
Al already plays an important role in how scientific experiments are conducted, how supercomputers run simulations, and how large datasets are analyzed to make predictions. As computing systems evolve past exascale capabilities toward zettascale and beyond, so will Al technologies.

Large language models will continue to influence scientific discovery processes, including hypothesis investigation, as will models that can analyze and interpret multimodal datasets. Al-driven automation will become more routine in laboratories and experimental facilities, producing data at unprecedented rates. Advanced manufacturing techniques augmented with Al will enable adaptive design processes and smarter production operations.

As the Department of Energy considers significant large-scale Al investments, the CogSim Institutional Initiative will ensure LLNL upholds a deliberate, focused vision for Al development and execution in addressing national security priorities. As part of this effort, Al3 will continue to coordinate multi-partner expertise focused on applications—such as through early access to proprietary commercial Al models—while nurturing the Laboratory's visibility and influence with sponsors and government partners.

LLNL-MI-2001157

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-ACS2-07NA27344, November 22, 2024



# Real-Time Artificial Intelligence

Surpassing the ability of humans to make effective real-time decisions involves combining and contextualizing data as it is acquired, developing plans, and taking actions in the face of never-before-seen scenarios.

Lawrence Livermore National Laboratory (LLNL) has made a breakthrough in scalable optimal planning that brings us closer to realizing decision-making capabilities superior to those of humans. The Laboratory has replaced expensive neural network architectures in favor of more compact and complete mathematical representations. By coupling real-time data streams and leveraging LLNL's highperformance computing, the Parallel Agent Dynamical Learning capability and associated data-driven workflows are being developed to provide responsive predictions and risk assessments on operational outcomes, without the offline training requirements and scaling limitations of artifical intellgence (AI) methods such as Large Language Models (LLMs) or reinforcement learning (RL).

In partnership with other national security laboratories and the U.S. Strategic Command, LLNL's Decision Superiority capabilities are poised for national impact.

## **Applications**

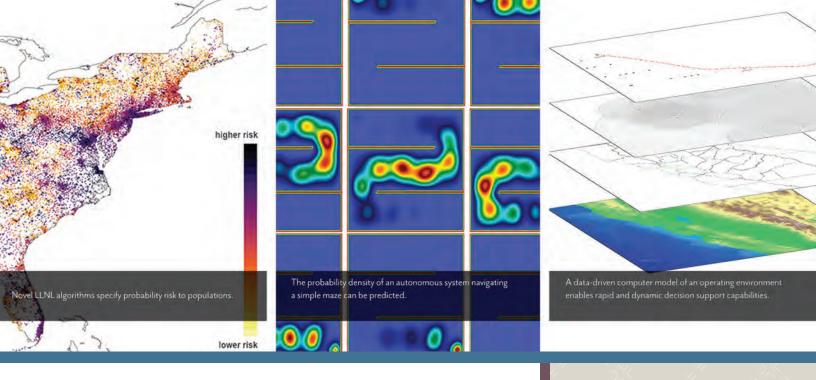
One of the most important unsolved problems in AI is how to plan for the future given incomplete information about the present. Doing so requires an ability to adapt quickly to changing circumstances beyond the range of eventualities in past training data. A new LLNL approach is enabling deployment of data-driven computational capabilities in real-world operations where new variables are being created exponentially in real-time. Traditional AI has limited utility to inform decision-makers at the speed required.

LLNL is pursuing an open research frontier in the numerical solution of integrable systems applied to mission-driven models. With advances in numerical speed and accuracy, new problem domains can be solved, including in combinatorial optimization, complex systems, and a variety of physical phenomena.

In applying such models to signal processing, data fusion, and optimal control tasks, the decision superiority capabilities are also impacting Al approaches to provide methods for faster training, more reliable uncertainties, and/or guaranteed performance with limited training data.

Applications of Decision Superiority include:

- Offering decision support for whole-of-government competition, integrated deterrence, and crisis management.
- Providing relevant context, warnings, and risk assessments for senior decision-makers through coupling with LLNL's high-performance computing (HPC) and open-source and government data streams.
- Supporting national security applications of computational science and capabilities in the newly created Decision Superiority Laboratory in the Global Security directorate.
- Strengthening the Strategic Advantage Mission Focus Area with scientific research led by the Decision Superiority Institutional Initiative.



Computational planning means solving a multi-agent optimal control problem. The LLNL Parallel Agent Dynamical Learning (PADL) code has achieved significant speedup in solving such problems. PADL provides changes in probabilities over time of optimal agent actions and outcomes and operates as part of an end-to-end decision support workflow. Multi-domain data feeds the Laboratory's Geospatial Information System for Knowledge and Rapid Decisions (GISKARD), which produces a computer model of the environment or decision space in which decision-makers must act. PADL enables near-real-time optimization over the synthesized decision space, producing courses of action, adversary assessments, and risk analysis to support human decision-makers. Examples of LLNL Decision Superiority accomplishments include:

- Demonstration of the most sophisticated computational model of deterrence known to U.S. policymakers.
- Benchmarking linear runtimes in numerically accurate solutions of multi-agent optimal control problems, in contrast with the exponential runtimes of current state-of-the-art methods.
- Deployment of decision support workflows on classified networks ready to support national security missions.
- Establishing an institutional partnership with the Department of Defense Chief Digital and Al Office (CDAO), responsible for overseeing data and Al infrastructure for the entire department.
- Supporting development of new program activities in areas of defense, non-proliferation, and deterrence analysis, in partnership with other NNSA laboratories.
- Creating new engagements between LLNL and the U.S. academic community in areas of applied mathematics and operations research.

#### The Future

Based on mathematical advances in dynamical systems, LLNL is creating scalable, stable, and robust modeling and forecasting capabilities that can resolve complex decisions with limited information. On the horizon for LLNL advances in this area is learning general embeddings of operational data to solve combinatorically hard planning problems. Efficiently representing these embeddings on conventional computing architectures is a gap that will drive evolution in computing architecture designs.

On a three-year timeline, LLNL Decision Superiority teams expect to demonstrate real-time planning capabilities at scale on LLNL high-performance computing systems. This will help expand modeling into social science domains, widely acknowledged as critical for managing future threats. Integrating the developing tools with humans will help build trust in the system.

Within five years, evolving LLNL capabilities will enable delivery of decision support products to users across the U.S. government and will foster transfer of capabilities to a broader LLNL mission set.

LLNL-MI-2001177
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-ACS2-07NA27344. December 4, 2024



# A Giant Leap Toward a Fusion Energy Future

Energy is at the heart of modern economies. As the world's energy demands continue to climb, new energy sources that are clean and plentiful are required. Fusion energy promises a virtually inexhaustible, safe, environmentally-friendly and universally available energy source, capable of meeting this need.

Fusion has powered the sun for billions of years, but humankind has yet to harness fusion energy on Earth in a controlled manner. The achievement of fusion ignition at the National Ignition Facility (NIF) demonstrates the fundamental basis of inertial fusion energy (IFE) and represents a giant leap toward a fusion energy future.

Working in synergy with Lawrence Livermore National Laboratory's (LLNL's) stockpile stewardship mission, the IFE Institutional Initiative is enabling the U.S. national, technical, and community leadership needed to build the foundational science and technology for IFE and support the Department of Energy's (DOE's) vision for accelerating the commercialization of fusion energy.

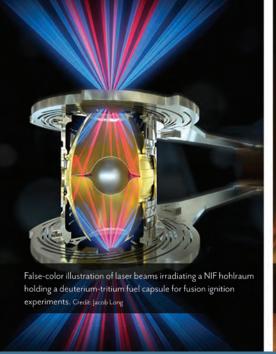
Institutional Initiatives reflect LLNL's "team science" approach and support a single institutional mission by anticipating issues of national importance.

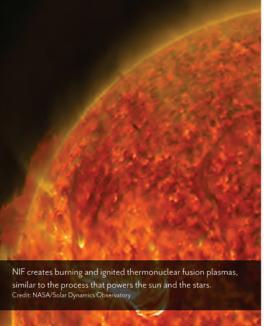
## **Applications**

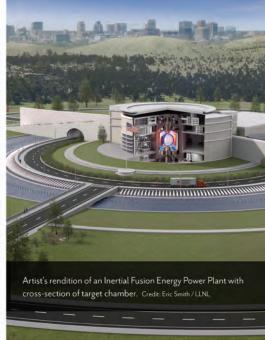
The U.S. is the world leader in both high energy density science (HEDS) and inertial confinement fusion (ICF). This is the result of significant, multi-decade investments by the DOE and the National Nuclear Security Administration (NNSA) to sustain the nation's nuclear deterrent and the possibility of fusion energy.

These investments led to the Laboratory's watershed achievement of fusion ignition in December 2022, when a NIF experiment produced more fusion energy than the laser energy used to start the reaction. This achievement—since repeated multiple times—has revitalized a national IFE program with the DOE Office of Science's Fusion Energy Sciences Program (DOE-SC/FES). Research and development (R&D) in IFE is strengthening the Laboratory's ability to achieve its core missions. These projects include:

- Developing novel high gain ignition target designs that could also be applied to stockpile stewardship missions.
- Establishing advanced full plant modeling capability for trade space studies and requirements setting to guide the U.S.'s path toward a fusion pilot plant, building on LLNL's system engineering capabilities.
- Developing and demonstrating next-generation diode-pumped solid-state lasers capable of meeting power plant technical and cost requirements, with spin-off applications to national security areas.
- Enhancing our understanding of relevant reactor materials survivability and lifetimes in extreme fusion environments and advancing their technical readiness level.
- Developing viable scale-up paths for mass manufacturing of ICF targets.
- Advancing high-repetition-rate HEDS by developing experimental subsystems capable of operating at greater than Hz rates with real-time feedback and optimization in partnership with the Cognitive Simulation Institutional Initiative.
- Developing a sustainable, world-leading IFE workforce that also strengthens LLNL's core mission delivery.
- Ensuring foundational technologies are effectively spun out to industrial partners.







LLNL is enabling the national, technical, and community aspects of growing a robust U.S. IFE program. The Laboratory's IFE Institutional Initiative provides inclusive leadership on national and international stages, builds up IFE efforts within LLNL in areas highly synergistic with stockpile stewardship, and supports the emerging public and private IFE landscape. Building on the groundbreaking achievement of ignition, LLNL has:

- Provided leadership for major DOE and community-driven fusion planning activities, including efforts under the Fusion Energy Sciences Advisory Committee, to support DOE's bold decadal vision to accelerate the commercialization of fusion energy.
- Built the technical basis and sustained advocacy to support the continued growth of the revitalized U.S. IFE program in partnership with DOE, congressional stakeholders, and the private sector.
- Chaired and delivered the Inertial Fusion Energy Basic Research Needs report for the DOE-SC/FES, laying out priority research opportunities for the nation.
- Established the STARFIRE (Science and Technology Accelerated Research for Fusion Innovation and Reactor Engineering) Hub, one of three DOE IFE Hubs, to advance foundational IFE S&T through DOE National Laboratories, academia, and industry.
- Established an IFE Collaboratory with ten other DOE National Laboratories and institutions to facilitate public/private partnerships, including hosting two Industry Days.
- Partnered and supported three private company awardees in the DOE Milestone program to design a pilot fusion power plant to advance technical and commercial viability.
- Completed an LLNL IFE Strategic Planning exercise with multi-directorate involvement and drafted a high-level U.S. IFE plan to support DOE roadmapping activities.
- Fostered a portfolio of R&D projects including high yield target designs, high-repetitionrate laser system technologies, and scalable 3D printing of foam targets.
- Organized an IFE summer school for undergraduate and graduate students and developed an IFE curriculum for deployment at six universities starting Fall 2024.
- Delivered a TED talk on the potential of fusion energy at the 2024 TED Conference and conducted wide-ranging outreach activities to advance the broader public understanding of fusion.

LLNL-MI-2001122

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

December 4, 2024

### The Future

In achieving ignition, the U.S. has taken the first pivotal step to IFE. Achieving fusion energy will require sustained, long-term investments and innovations in multiple fields to enable a viable energy source.

LLNL and its partners will continue to grow a robust and coordinated U.S. IFE program spanning the public and private sectors to build pilot power plants. Key components will include:

- Integrated plant design to drive S&T to close existing gaps and set requirements for fusion pilot plant concepts.
- National hubs with the necessary new facilities to advance component technologies and foundational science.
- Access to unique, world-leading NNSA and DOE facilities to provide near-term data and reduce risk.
- A proactive workforce development effort spanning all levels and inclusive public engagement in fusion.

U.S. leadership in IFE could profoundly transform long-standing energy geopolitics, strengthen energy and climate security, and bolster national security for the U.S. and allied partners. Building on the historic achievement of fusion ignition is a worthy scientific and engineering grand challenge.



## **Accelerating Science**

From Wall Street to the White House, artificial intelligence (AI) is more than a buzzword. It is a rapidly growing—yet little understood—field that has changed the world in numerous ways. At Lawrence Livermore National Laboratory (LLNL), we dig deep into all aspects of AI, investigating its capabilities alongside vulnerabilities. We develop sophisticated AI technologies while leading the conversation about using AI to advance science and address national security needs.

Amid headlines about AI startups, products, and ethics, challenges remain regarding AI safety and security—with effective solutions yet to emerge from commercial companies. As a national laboratory with a high-stakes mission to steward critical technology, we are concerned with these issues, so fundamental research is a cornerstone of our AI exploration. Additionally, our experimental facilities, high-performance computing systems, and large multimodal datasets provide a robust proving ground for developing and testing new techniques.

Driven by national security and our service-oriented role, LLNL has demonstrated leadership in using Al to tackle scientific challenges, while also creating an important link between academia and industry. This also positions LLNL to help the Department of Energy and the National Nuclear Security Administration contribute to Al-related national security solutions.

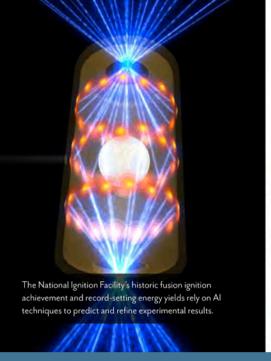
## Transformational Research

Al has great potential to transform national security science in mission-critical applications, such as those related to the strategic deterrent, intelligence gathering, and nuclear nonproliferation. It allows us to combine copious simulation predictions and detailed experiments to form an incredible model of our physical world. But can the model be trusted when conditions in the lab or the field differ from the training data? Can the model make reliable predictions about key situations it has not previously encountered? LLNL is pioneering new Al technologies that meet the high standards necessary for our national security missions.

To effectively harness the power of—and increase confidence in—this transformative technology, LLNL's foundational AI research encompasses a full spectrum of safety and security considerations:

- Al for mission-critical science: Commercial Al solutions are impressive in their domain but not yet capable of addressing foundational challenges of national security science. We build specialized Al solutions for our critical science missions, pushing Al to handle any scientific data modality.
- Robustness and safety: Mainstream AI solutions are often brittle and produce nonsensical results for even minor variations on the inputs. We created small models with better adversarial robustness than larger models can achieve.
- Generalization and uncertainty: Many Al techniques are unable to generalize to unknown situations yet are overly confident of their predictions. Our novel frameworks and algorithms generate reliable uncertainties for high-confidence decision making.
- Interpretability and trust: Understanding how an AI model makes decisions is crucial to extracting scientific insights, instilling trust in subsequent decisions, and guarding against unintended biases. We explore "black box" models by visualizing high-dimensional design spaces.

The most effective AI models are resilient to outlying or anomalous data, reliable with trusted datasets, and robust against noise. LLNL is developing AI tools to address these problems, which leading companies have not been able to solve, and with results that outperform state-of-the-art models.





#### Al in Action

LLNL's leadership in AI requires robust community engagement, both inside and outside the Lab. Through our AI Innovation Incubator, we form public/private partnerships and share our interdisciplinary scientific challenges with industry leaders. Our Data Science Institute supports our workforce through educational and collaborative opportunities. Additionally, we mentor the next generation of AI experts through student internship programs. These activities along with strategic, multi-year investments in AI research are already making a difference as we integrate AI into a wide variety of applications:

- Inertial confinement fusion: We combine Al surrogate models with simulations and data to predict fusion experiment performance and improve laser shot designs. The National Ignition Facility's diagnostic tools generate datasets for every shot, which are fed into Al models to inform future shots.
- Advanced manufacturing: We augment manufacturing processes with generative Al techniques
  enable adaptive design and smarter production operations. We are working with industry partners to
  build laboratories that autonomously manufacture parts and optimize designs.
- **Drug design:** We co-founded a consortium that develops AI tools to accelerate the drug discovery pipeline. These tools characterize billions of compounds, so only the most promising molecular combinations—those targeting cancer cells or viruses like COVID-19—move on to the costly experimental phase.
- Cancer modeling: RAS proteins are a family of proteins whose mutations are linked to more than 30% of human cancers. We developed an Al-based simulation framework that models RAS protein biology at different spatial and temporal scales: from nano- to milliseconds and from nano- to micrometers.
- **Strategic deterrent:** We built Al models to assess the reliability of the nation's nuclear stockpile. These models accelerate precision simulations, tune experimental facilities (e.g., Scorpius accelerator), guide optimized system designs, and distill information from empirical observations.
- Image reconstruction: Computed tomography (CT) reveals an object's interior by piecing together x-ray images. We developed AI tools to 3D-reconstruct an object for better anomaly detection in settings where only limited CT views are available, such as hospitals and airport security screening.
- **Materials synthesis:** We created AI techniques to expedite the discovery, optimization, and deployment of different types of materials, such as high explosives. These projects include using machine learning and computer vision to predict which physical features are important.
- Model safety and trust: We developed neural network compression approaches that show for the first time that AI robustness and efficiency are not mutually exclusive. These smaller AI models outperform significantly larger models from industry leaders.

#### The Future

The only certainty in AI is that opportunities and challenges abound. At LLNL, we recognize the need to balance innovation and preparedness in this burgeoning field, especially regarding the nation's security and stability. Whether improving cybersecurity infrastructures, boosting the accuracy of clinical predictions, or developing tools that explain how Al models work, our researchers evaluate and leverage new Al paradigms and technologies (e.g., the advent of large language models) in the context of our mission. Additionally, we are planning activities to collaborate with other national labs, including increased data sharing. Under LLNL's Cognitive Simulation Institutional Initiative, we will uphold a deliberate, focused vision for Al development and execution in addressing national security priorities.

#### Learn More

LLNL's Al research includes these frequently cited papers:

- Diffenderfer J., et al. "Multi-Prize Lottery Ticket Hypothesis: Finding Accurate Binary Neural Networks by Pruning a Randomly Weighted Network." International Conference on Learning Representations (ICLR), 2021.
- Xu K., et al. "Automatic Perturbation Analysis for Scalable Certified Robustness and Beyond." Neural Information Processing Systems (NeurIPS) Conference, 2020.
- Thiagarajan J.J., et al. "Single Model Uncertainty Estimation via Stochastic Data Centering." Conference on Neural Information Processing Systems (NeurIPS), 2022.

Learn more about our research in highimpact publications along with our Alrelated patents, open-source datasets, and open-source software:



LLNL-ML-859966rev1
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. January 30, 2024



## Scientific Expertise on Call

As a long-established Department of Energy (DOE) / National Nuclear Security Administration (NNSA) partner and member of the interagency nuclear and radiological emergency-preparedness and response community, Lawrence Livermore National Laboratory (LLNL) provides round-the-clock expertise and technical capabilities. Laboratory teams support civil-emergency scenario planning, crisis assessment and analysis of chemical, biological, radiological, nuclear, and explosive (CBRNE) threats against the U.S., and research and develop tactical tools for military operations and the intelligence community.

The Laboratory's trained, certified interdisciplinary teams of subject-matter experts possess a unique collection of skills, experience, and abilities across a range of disciplines from atmospheric modeling to weapons physics and data science and can be deployed on-site or off, within minutes, 24 hours a day, seven days a week.

LLNL's multidisciplinary teams and facilities respond to hazardous atmospheric releases, characterize and defeat nuclear threats, or, should a detonation occur, provide forensic and consequence management assistance to U.S. government officials as well as state and local authorities.

## **Applications**

LLNL provides U.S. interagency response support against a range of nuclear, radiological, chemical, biological, explosive, and cyber threats. Various LLNL response teams provide levels of support, including 24/7 crisis assessment and forensic analysis. The Laboratory applies its response expertise in the following areas:

- LLNL is one of the three DOE laboratories that directly supports the Nuclear Emergency Support Team (NEST), NNSA's multi-mission, nuclear-emergency response capability that leverages DOE's world-class scientists and technical experts to contend with the nation's most pressing radiological and nuclear challenges. NEST is the umbrella designation that encompasses all DOE/NNSA radiological and nuclear-emergency response functions, some of which date back more than 60 years.
- NEST's National Atmospheric Release Advisory Center (NARAC) responds 24/7 to hazardous atmospheric releases anywhere in the world—predicting their evolution, exposure levels, and trajectories to protect the public and the environment. NARAC has developed an operational urban-dispersion capability and a fallout model based on first-principles physics and chemistry.
- One of two U.S. laboratories with international certification to handle chemical warfare agents, LLNL's Forensic Science Center provides sample analysis across the chemical, biological, radiological, nuclear, and explosive (CBRNE) threat space.
- LLNL and Los Alamos serve as national laboratories for the Bulk Special Nuclear Materials Analysis Program, a U.S. interagency program that ensures accurate analysis of nuclear material.
- The Counterproliferation, Analysis, and Planning System strengthens CBRNE capabilities across the Department of Defense by providing intelligence analysis and reach-back support to the intelligence community and combatant commands.
- Infrastructure protection and security experts at LLNL evaluate electrical grids, oil refineries, natural gas networks, railways, ports, and waterways for physical and cyber security. Specifically, the Rapid Impact Vulnerability AnaLysis (RIVAL) response leverages critical infrastructure expertise, intelligence information, and modeling and simulation capabilities. These resources evaluate emerging cyber threats, portray potential scenarios, reveal potential impacts, and recommend mitigation strategies.
- International Nuclear and Radiological Security teams work worldwide to secure and protect nuclear and radiological materials from theft, sabotage, and terrorism.







LLNL's decades-long record of emergency preparedness and response relies on its interdisciplinary teams of subject-matter experts who possess a keen understanding of risks and threats; preparation and execution of policies, plans, and procedures; and development of innovative technologies to prevent, mitigate, and respond to threats. LLNL has provided urgent support to the U.S. Government during several recent incidents and emergencies and for emergency preparedness including:

- Ukraine (2022): NEST continuously monitors data from radiation detection sensors in Ukraine and the surrounding region to ensure real-time situational awareness of nuclear facilities. Sensor data provides early warning of an emergency at these facilities and allow DOE/NNSA scientists to provide critical technical guidance to Ukrainian partners to inform measures to protect public health and safety.
- Plutonium Finishing Plant at Hanford (2018): Assessments of potential contamination at the Plutonium Finishing Plant at the Hanford Site in Washington state were made by NARAC using a fast-running, urban-dispersion model to determine if contamination levels warranting controls might extend beyond established radiological boundaries.
- Ruthenium Detections Across Europe (2017): When a mildly radioactive plume of ruthenium-106 appeared in the atmosphere across Europe, NARAC quickly estimated probable source locations and strength using a machine-learning tool.
- Apex Gold (2016): LLNL hosted the first, minister-level exercise to identify national and international actions to address a simulated nuclear crisis and advise heads of government how to best prepare 24/7 response to a nuclear-security crisis.
- PG&E Substation Sniping (2013): After a domestic terrorism incident at an electric power station in California, LLNL conducted immediate after-action analysis, assessed security vulnerabilities, and recommended security enhancements.
- Fukushima Daiichi Nuclear Disaster (2011): LLNL deployed NEST's Radiological Assessment Program team, in conjunction with NARAC's ongoing plume modeling predictions, to analyze radiological samples to inform on public health and safety. This 24/7 effort was sustained for many weeks after the disaster.

## The Future

LLNL continues to advance its technical capabilities and contribute to the nation's credible response posture by applying advances in high-performance computing and artificial intelligence as well as by rapidly gathering and interpreting intelligence and assessing credible threats.

LLNL directly supports the U.S. response infrastructure by training first responders to improve their effectiveness and reduce response times.

LLNL subject-matter experts are developing high-fidelity training materials and leveraging next-generation technologies such as augmented reality to advance first-responder training.

As LLNL researchers continue to develop informed innovative technologies, the Laboratory's 24/7 operational technical support will be further enhanced to provide increased confidence for timely and effective national emergency response.

LLNL-MI-858683

This work performed under the auspices of the U.S. Department of Energy by awrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

December 22.2023



## LLNL's Economic Impact

Lawrence Livermore National Laboratory (LLNL), located in Livermore, California, is a science and technology research and development facility focused on solving some of our nation's greatest challenges. Managed by Lawrence Livermore National Security, LLC (LLNS), LLNL has an annual budget of nearly \$3.3 billion and has roughly 9,600 LLNS employees. It is largely funded by the Department of Energy's National Nuclear Security Administration.

LLNL's economic impact in California manifests through payroll to employees and procurements awarded to local companies. The Laboratory stimulates commercial activity through the transfer of its technologies to licensees ranging from startups to FORTUNE 500° companies. LLNL also develops research-based public-private partnerships to improve business access to world-class scientific capabilities to help them improve their technologies.

In fiscal year 2024, LLNL awarded more than \$1.07 billion in procurements to businesses, both in California and across the nation, for a broad range of products and services that support the Laboratory's overall mission. Since 2019, roughly \$747 million worth of products based on LLNL technology have been sold worldwide.

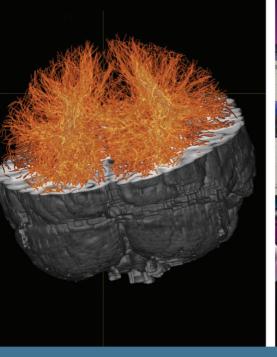
### California Success Stories

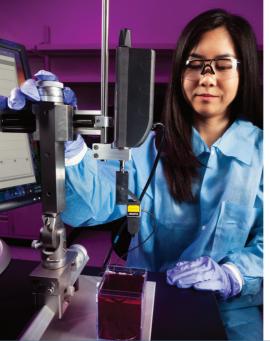
**High-Density Hydrogen Storage:** Developed in collaboration between LLNL and San Francisco-based startup Verne Inc., a cryo-compressed hydrogen storage system suitable for heavy-duty vehicles was successfully demonstrated. This system is the first of its kind scaled large enough for semi-trucks, marking a milestone in hydrogen storage. This benchmark is three times greater than what has been previously demonstrated with any single cryo-compressed hydrogen storage system and roughly equivalent to a one-megawatt-hour battery system, yet in a lighter and more compact storage unit.

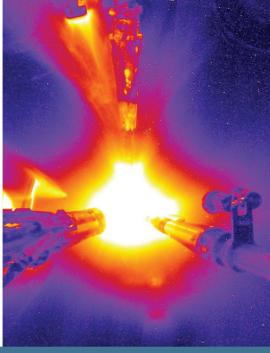
**High-Peak-Power Laser Peening:** Pioneered at LLNL in partnership with Curtiss-Wright's Metal Improvement Company (MIC), high-peak-power laser peening for commercial applications in manufacturing started at the MIC R&D center in Livermore. Beginning with engine blades for aircraft to decrease failure rates and improve airline safety, the applications have expanded to improve turbine blades for electrical generation, provide crack-free life extension to military fighter jets, and support hydrogen storage capabilities as well as fuel storage for nuclear power plants.

Nucleic Acid Detection and Analysis: Founded in 2008 by an LLNL biodefense researcher, a Bay Area-based biotechnology firm converted LLNL's anti-bioterrorism detectors into genetic screening tools. These tools use oil-emulsion to anatomize single samples into thousands of equivalent, nanoliter droplets. As a result of the Digital Droplet™ PCR technology initiated at LLNL, transformed by QuantaLife, Inc. and later expanded by Bio-Rad Laboratories Inc., researchers can now delve deeper into a wide range of genetic mysteries, including sequential mutations, cancer progressions, and pathogen adaptations.

#### LLNL FY24 Fueling California's Economy **PROCUREMENTS** BY COUNTY (Top 10) CA PROCUREMENT AWARDS Alameda Contra Costa \$25M San Joaquin San Francisco TOTAL PROCUREMENT AWARDS San Máteo Santa Clara San Diego \$9M 61 companies with active commercial Ventura licenses, 35 based in California Los Angeles Orange ■ \$1.51 billion total California payroll







### LLNL as a Business Partner

The Laboratory focuses on innovation initiatives that will develop public-private partnerships and grow high-technology business opportunities in the Tri-Valley and greater San Francisco Bay region. Furthering these goals are LLNL's relationships with regional organizations such as the California Clean Energy Fund, Bay Area Council, East Bay Economic Development Alliance, Silicon Valley Leadership Group, and Innovation Tri-Valley Leadership Group.

LLNL's Innovation and Partnerships Office (IPO) spearheads the Laboratory's engagement with industry. Whether through technology commercialization, entrepreneurship encouragement, or business development activities, the primary mission is to grow the economy by advancing the development and commercialization of scientific discoveries.

IPO has active commercial licenses with 61 companies as well as dozens of cooperative research and development agreements (CRADAs). Licensing and royalty income topped \$4.9 million in FY24, while roughly \$747 million worth of products based on LLNL technology have been sold since 2019. LLNL-licensed technologies have enabled the launch of numerous new businesses that help drive economic growth locally, regionally, and beyond. Additionally, the Laboratory participates in events and organizations that support technology innovation and business development. Here are some examples:

- University Partnerships: LLNL and Stanford University collaborate to create multi-scale models and prototype devices for the electromechanical production of chemicals from CO<sub>2</sub>. The project aims to improve carbon capture, storage, and utilization technologies to help reduce both CO<sub>2</sub> and fossil fuel reliance.
- Industry/Non-Governmental Organizations: The High Performance Computing for Energy Innovation program (HPC4EI) offers U.S. industry access to LLNL's superior computing power to improve their global competitiveness. LLNL works with Santa Clara materials engineering firm Applied Materials to improve a process for depositing thinfilm materials on wafers used in LED lights.
- Community Partnerships: LLNL supports the i-Gate innovation hub, located in the city of Livermore, California, for regional entrepreneurs.
- State Government Partnerships: The Laboratory's newly appointed Senior Advisor for State Government Affairs liaisons with a broad range of state leaders to help inform science and technology-based policymaking.

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## **Expanding Partnerships**

As a public-facing open innovation space and a portal to both LLNL and Sandia National Laboratories (SNL-CA), the Livermore Valley Open Campus (LVOC) was created to drive mutually beneficial collaboration and scientific and technological discovery by leveraging scientific capabilities, renowned expertise, and unique facilities. Along with strengthening the Laboratories' national security missions, LVOC:

- Empowers multidisciplinary partnerships to advance science and innovation
- Creates spin-in/spin-out opportunities for all users
- Bolsters the U.S. economy by developing and refining new technologies
- Contributes to science education and strengthening local and scientific communities

LVOC's campus is ideal for team science by providing spaces and facilities for researchers and entrepreneurs to gather.



LVOC's campus bridges Sandia and Lawrence Livermore National Laboratories. This unique partnership allows industry and academic collaborators to tap into the resources of both facilities, creating a bridge into some of the world's most advanced science and technology.