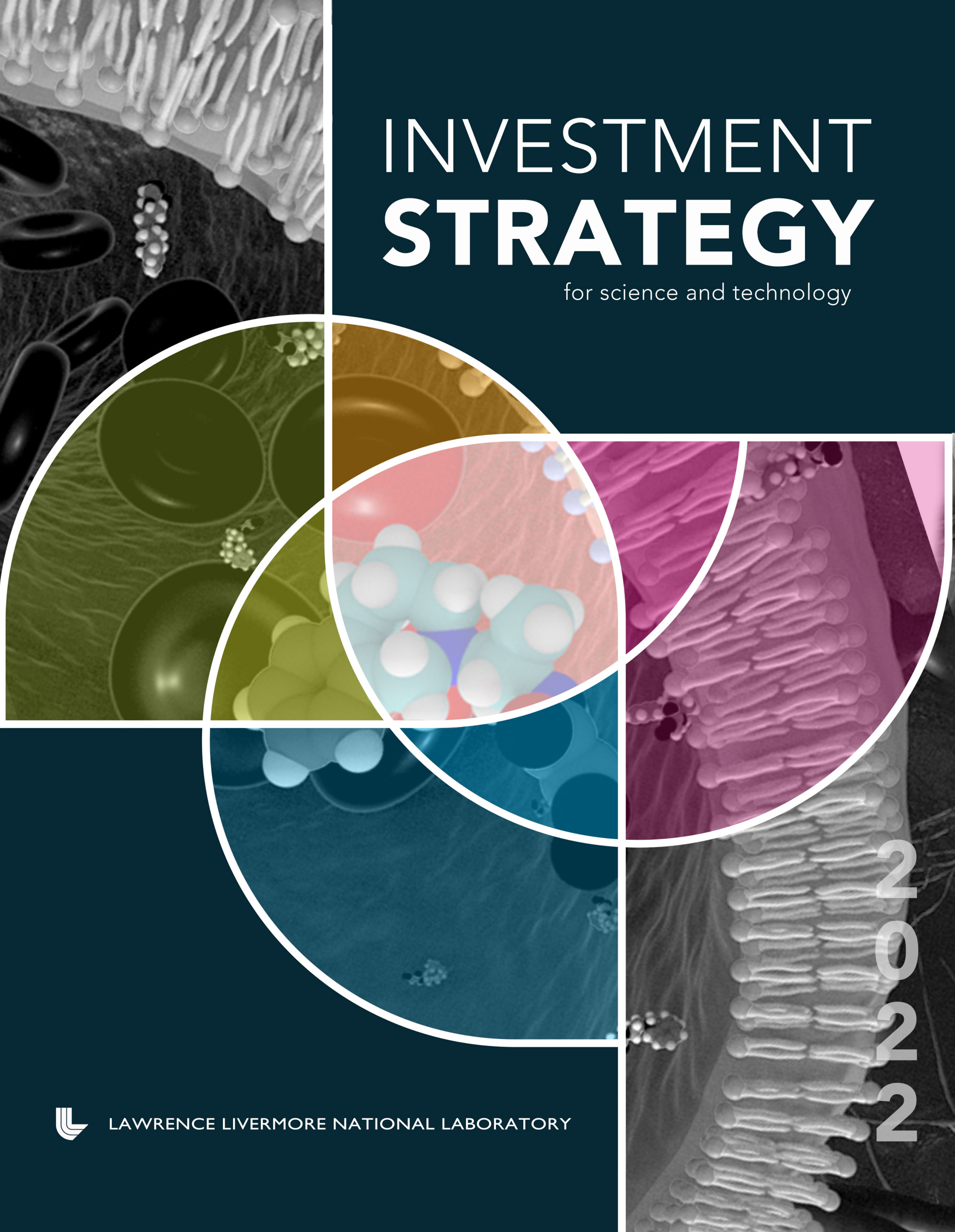
INVESTMENT
STRATEGY
for science and technology



2022

LAWRENCE LIVERMORE NATIONAL LABORATORY

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Science and Technology on a Mission

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Deputy Director for
Science and Technology

Our founders created Lawrence Livermore National Laboratory (LLNL) as a "new ideas" lab, a place where innovative science and technical solutions to the nation's most difficult security challenges are created. We continue this tradition, living our motto, "Science and Technology on a Mission," by pushing the frontier of what is or might be scientifically and technically possible. Team science is a hallmark of LLNL. Effective team science is enabled through a healthy research culture of respect, openness, interdisciplinary teaming, workforce diversity, and collaborative approaches. Mission delivery requires talented and committed staff, state-of-the-art facilities and equipment, and robust partnerships with colleagues at other laboratories, universities, industry, biomedical firms, and government organizations. These factors have been essential to the Laboratory's many achievements and continue to be indispensable for the Laboratory's vital missions and the advancement of science and technology (S&T). Our internal institutional investments—and, in particular, our Laboratory Directed Research and Development (LDRD) Program—support the exploration of new ideas that anticipate future needs within our national security missions.

The 2022 LLNL Investment Strategy for Science and Technology outlines the priorities for this year's LDRD program investments and informs decisions on other institutional investments including scientific facilities and equipment. The strategy describes science and technology challenges from a mission perspective and looks ahead to where pushing the boundaries of new science, technology, and innovation could lead. Our objective is to invest to sustain a vibrant set of scientific and engineering capabilities, meet long-term mission needs, and provide agility to respond to as-yet-unknown challenges.

Under the leadership of our director, Kim Budil, we have been examining our laboratory's mission space and exploring how we can better advance our nation's national security. Teams of thought leaders have developed strategies in key areas that build on LLNL's strengths to create new and enhanced mission focus areas to address our national security mission. I'd like to highlight these focus areas in our investment approach this year.

Nuclear deterrence remains a key component of the nation's security and a top priority for LLNL. Our work to modernize the stockpile and provide expertise to the annual stockpile assessment is essential to our work. Even while current nuclear threats continue, new and evolving threats are emerging and demand different responses. This requires us to assess the future of nuclear deterrence and modernize existing capabilities by integrating agile designs with state-of-the-art materials, advanced manufacturing techniques, and a unique confluence of experimental and computational facilities.

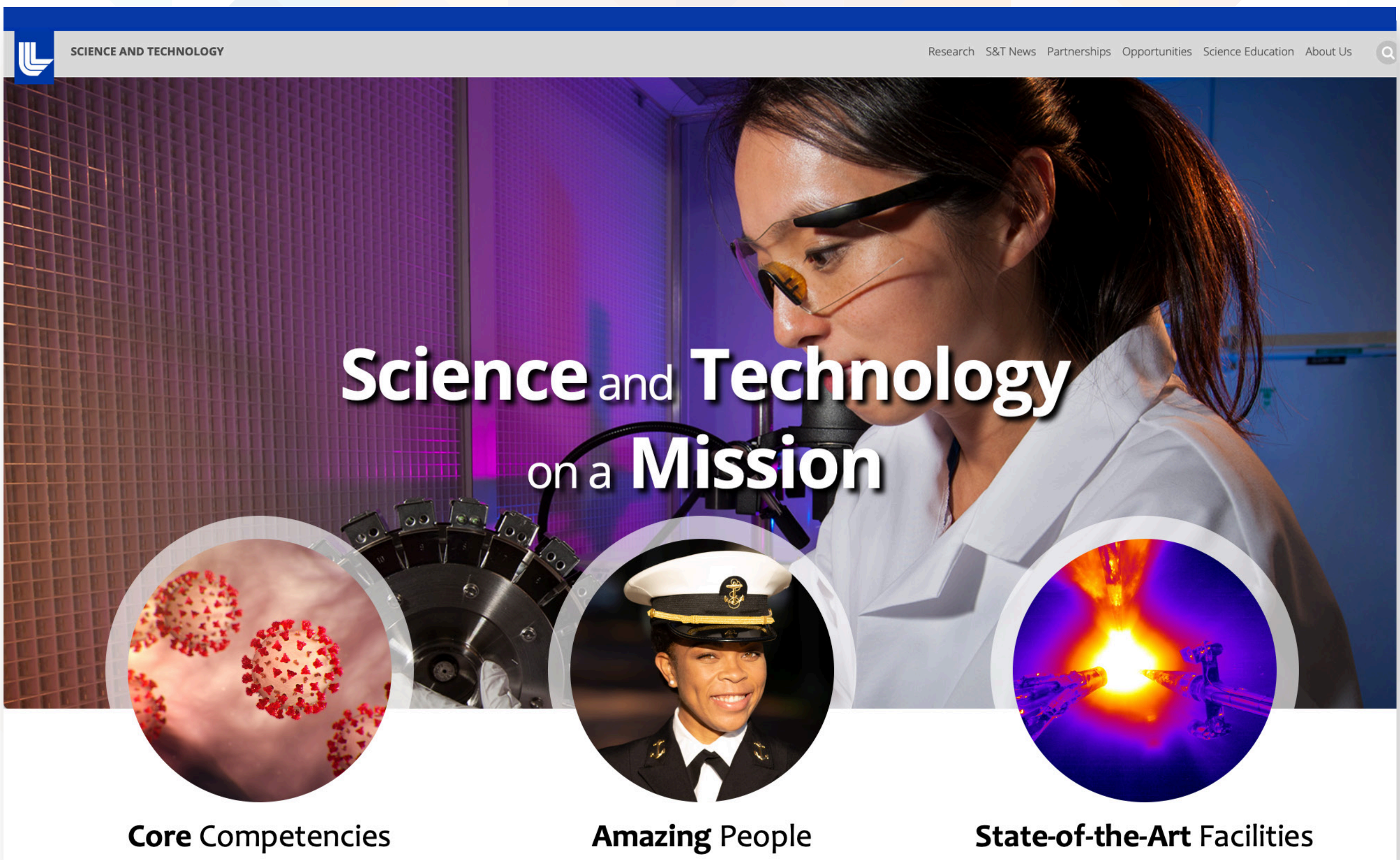
The stability of nuclear deterrence is being stressed by the intensification of global competition in emerging technologies including artificial intelligence, advanced computing, communication and network technologies, conventional defense, and cyber and space technologies. To support our national security, LLNL must help maintain national leadership in technology development. It must also integrate new technological capabilities and tools into coordinated assets that act intelligently and more rapidly, and that possess resilience to any threat.

The COVID-19 crisis has highlighted additional threats to our national security spanning chemical, biological, proliferation, and counter terrorism. Our COVID-19 work continues to advance computational therapeutics designs. We are also investing to build high throughput tools to experimentally validate candidate designs towards better medical countermeasures to broad forms of pathogens. LLNL's skills in all-source intelligence is important to provide timely and actionable information linking to new tools in artificial intelligence (AI), high-performance computing (HPC), and manufacturing for innovative solutions.

Climate change will pose a threat to national security for decades to come as the risks, often at the local and regional scale, from disease, extreme events, water scarcity, wildfires, and other impacts increase in number and severity. Central to many of these impacts are energy and water infrastructures; LLNL is developing Earth system modeling tools to anticipate climate-caused risks to these infrastructure systems and enable pathways and solutions to reduce impacts. Concurrently, the Laboratory is also integrating materials science with computational design to develop technologies that remove carbon dioxide from the atmosphere and ensure these technologies perform at the scales needed for an impactful global solution.

LLNL places a high priority on engaging in these national endeavors and we are enthusiastic about your ideas to meet the challenges at these frontiers. The descriptions of our mission, Director's Initiatives, core competencies, and mission research challenges highlight our capabilities and research and development—priorities that overlap with these areas. I hope you enjoy this description of the many opportunities before us, find related information on the Laboratory's science and technology website, st.llnl.gov, consult with your colleagues, and reach out with any questions.

We are grateful for the ability to make strategic investments that sustain Lawrence Livermore National Laboratory as a national resource for innovative solutions to tough, important national security challenges. And we are determined to use these investments to keep the Laboratory an exciting and meaningful place to work for top-flight scientists and engineers.



A Strategy for Science and Technology Investments

Lawrence Livermore National Laboratory (LLNL) pursues "Science and Technology on a Mission." We have an enduring, demanding mission and a bold vision for the future of the Laboratory:

MISSION: To strengthen U.S. security through the development and innovative application of world-class science and technology (S&T) to meet long-term mission needs and as-yet-unknown challenges in the future.

VISION: LLNL will lead in developing and applying the S&T needed to overcome challenges to national security, international stability, and human progress.

Delivering on this strategic vision requires a world-class workforce, state-of-the-art facilities and equipment, and strong partnerships with academia, industry, and government organizations. All have been essential to the Laboratory's many achievements and are essential to supporting the Laboratory's emerging mission needs and the advancement of science and technology.

Investment Approach

The Laboratory's investment approach considers the science challenges from the mission need perspective and it looks ahead to where pushing the boundaries of technology and innovation could take us. The eleven mission research challenges capture the 'mission pull' and the seven core competencies capture the 'technology push' points of view The Director's Initiatives address areas of emerging national importance that merit special attention. Together they inform the investments needed to sustain a vibrant technical workforce base, meet long-term mission needs, and provide agility to respond to as-yet-unknown challenges.

Our internal institutional investments in General and Administrative (G&A) support, Institutional Strategic Support (ISS)—and especially the Laboratory Directed Research and Development (LDRD) Program—provide critically needed support to explore new ideas that anticipate the future needs of our security mission. In addition, part of Site Support funding is used to manage, maintain, and upgrade general-purpose facilities and property.

Investment in development of our workforce and team science is a vital component of our success. We continue to expand the definition of team through a healthy research culture of workforce diversity, inclusion, respect, openness, interdisciplinary teaming, and external partnerships.

> *At LLNL, we apply cutting edge science and technology to address the most significant challenges facing the world today, working each day to translate our innovations into meaningful impact.*
>
> — Kimberly S. Budil, LLNL Director

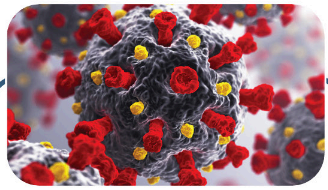
Delivering on our mission requires fostering these values and strong partnerships with universities, industry, research institutions, and government organizations. These collaborations take advantage of the complementary strengths of LLNL and its partners. LLNL undertakes activities and initiatives—such as the Livermore Valley Open Campus (LVOC)—to engage prospective partners and build strong relationships with them.

Laboratory Missions and Mission Research Challenges

The Laboratory's missions and investment priorities align with the Department of Energy's (DOE) and the National Nuclear Security Administration's (NNSA) strategic plans, including the NNSA's report, "Fiscal Year 2021 Stockpile Stewardship and Management Plan – Report to Congress." They respond to an evolving budgetary, policy, science and technology, and national security landscape. The Laboratory's mission space consists of four interrelated mission areas.

Lawrence Livermore's Mission Areas

Nuclear Deterrence



Threat Preparedness and Response

Climate and Energy Resilience

Integrated Deterrence and Competition

Nuclear Deterrence

Develop the appropriate S&T capabilities needed to assure the future safety, security, and reliability of the U.S. nuclear stockpile in an ever-changing threat environment:

- Develop an enhanced understanding of the performance of the nuclear explosive package, including details about manufacturing, build, aging, stockpile-to-target sequence (STS), and lifecycle environment.
- Advance the state of the art in experimental facilities, diagnostics, simulation capabilities, and high-performance computing (HPC) platforms to support future assessment and certification challenges.
- Enhance surveillance capabilities to more thoroughly and cost-effectively characterize the health of the stockpile. Enhance surveillance capabilities to characterize the health of the stockpile without significant destruction of assets.
- Advance and extend the use of existing underground test (UGT) data through improved scientific understanding and application of modern data science algorithms.
- Enable the modernization of the NNSA production enterprise by building S&T tools, developing advanced manufacturing technologies, rapid prototyping, and reimagining processes to improve efficiency.
- Invest in and apply systems analysis, wargaming, advanced modeling, and foundational research to evaluate enduring, emerging, disruptive, and prospective challenges facing key national security stakeholders for integrated nuclear and non-nuclear deterrence and competition.

Pertinent Mission Research Challenges: Nuclear Weapons Science; High Explosives Physics, Chemistry, and Material Science; Forensic Science; and Nuclear Threat Reduction.

Threat Preparedness and Response

Counter the threat of natural and man-made weapons of mass destruction (WMD) and enhance global security by providing unique capabilities, expertise, and innovative solutions to anticipate threats, reduce risk, and build resilience:

- Conduct technically informed intelligence analysis to identify emerging chemical, biological, radiological/nuclear, and explosive (CBRNE) threats to preclude technical surprise and to understand adversary capabilities.
- Improve capabilities to identify WMD proliferation and production pathways, monitor potential proliferators, and support arms control treaty development, negotiation, and verification.
- Support the national security community with rapid data collection and analysis, data science applications, and sensor capabilities that enhance awareness of emerging and evolving threats, and improve timely and confident predictions through advanced modeling and simulations to support preparedness and consequence mitigation.
- Detect and respond to terrorist threats and cases of alleged use, and effectively respond to and manage consequences of CBRNE incidents. Bolster the advancement of forensic science and technologies to aid in attribution of WMD.

Pertinent Mission Research Challenges: Biological and Chemical Countermeasures; Forensic Science; Nuclear Threat Reduction; Quantum S&T; High Explosive Physics, Chemistry, and Material Science; and Space Science and Security.

Climate and Energy Resilience
Secure and expand the supply and delivery of affordable, clean energy with technologies resilient to evolving natural and adversarial risks:

- Enhance our understanding of earth and energy systems through improved simulations and data gathering, analysis of climate, weather, and malicious risks, and assessments of mitigation strategies.
- Enable access to diverse domestic energy resources together with efficient, reliable energy storage and delivery systems resilient to physical and cyberattacks as well as natural hazards.
- Lead in the science, methods, and technologies that reduce the accumulation of atmospheric carbon dioxide (CO_2) and other greenhouse gases, capture and recycle CO_2 into innovative, value-added products, and indefinitely store CO_2 in terrestrial, soil, and geologic systems.
- Advance scenario modeling integrating regional climate projections and potential impacts to infrastructure, water availability, and other critical resources at spatial and temporal scales required by decision makers.

Pertinent Mission Research Challenges: Cybersecurity and Cyber-Physical Resilience; and Energy and Resource Security.

Integrated Deterrence and Competition
Create strategic advantage for the U.S. and its allies and partners in the global dynamics of deterrence and competition by providing networked mix of policy, technology, and operational concepts to flexibly manage escalation and bolster defensive capabilities:

- Conduct systems analysis and algorithmic wargaming of enduring and emerging deterrence challenges to identify and evaluate opportunities for deterring and managing escalation and prevailing in crisis and regional conflicts.
- Assess Red and Blue capabilities and strategies through technically informed intelligence analyses and physics-based modeling to help shape operational requirements, concepts, and plans.
- Exploit high-performance computing and artificial intelligence to aide decision making in complex threat environments; understand the multiple pathways for effective coordination of assets; and prioritize needed forms of integration for effect within a coherent risk framework.
- Develop new capabilities to support advanced military systems including cyber and electronic warfare, hypersonic, kinetic, and directed energy systems; advanced manufacturing capabilities; artificial intelligence and machine learning methods; and other enabling technologies.
- Develop methods for monitoring and verification of nuclear weapons, advanced conventional weapons, and space- and cyber-warfare domains. Establish technological approaches, data protection of sensitive information, and classifying and tracking weapons systems to support the advancement of compliance and transparency frameworks, such as arms control treaties and other agreements on international norms of behavior.

Pertinent Mission Research Challenges include but are not limited to: Space Science and Security; Quantum Science and Technology; Nuclear Weapon Science; High Explosives Physics, Chemistry, and Material Science; Nuclear Threat Reduction; Biological and Chemical Countermeasures; Directed Energy; Forensic Science; Cybersecurity and Cyber-Physical Resilience; Energy and Resource Security; and Science of Materials in Hypersonic Regime Conditions.

These four mission areas, altogether, reference ten pertinent Mission Research Challenges that reflect the mission pull perspective. These Mission Research Challenges identify urgent national security needs for which LLNL has special S&T strengths. Applying these strengths, the Laboratory strives for breakthroughs that will “make a difference.” The goal is to create vital new capabilities and game changing advances in our national security programs.

These Mission Research Challenges and associated research and development (R&D) thrusts are described in detail on pages 12, 13, and 37–51.

Director’s Initiatives

Director’s Initiatives (DI) focus on identified research areas that merit special attention. They position the Laboratory to address an important emerging national need. These selected multi-year activities strengthen specific science, technology, and engineering capabilities through institutional investments in research, workforce development, and infrastructure. Initiatives target new missions and opportunities and build new core competencies. The DI leader provides the strategic vision and guidance and integrates the portfolio of work.

The current Director's Initiatives listed below are described further on pages 8–16:

Accelerated Materials and Manufacturing—creating a more agile, responsive, and integrated material development, manufacturing, and qualification ecosystem to meet NNSA and national needs.

Cognitive Simulation—combining machine learning, high-performance simulation, and empirical data to improve prediction for national security applications.

Engineering the Carbon Economy—supporting the S&T innovations and collaborations that create global-scale CO_2 removal and climate change mitigation solutions in the new carbon economy.

Predictive Biology—enabling a new, precision approach to data- and simulation-driven threat characterization, diagnosis, and intervention development.

Space Science and Security—combining all-source intelligence analysis, cutting-edge modeling and simulation, and novel hardware to advance space science and enhance space security.

Laboratory Core Competencies

In support of these mission areas and to ensure the continued preeminence and quality of the Laboratory's science and technology, institutional investment priorities strengthen LLNL's science and technology base. They focus on a set of seven core competencies that are crucial to mission success. These core competencies are essential to the Laboratory's many outstanding achievements—and are vital to the continued success of its missions and the advance of science and technology.

Each core competency is a defining capability or signature expertise in which the Laboratory is a recognized leader in the field. The core competencies are listed below and further described on pages. 15–36:

Advanced Materials and Manufacturing—meeting NNSA and national needs for the rapid, cost-effective development

Institutional investments aim to strengthen the Laboratory's science and technology base and, in particular, focus on a set of seven core competencies that are crucial to mission success.

of advanced materials and manufacturing processes and systems.

Bioscience and Bioengineering—working at the interface of biology, engineering, and the physical sciences to address national challenges in biosecurity, chemical security, bioenergy, and human health.

Earth and Atmospheric Science—advancing the frontier in Earth and atmospheric sciences to develop innovative capabilities that drive the Laboratory's energy and national security missions.

High-Energy Density Science—providing international leadership in studying and controlling matter under extreme conditions of temperature and pressure.

High-Performance Computing, Simulation, and Data Science—advancing computation to understand and predict the behavior of complex systems through:

- **High-Performance Computing (HPC)**: providing leadership in the technically challenging drive toward exascale-class computing.

- **Computational Science and Engineering**: developing and applying higher fidelity and more reliable simulations in scientific discovery and engineering.

- **Information Systems and Data Science**: creating scalable capabilities to manage and recognize patterns in big data.

Lasers and Optical Science and Technology—designing, building, and reliably operating complex laser systems that dramatically advance the state of the art for strategically important applications.

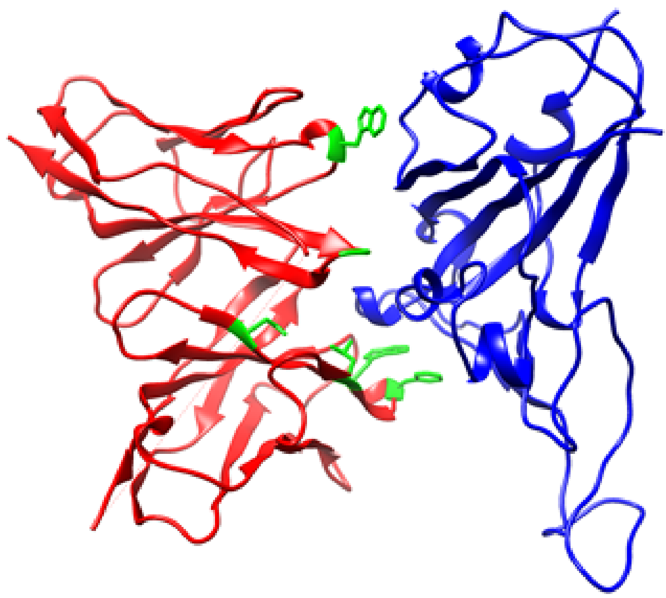
Nuclear, Chemical, and Isotopic Science and Technology—advancing fundamental understanding, scientific capabilities, and technologies in nuclear and particle physics, radiochemistry, analytical chemistry, and isotopic signatures to support LLNL's multifaceted national security mission.

Predictive Biology

Enabling a new, precision approach to data- and simulation-driven threat characterization, diagnosis, and therapeutic development.

The past 18 months have effectively demonstrated the power of emerging biothreats to disrupt and degrade our national security and well-being. The COVID-19 pandemic has exposed shortcomings in our ability to anticipate and respond to biothreats. We know that we will face future threats of at least this magnitude; human contact with natural environments is accelerating the rates of zoonotic spillover events and rapid advances in biological and information technologies are enabling growing numbers of groups around the world to work with, study, and engineer new novel pathogens.

A tested and validated predictive biology framework will enable a new, precise, data-driven, simulation-based approach to threat characterization, diagnosis, and accelerated therapeutic development. The convergence of advances in the life sciences, innovative experimental platforms and sensors, and high-performance computing is transforming health care and can enable new science-driven responses to challenges in our national and health security. Bringing together cross-disciplinary partnerships ("team science") with deep capabilities in these technical areas and focusing on substantive R&D collaborations at scale is the path to rapid progress.



High-performance simulations guided by machine learning and experimental feedback enabled computational re-engineering of a SARS-CoV-1 antibody (left in red) to neutralize the SARS-CoV-2 spike protein (right in blue).

This approach is only possible if we bring together the nation's leading capabilities in the life sciences, precision experimental measurements, and high-performance computing. If successful, this approach will be transformative.

Integrating biological simulations, data-driven artificial intelligence, and machine learning

New approaches to integrating simulations of biological mechanisms and processes with advances in data-driven artificial intelligence and machine learning are opening new possibilities for more accurate predictions and a deeper understanding of uncertainties. These advances depend on the foundation of high-performance computing and data science at LLNL. These new models are fueled and grounded by a growing ability to synthesize/engineer complex biological systems (both prokaryotic and eukaryotic) and make novel, precise, accurate measurements of complex system functions.

LLNL is developing a world-class capability in engineering biology, building on strengths in microfabrication, advanced manufacturing, and precision experimental biology. Although these technologies fuel advances in predictive biology, the extreme complexity and scale of biological and health data expands the frontiers of LLNL computing and biotechnologies, providing significantly enhanced capabilities back to our core missions.

A public–private partnership approach

Developing an integrated multidisciplinary ecosystem of biological sciences, computing and data analysis, and precision measurement technology will require a public–private partnership of the best national capabilities in biomedicine, biotechnology, and computing. These partnerships will be centered on a "co-design" methodology in which we design new capabilities and tools using integrated life sciences measurements, and computing expertise. The capabilities developed in this initiative will support new biosecurity and human health stewardship tools and methods, providing the U.S. with enhanced capabilities to respond to these growing priorities.

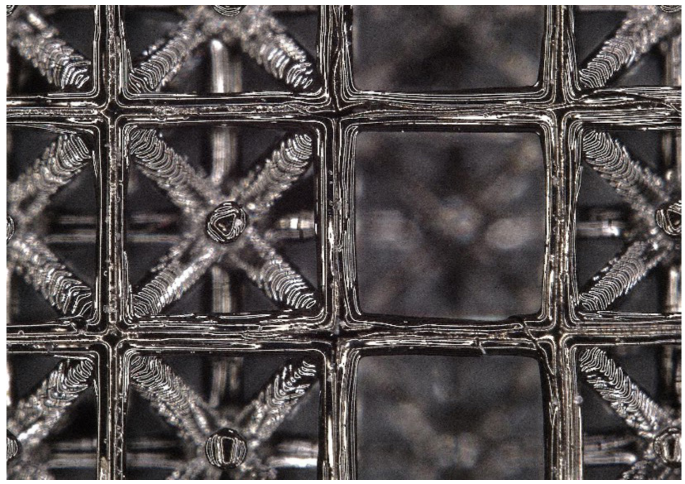
Engineering the Carbon Economy

Investing in S&T innovations and partnerships that produce global-scale carbon dioxide removal solutions to unlock climate change mitigation strategies for the new carbon economy.

Climate scientists predict that even after we achieve carbon-free electricity and most industry and transportation is emission-free, the world will still be about 25 percent short of the carbon dioxide (CO_2) reductions necessary to limit the global mean temperature increase to no more than 2°C. The remaining gap is caused by agriculture, other transportation such as airplanes and ships, and the fact that the transition to a carbon-free energy system will not be fast enough. Importantly, the individual and aggregated effects of this temperature rise to U.S. national security, including defense-, energy-, resource-, and economic-security, are not fully understood. To create a "stable 2°C world," most models predict that by later in this century we will need to remove ten gigatons of CO_2 per year. For scale, the world currently harvests about a gigaton of grain, and moves about two gigatons of oil per year. An endeavor of this magnitude is unprecedented, and requires new technology, new collaborations, and ultimately new companies that are engaged in the business of cleaning the atmosphere. The LLNL Carbon Initiative is helping create the science, technology, and collaborations that support global-scale CO_2 removal. The timeline for this next phase of climate technology brings it to full scale after carbon-free energy is widely available, but LLNL is acting now because the enormous size of the activity requires us to create technology innovations today.

A new carbon-recycling economy: valuable products from CO_2

Renewable, carbon-free electricity is an important resource for achieving dramatic carbon reductions. It will permit us to make many carbon-based fuels and products not from fossil carbon, but from CO_2 that we have harvested from the atmosphere. LLNL is inventing new electro-, thermal-, and biochemical approaches for making fuels and industrial chemicals and feedstocks, such as ethylene (C_2H_4) and ethanol (C_2H_5OH), from CO_2. Using LLNL's advanced materials and manufacturing capabilities, researchers have printed three-dimensional (3D) reactors that operate under benign conditions and have unparalleled performance—these are the first steps for turning CO_2 from a deleterious waste product into a valued resource in the new carbon economy. LLNL's unique multidisciplinary approach is a distinguishing feature and competitive advantage, and it is imperative that LLNL continue to make significant investments in this fast-growing field and expand its partnerships in this area.



A design-optimized, three-dimensional, micro-architected electrode based upon LLNL's novel cellular fluidics technology developed for CO_2 electrolysis.

Enhancing our soil by returning carbon to the Earth

Much of the carbon dioxide removed from the atmosphere will ultimately be stored in the earth. Soil carbon is a huge sink for atmospheric CO_2 that modern agriculture has depleted, particularly in the U.S. heartland. By understanding the science that caused the highly productive carbon-rich soils of the central U.S. plains to form originally, we are working to engineer agricultural and agronomic approaches that will return carbon to soil in long-lived forms. This can improve the atmosphere, and make farmland more fertile, allowing marginal land to be returned to a more productive state.

Prioritizing investments with informed decision making

The choices that must be made in our complex energy and agriculture system require thoughtful evaluation of the best ways to combine and prioritize our approaches. How can we achieve our climate goals, while encouraging new jobs and industries, building better farms, and protecting our national interests all while keeping the costs manageable? The Carbon Initiative is using system analysis to lead us to win-win solutions.

LLNL will work with partners to shape a new carbon future
Working with our partners to define the research and development pathway to reach optimal real-world solutions is an LLNL strength, and we are applying it to understand solutions like:

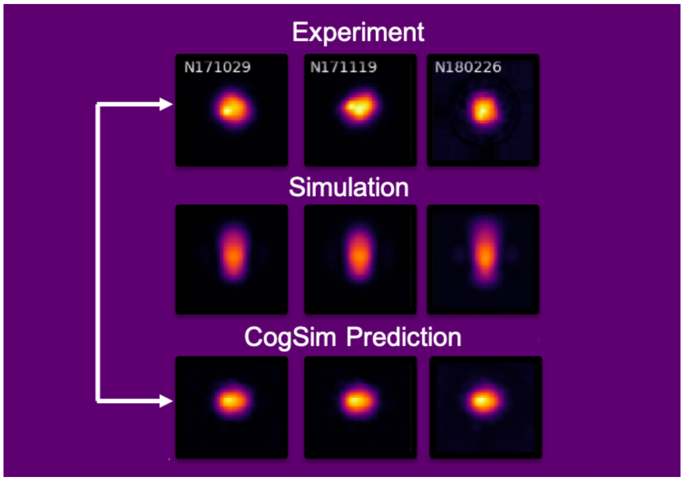
- Additively manufactured 3D reactors that combine structure and materials in unparalleled ways to achieve improved performance for metrics such as yield, productivity, conversion, efficiency, selectivity, and stability.
- Carbon capture from biofuel production to enable negative emissions fuels—fuels that when burned, emit less carbon than was permanently stored during their production.
- Combine carbon capture and conversion processes to advance the emerging research area of “reactive capture.”
- Investing in the “Science of Scaleup” with a focus on early identification of emergent scaling phenomena along with creation of an institutional strategy and accompanying ecosystem, including a “Prototyping Enclave,” will help bridge the “valley of death” and accelerate technology deployment.
- Storing CO_2 in existing California oil reservoirs to utilize the infrastructure and expertise present across California.

LLNL works with industry, academia, and other government entities to develop unique visions and turn them into reality in time to meet climate and national security goals. Technology comes from many sources, as LLNL creates the next generation of partnerships and industries required to implement these new technologies.

Cognitive Simulation

Combining artificial intelligence, high-performance simulation, and empirical data to improve prediction for national security applications.

We are exploiting rapid advances in simulation science, artificial intelligence, and high-performance computing (HPC) to transform a broad spectrum of predictive modeling applications. These transformations are enabling new science-driven responses to high priority national challenges ranging from nuclear security to precision health care. The centerpiece is the development of "cognitive simulation" systems. These systems combine artificial intelligence, HPC, and simulation to enable new approaches to predictive analysis for complex data-driven problems.



Cognitive simulation models use experimental data to correct simulation predictions. Here, a CogSim model ingests image data from past National Ignition Facility experiments to make predictions of real experiments.

Mission needs to model complex systems
To meet mission needs, our simulation tools model ever more complicated full-system behaviors and predict their response to changes and perturbations. At the same time, our simulation and experimental advances have produced overwhelmingly large and rich data sets that necessitate a rethinking of our existing tools and approaches.

Innovative tools for modern problems
Cognitive simulation (CogSim) models use artificial intelligence to combine our rapidly expanding simulation capabilities with precise empirical data sets. These new models have the ability to incorporate, adapt to, and guide experimental observations. Cognitive simulation systems enable entirely new approaches to ensure our national security, economic growth, and the health of our citizens.

Cognitive Simulation Initiative objectives
The initiative's objective is to accelerate the integration of artificial intelligence, high-performance simulation, and empirical data for our national security missions. Inertial confinement fusion (ICF) and weapons science are being used as driver applications. The results from these drivers then seed new opportunities across missions. Examples include atmospheric release prediction, AI-driven manufacturing, and biosecurity projects modeling disease spread and drug design.

Improved predictive models
The driver applications are employing cognitive simulation to improve predictions by coupling large ensembles of simulations with more limited quantities of experimental data. The improved models also deliver better detailed quantification of uncertainty, and quantitative measures of the value of past and future experiments. They also provide us a vehicle to drive new partnerships that couple industry leaders in AI with the Laboratory's national security mission and experts with the rapidly evolving field of AI for science.

Amplification of computing power
Cognitive simulation is driving learning algorithms and computational workflows that push today's most advanced computers to their limits. The algorithms also incorporate new methods that accelerate existing simulation capabilities and highlight needs for future platforms. We are using our cognitive simulation models in collaboration with manufacturers of novel computer processors to explore the coupling of AI accelerators with traditional HPC for next-generation supercomputing.

New AI-driven design methods
These CogSim models integrate seamlessly with integration of empirical data for improved performance and increased confidence. The underlying algorithms and workflows provide a testing ground for developing experimentally validated capabilities that can be used for other stockpile

stewardship applications where design, testing, and validation are more difficult. These same methods are also opening new classes of experiment to gather huge amounts of data. They are the foundation for new, "self-driving" high-repetition rate laser systems that automatically design and execute experiments.

Leading advances in scientific approaches

The CogSim initiative has developed the new AI Innovation Incubator (AI3) at LLNL to serve as an integrating center for LLNL AI and CogSim strategy development. AI3's principal aim is to coordinate strategic development of advanced AI tools and techniques with industrial collaborators. The AI3 collaboration hub has built an ecosystem of public–private partnerships with an ensemble of companies ranging from the world's largest tech businesses to leading-edge computer hardware vendors and precision manufacturing equipment producers. AI3 and its corporate partners' work has been curated to advance key Laboratory AI needs covering generative AI models for drug discovery, AI-driven automation for advanced manufacturing, and much more. Using the collaboration hub projects, AI3 is delivering multiple lasting benefits to the Laboratory AI ecosystem: a state-of-the-art open software stack in collaboration with RADIUSS (Rapid Application Development via an Institutional Universal Software Stack); an AI subject-matter-expert team to help reduce time to solution for AI-driven program work; and large-scale data sets for the development and improvement of Laboratory and broader scientific AI. These strategic partnerships provide LLNL with access to some of the world's most cutting-edge commercial AI. At the same time, our industrial partners are able improve their own software stacks and hardware by exercising them against challenges at DOE scale.

Space Science and Security

Combining all-source intelligence and engineering analysis; cutting-edge modeling, simulation and data science with high-performance computing; and novel hardware, observations, and experiments to advance space science and enhance space security.

The Space Science and Security Director's Initiative was launched in recognition of the importance of outer space in the pursuit of U.S. national security, economic, and scientific objectives. It builds on the Laboratory's longstanding involvement and deep expertise in space science. Unfettered operation in space is vital to U.S. interests across multiple areas:

- **Military**—for intelligence, surveillance, and reconnaissance (ISR) and for secure and assured military and government communications.
- **Intelligence**—for indications, warnings, threat detection, and technical intelligence.
- **Civil**—for astrophysics, cosmology, planetary science, and earth science.
- **Commercial**—for communications, financial transaction processing, entertainment, and increasingly, for space platform-derived business information.

Space Security

Space is becoming more congested and contested. The emergence of low-cost commercial launch and small satellite constellations have democratized access to space and led to the deployment of mega-constellations for commercial communications. The increasing number of space objects, both active and inactive, is taxing our capacity to monitor space activity. Our adversaries are moving quickly to deploy new space and counterspace capabilities and some of these threaten our ability to operate in this environment.

LLNL has responded to this changing landscape by growing its efforts to support U.S. space defense and resilience with several mutually supportive elements:

- **All-source intelligence and engineering analysis**—employed to anticipate and respond to emerging threats. LLNL analysts work in multidisciplinary teams to analyze and evaluate technologies and threats while applying their engineering rigor and multidisciplinary subject matter expertise.

LLNL researchers work on LLNL's payload software for the Tactically Responsive Launch-2 spacecraft, launched with Space Systems Command, Space Dynamics Laboratory, and the Air Force Research Laboratory.

- **Advanced modeling and simulation (M&S) tools**—used to quickly evaluate and improve potential mission concepts. LLNL excels in applying physics-based M&S tools to complex problems using high-performance computing resources. The Laboratory's scientists and engineers use these tools to understand the performance of sensors, satellites, and system architectures.
- **Data science for space domain awareness**—assist in tracking space debris and adversary space threats. LLNL scientists are developing data analysis techniques including machine learning algorithms with robust uncertainty quantification.
- **Novel hardware**—primarily for small satellite platforms. LLNL has pioneered the development of space-based optical payloads and enabling technologies for very small satellites. Our optics technologies are being applied to ISR space domain awareness, persistent surveillance missions, as well as missile and hypersonic vehicle detection and tracking.

Space Science

Leveraging unique LLNL capabilities and expertise developed for programmatic applications, space science groups address fundamental scientific questions in astrophysics and planetary science such as

- How does the universe work?
- How did the Sun and our Solar System form, and how long did this take?
- Are we alone? Is there something unique about the Solar System compared to extrasolar planetary systems that enabled life to develop here?

This work involves a variety of research approaches, including technology and instrument development for ground- and space-based observatories; observations and laboratory experiments; and data analytics and modeling. LLNL has established efforts in cosmochemistry, optical astronomy and cosmology, x-ray astrophysics and laboratory astrophysics, planetary defense, and particle astrophysics, with technical expertise in adaptive optics, optical/infrared instrumentation, extreme ultraviolet (EUV) and x-ray optics, x-ray spectrometers, and gamma-ray spectrometers.

Space science activities at the Laboratory span multiple directorates and leverage LLNL core competencies and facilities to provide unique contributions to the scientific community. Science objectives above align with themes and priorities identified by decadal surveys (e.g., Astro2020) and are tightly coupled to several mission research areas at LLNL, including space security, nuclear forensics, and nuclear nonproliferation. LLNL contributes to and leads projects ranging from single-investigator efforts to large international collaborations, with a goal to recruit and train the next generation of space scientists to support our programs.

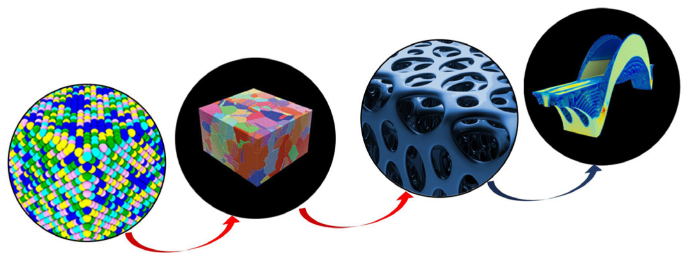
Accelerated Materials and Manufacturing

Creating a more agile, responsive, and integrated material development, manufacturing, and qualification ecosystem to meet NNSA and national needs.

The Accelerated Materials and Manufacturing Initiative and the Advanced Materials and Manufacturing Core Competency are focused on meeting NNSA's needs and the broader national need for rapid, cost-effective development of advanced materials and manufacturing processes and systems. The initiative in combination with the core competency area are pursuing the underlying science and developing the technologies to create a more agile, responsive, and integrated material development, manufacturing, qualification, and deployment ecosystem. An integrated approach creates opportunities to reduce cost, infrastructure footprint, and development times, as well co-design and co-optimize performance for requirements at the system level. Specialized materials (e.g., with graded porosity, graded composition, radically enhanced geometric complexity, etc.) and components with previously unattainable properties are needed for Laboratory missions and have potential for much wider application. In many cases, new models, design methodologies, fabrication processes, and diagnostic technologies must be developed to manufacture and qualify materials and components to meet these needs.

Many successes in meeting national and global security needs have come from LLNL's multidisciplinary approach to developing innovative new materials, characterization methods, and manufacturing processes. Progression from discovery of a new material, or the invention of a new fabrication process, to a deployable product often takes a decade or even more. Our goal is to deliver materials and components with tailored properties on an accelerated schedule and at reduced cost, with a special focus on energetic materials, actinides, optical and target materials, composites, polymers, porous, and other functional materials needed for our national security stakeholders.

Our R&D priority is to rapidly design, create, and qualify novel materials, structures, and advanced manufacturing methods. Underlying this priority is the need to predictively understand materials processing–structure–property–performance relationships using a combination of computational and experimental tools. Our R&D will build on, extend, and integrate foundational capabilities at LLNL for validated predictive simulations, tailored materials synthesis, characterization and testing, design optimization, and precision and additive manufacturing. By bringing these capabilities together in a national laboratory setting, we provide a holistic approach to meeting current and future national security needs. Specific R&D thrusts include:



Materials design and optimization fill foundational gaps to fully realize the potential of advanced additive manufacturing.

Feedstocks and tailored synthesis
National security missions require materials that are in many cases not commercially available. Through tailored synthesis the aim is to produce these functional materials with controlled morphology, phase, composition, and interfaces. Advances in computational material synthesis are needed to understand the chemical reactions that control material creation with desired functionality. New methods are needed to accelerate the creation of bespoke feedstocks and tailored materials with designed functionalities. Synthesis and processing methodologies to maximize production yield of these custom materials and feedstocks must be seamlessly integrated with in-situ characterization tools. The science of scale-up—taking bench-scale quantities of exquisite feedstocks to scales for use in fabricating components (typically greater than kilograms)—is a focus. Applying data science and machine learning methods to materials discovery and synthesis is an emerging area of interest and codesign of feedstocks for specific fabrication processes is always critical.

Manufacturing process development
Advancements in manufacturing processes require developing fundamental understanding of the underlying science, which leads to improvement of these processes, as well as invention and development of new, scalable processes

with capabilities such as precision-controlled 3D micro- and nanoscale features, mixed material structures, and radically improved throughput. Embedded sensors combined with machine learning models to enable feed-forward process control can vastly improve the predictability and precision of manufacturing processes and reduce the time and cost for part qualification. Additionally, inventing and developing processes with enhanced capabilities, such as for bioprinting and other emerging fields will be critical. Future capabilities in atomic-precision assembly of materials to create novel functionalities are also of interest and would further broaden design space. Along with using these processes to create architected materials, process development has been the core thrust of the Center for Engineered Materials and Manufacturing.

Optimal design
As materials and manufacturing processes are advanced to provide enhanced geometric and material flexibility, so too must design methods. We can no longer rely on a human designer with a drafting software package to provide the sophisticated, nonintuitive designs required by our applications and made possible with new manufacturing processes. Consequently, advanced inverse design methods, such as gradient-based topology optimization and/or statistical exploration of the design space, are being pursued by the Center for Design Optimization. Not only will these methods apply to designs of components and material architectures but can also be used for optimizing the manufacturing process itself to tune local material properties. The potential for multiscale optimization using an integrated process-architecture co-design could lead to novel component performance capabilities that dramatically expand design phase space.

Advanced and in-situ characterization
The accelerated development and optimization of new materials, processes, and components require continued access to and development of state-of-the-art materials characterization equipment and expertise as well as advanced inspection methods. This includes new capabilities for 3D imaging, spectroscopy, and scattering, where each would have unprecedented sensitivity that span atomic to macroscopic length-scales and multiple timescales. Developments in materials characterization are further enhanced by complementary consideration of rapid data analysis and modeling tools, including addressing issues associated with generating, storing, transmitting, and analyzing massive datasets, as well as developing complementary simulation-enhanced characterization methods. In-situ and in-operando techniques are required to probe material properties and performance under relevant ambient and extreme conditions that arise during fabrication, processing, and/or operation. Additionally, in-situ diagnostics play a pivotal role in advancing the state of the art in manufacturing and the associated qualification of processes, materials, and components.

Predictive simulations and performance modeling
To achieve rapid design-to-qualification of components, advances are needed in validated predictive material-, component-, and system-level models over a broad range of material sets, spanning atomistic scale to continuum levels, and spanning static to dynamic and chemically reactive timescales. These advances will require both high-fidelity and reduced-order process models to decrease the time from concept to application. A combination of first-principles simulation, data informatics, and machine learning are needed to make service-life predictions under varying and sometimes uncertain use cases. In general, predictive modeling needs to evolve from describing ideal systems to describing real systems with multiple levels of complexity. Materials compatibility and function associated with surfaces and interfaces comprise a particular frontier area for advancement.

Scale-up and qualification
Nonlinear scale-up challenges require in-depth analysis and detailed understanding of processes that affect the transition from benchtop to full-scale advanced manufacturing. To transition new materials and processes to our programs, we must be able to qualify them in an accelerated fashion. Consideration of the cradle-to-grave lifecycle of a material, component, or system is critical to achieve both efficient use of materials and reliable scale-up for end-use.

Expanded partnerships
Expanding our strategic partnerships with academic institutions, U.S. industry, federally funded research and development centers, and NNSA laboratories and production facilities will benefit LLNL's advanced materials and manufacturing efforts through the communication of best practices, new ideas, and improved processes and will also act as a pipeline for new talent. In addition to leveraging unique materials synthesis and characterization on the main LLNL campus, external partnerships have flourished in the new Advanced Manufacturing Laboratory (AML) in the Livermore Valley Open Campus (LVOC), where Laboratory staff can work side by side with academic and industry partners on materials and manufacturing projects of joint interest. "Spinning out" LLNL technologies to U.S. industry and "spinning in" the best ideas and practices from the external community, both academia and industry, will benefit the Laboratory's programs ranging from stockpile stewardship to energy security.

High-Energy-Density Science

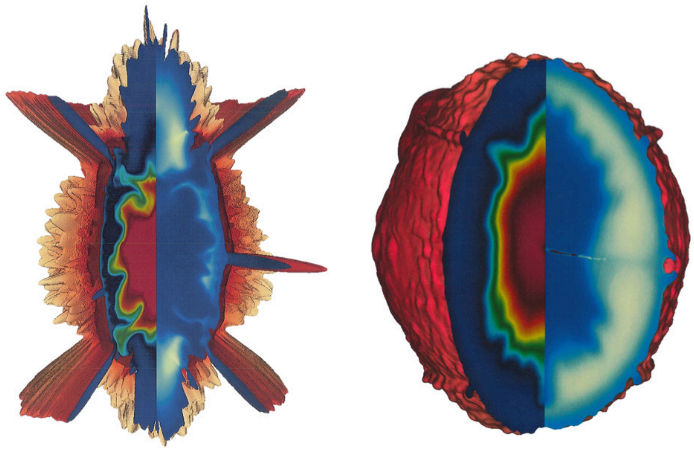
Providing international leadership in studying and controlling matter under extreme conditions of temperature and pressure.

High-energy-density (HED) science is the study of matter and radiation at conditions of high pressure or temperature or under the influence of a strong external perturbation, such as an intense laser, particle beam, pulsed power, impact, or radiation source. These are the conditions seen in the cores of the giant planets or in a burning plasma at the National Ignition Facility (NIF) or in the core of the sun.

A multidisciplinary field, HED originated from the design of nuclear weapons, the pursuit of controlled fusion energy, and the interpretation of astrophysical observations. HED science has been a core competency of the Laboratory since its founding, supported by world-leading experimental and simulation capabilities.

LLNL is home to NIF, the highest energy laser in the world, where unique conditions of temperature and pressure, otherwise only found inside stars, planets, and nuclear weapons can be attained. NIF brings world-leading expertise in creating and diagnosing HED matter, the ultrafast dynamics of strongly driven materials, solid-state and warm dense matter at terapascal pressures, the atomic physics of charged ions, plasma opacity and equation of state, plasma physics, laser–matter interactions, radiation transport, hydrodynamics and instabilities, inertial confinement fusion, and associated simulations, targets, and diagnostics for HED experiments.

LLNL researchers also have access to a range of worldwide facilities to conduct HED experiments, some with unique diagnostic opportunities and others that serve as early testbeds for the higher temperatures and pressures that experiments can reach at NIF. These testbeds include both large and mid-size facilities such as the Jupiter Laser Facility at LLNL; Omega; the Z-machine; the Linac Coherent Light Source; the Dynamic Compression Sector at the Advanced Photon Source; European and Japanese x-ray free electron lasers (XFELs); and the Extreme Light Infrastructure including the LLNL-constructed HAPLS (High-Repetition-Rate Advanced Petawatt Laser System) laser. LLNL is also home to world-class high-performance computing facilities. High-resolution, predictive simulation of HED conditions requires advances in modeling and algorithms that leverage LLNL's high-performance computing resources.

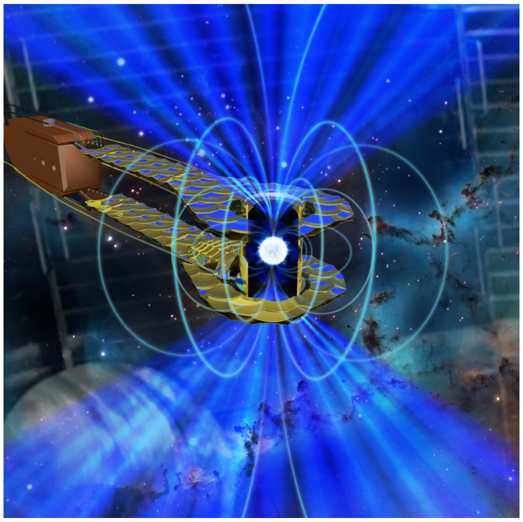


State-of-the-art 3D capsule-only simulations track the results of NIF experiments and performance improvements: High Foot 2014 (left), Big Foot 2018 (right).

Science Drivers

Understanding matter at HED-like conditions is a challenging problem with important applications in Laboratory missions. Maintaining the nuclear weapons stockpile in the absence of nuclear testing; the intellectual challenge of understanding matter and chemistry at extreme conditions seen in planets and stars; and the quest for creating, sustaining, and controlling burning plasmas are the three critical science drivers for HED science. These drivers identify and prioritize the S&T investments LLNL is to make. The research of extreme states of matter and fusion plasmas through HED science provides a foundation for executing LLNL's core mission of stockpile stewardship as well as the longer-term possibility of fusion energy and other beneficial technologies.

- The Stockpile Stewardship Program (SSP) uses the latest science and technology for qualifying newly manufactured components and assessing an aging nuclear weapons stockpile without relying on nuclear testing. The science responsibilities include developing, validating, and deploying high-fidelity, physics-based capabilities to predict, assess, and certify nuclear weapons performance. One of the key challenges for the ongoing modernization effort is finding new ways to bring modern technology into the enterprise to enable resilience and responsiveness. To meet this objective, we must enable impactful assessments utilizing HED capabilities on an ever-faster schedule.



NIF can create plasma conditions needed for directly probing the properties of materials in white dwarf stars. Kritcher, A.L., et al. *Nature*, 2020.

- HED science stands alone as a scientific discipline. Its complex multiphysics nature makes it an intellectually challenging area of research. Matter at these conditions exhibits a wide range of interesting phenomena: high pressure or high fields, which distort atomic and material structure; high energy densities, which create complex chemistry; slightly ionized materials that are in between regimes well-described by existing methods; highly ionized materials, which generate strong electromagnetic fields and emit copious radiation, influencing hydrodynamics; and plasmas, which exhibit a rich variety of collective and coherent behavior.

- One of the highest priorities is to develop the science for creating, predicting, controlling, and exploiting burning fusion plasmas. This work includes gaining a better understanding of what it will take to achieve ignition within the laboratory and pursuing innovative and cost-effective technological solutions that would lead to high yield. Such plasmas are particularly important to the SSP because thermonuclear burn involves complex processes that occur in both weapons and inertial confinement fusion (ICF) capsules and are not well understood. Computational simulations are extremely complex, with many calibrated parameters. NIF experiments will provide better understanding of the underlying physics and reduce uncertainties in weapon performance. The results of these experiments will be used to improve first-principles models. They will also better establish calibration parameters for simplified physics models that must still be used because full-physics calculations are too complicated for even the fastest computers. Furthermore, this work lays the technical and physics foundation for inertial fusion energy (IFE).

R&D Priorities

Properties of Matter at Extreme Conditions

Stockpile stewardship in the absence of nuclear testing requires a broad and deep understanding of materials response at extreme conditions. Complex physics interactions over a variety of length and time scales must be well-understood in regions that are difficult to access and diagnose. Examples include shock-induced chemistry, plasticity, nucleation processes, and phase transition kinetics; high-strain-rate phenomena and strength effects; high-pressure and high-temperature synthesis and characterization of novel materials; equations of state; and properties of matter under extreme conditions. To build the high-fidelity physics-based capabilities needed for assessment and certification, these detailed physics and scaling laws and their limits must be understood across time scales ranging from picoseconds (ps) to seconds, and length scales ranging from the atomic to the bulk. Further, in regions that are inaccessible with current technology, detailed models supported by appropriate scaling laws from experiments and strong physicochemical theories must be developed.

- Time resolved measurements will be an essential driver over the next 3 to 10 years for multiple research topics. Resolution will need to be as fine as ps for some studies (e.g., chemistry), while duration may be as long as μs-ms for others (e.g., thermal transport, kinetics).

- Increased attention should be given to understanding and demonstrating appropriate scaling laws for physical models, computational models, and materials' response. In particular, we must better link the nanoscale to the bulk through refined mesoscale models, and tie response models together across wide pressure-temperature ranges (100 GPa–1 TPa).

- R&D investments in experimental diagnostics are needed for in-situ probes such as high-energy radiography/imaging, x-ray diffraction, extended x-ray absorption fine structure (EXAFS), and widely applicable temperature diagnostics. The ability to quantitatively measure spatial variation in velocity, density, temperature, and chemistry will enable improved modeling capabilities. Thus, additional investments are needed in developing platforms combining multiple diagnostics at multiple length scales. Ideally, diagnostics should be fieldable and cross-validated at multiple platforms.

- The span of HED experiments covers cold dense, warm dense, and hot dense matter. An improved understanding of the structure, constitutive properties, and equation of state of dense solids, fluids, and plasmas would improve our knowledge of various materials' response.

- Also needed are the development of XFEL-specific HED diagnostics to address numerous scientific gaps in dynamic mesoscale material response, such as dynamic tomography, 3D orientation imaging microscopy, dark field x-ray microscopy, and inelastic x-ray scattering.

- High-repetition-rate long-pulse lasers are currently planned to be installed at the brightest x-ray sources. They provide unprecedented opportunities to map out phase boundaries and large regions of phase space and to detect low-signal phenomena.

- R&D investments in high-throughput target fabrication and diagnostics, data analytics and machine learning, and rapid simulation and feedback control will be required to harness this potential.

- As models improve, increased research emphasis should be given to increasing complexity. For example, understanding material interactions under extreme conditions, and the roles of competing physics, in one P-T regime compared to others.

- Target fabrication capabilities must evolve to keep pace with HED experimental demands. Currently, the most urgent development needs lie in metrology and foam synthesis. In metrology, improved nondestructive methods for depth profiling and compositional analysis must be developed. For foams, methods that enable more control over morphology and local composition are desired. Additionally, there is an ever-growing development need for capabilities that allow fabrication of high-quality targets to take advantage of emerging high repetition laser sources.

Properties of hot dense matter

The atomic, thermonuclear, nuclear, and radiative properties of hot matter encompass all the physics and engineering aspects of obtaining full ignition. Included are dense plasma absorption and emission spectroscopy; radiation heating; opacities; spectral line shapes; dense plasma effects and the breakdown of the isolated atom picture; nonequilibrium atomic kinetics and radiation transfer; and detailed x-ray spectra simulations.

In addition, plasma transport properties such as electrical and thermal conductivity, viscosity, and charged particle stopping are important. Properties of hot dense matter also encompass thermonuclear and nuclear processes in dense plasma environments. Examples of the phenomena of interest are plasma screening, non-Maxwellian ion distributions (kinetic effects), nuclear excitation by electron capture, and big-bang nucleosynthesis.

All these phenomena occur in a moving fluid that absorbs and emits electromagnetic radiation, and in so doing modifies its dynamical behavior (radiation hydrodynamics). This is the area of integrated physics that relies on physics models and data coming from materials at extreme conditions and properties of hot dense matter. Of particular interest is the role of hydrodynamic instabilities in fusion plasmas.

In the pursuit of ignition, it is crucial to understand how various heating and cooling mechanisms, hydrodynamic mixing, and engineering features (such as laser drive and target and hohlraum design) impact capsule performance. Some needs include:

- Improved hydrodynamic mix models, validated with experiment.

- Integrating reduced-order models into design codes that allow incorporating detailed microphysics in hydrodynamic simulations.

- A better understanding of dense plasma effects on atomic, nuclear, and thermonuclear processes in hot, dense, and high neutron flux environments, both for basic science and mission science applications.

- With the advent of exascale computing, use high-fidelity physics codes such as particle-in-cell (PIC), quantum, and classical molecular dynamics, to develop improved microphysics and mesoscale models that feed into reduced-order models for design codes. An important application is a proper treatment of high-Z/low-Z mixtures for all transport processes in hot dense matter.

- Obtaining focused physics data (e.g., opacities, electron-ion coupling, stopping power, nuclear processes) for model validation purposes in the hot dense plasma regime is extremely challenging due to the coupled nature of hot dense matter. Increased R&D investment is needed in platforms, and improved diagnostics are critical. Time-resolved multichannel spectrometers and proton spectrometers are examples of the latter.

- New experimental platforms, including capsule and hohlraum designs and diagnostics, are a high priority. High energy neutron, x-ray (~1 million electron-volts, MeV), and gamma-ray imaging for a wide range of capsule designs, including those with high-Z pushers, will be needed to gain a better understanding of the convergence properties of these capsules. Radiochemical techniques and the use of proton activation as a mix diagnostic show promise. The challenge will be whether target fabrication with the necessary materials is possible.

- Advanced diagnostics that can provide insights into conditions in burning deuterium–tritium (DT) plasmas, including neutron, x-ray and gamma emission as function of time and space with high temporal (~10s ps) and/or high spatial resolution (~μms). These diagnostics need to operate in very harsh background and EMP environments generated by MJ neutron yields in ICF experiments.

- In many ICF implosions, the distinction between kinetic and hydrodynamic effects is blurry. A metric identifying when kinetic effects matter to a design code will be needed. Incorporating kinetic effects into design codes through either kinetic equation approaches or by adding additional moments to the radiation-hydrodynamic equations would improve predictive capability in this regime.

- Experiments and simulation generate large amounts of data and information that must be analyzed to gain understanding and draw conclusions. Data analytics and machine learning have recently become useful tools for researchers in HED physics and we expect these to continue to grow in importance.

- Quantum computing formally includes and supersedes classical computing. Quantum algorithm theory currently shows that many if not most classical algorithms for treating multiphysics phenomena in the HED regime can be expected to see quadratic or better speedups over what is possible with known classical algorithms. If and when large-scale fault-tolerant universal quantum computing becomes a reality, this will significantly impact time to solution and numerical accuracy of nearly every aspect of HED simulation.

Laser–plasma interaction and applications

The study and manipulation of laser-produced plasmas in nonrelativistic and relativistic intensity regimes is important for many applications in HED science. At high laser intensities, extreme plasma conditions that mimic astrophysical conditions, such as gamma-ray bursts, can be created. These give rise to copious emission of hard x rays and energetic particles, which are both of fundamental and practical interest. The intense electric and magnetic fields found in such relativistic plasmas also have the potential to be harnessed and applied to other areas of science (e.g., compact accelerators and radiation sources):

- A predictive modeling of laser–plasma interactions suitable for hohlraum physics studies and the development of plasma optics. Another need is incorporating into beam-propagation codes the kinetic and nonlinear effects important to NIF laser–plasma interactions as identified in PIC and Vlasov codes. Beam propagation codes must also be coupled to rad–hydro codes.

- The precise temporal and spatial manipulation of the interaction of high-intensity and ultrashort (sub-picosecond) laser pulses with matter. This includes novel diagnostics for characterization of the laser input and full development of a short-pulse simulation capability in support of NIF–ARC (Advanced Radiographic Capability) and smaller-scale facility experiments.

- Secondary sources of particles and photons based on laser–plasma interactions have potential for HED science and stockpile-stewardship-related applications and diagnostics. In particular, multi-modal radiography using concurrent x-ray and neutron sources has the potential to enable studies of HED materials at both static and dynamic conditions undergoing complex and rapid temporal evolution.

- With the emergence of high-repetition-rate, high-intensity short pulse lasers, HED experiments at high-rep-rate will be transformative for the science of laser–

plasma interactions and applications. The integration and development of high-throughput targets and diagnostics, cognitive simulation with advanced design optimization loops that rapidly integrate empirical data, and feedback control, and advanced computational hardware (application-specific integrated circuits (ASICs) and edge computing) will be required to harness this potential.

Inertial Fusion Energy

Fusion energy offers a long-term vision for enduring energy and climate security for the U.S. and the world. Recent results on the NIF that have demonstrated propagating burn and significant yield amplification establish the technical feasibility of energy gain via the laser-driven indirect drive concept. This and continued progress toward improved ICF and HED performance on multiple platforms, investments in rep-rate HED science and technology, and LLNL's substantial capabilities in large-scale system design and engineering position LLNL to uniquely drive forward the foundations needed for inertial fusion energy. Some of the key science and technology developments needed for feasible and economically attractive IFE include:

- Fundamental HEDP science, including, driver-target energy coupling, beam–plasma interaction, hydrodynamics, transport properties, material properties at extreme conditions, atomic and nuclear physics at HEDP conditions, and novel sources of particles and photons.

- High-gain target physics, including: an understanding of physical limits on design parameters applicable across drivers, unique designs for specific drivers, and advanced concepts for increasing gain.

- Drivers, diagnostics, and enabling technology, including reactor-relevant driver development, advanced laser technology and architectures, high-repetition-rate drivers, facilities, diagnostics, and targets, machine learning and cognitive simulation, and reactor engineering and economics.

High-Performance Computing, Simulation, and Data Science

In support of mission needs, advancing computational capabilities to understand and predict the behavior of complex systems by:

- *Providing leadership in the technically challenging drive toward exascale-class computing and future systems with increasing heterogeneity.*
- *Developing and applying higher fidelity, realistic, and reliable science and engineering solutions.*
- *Leveraging AI technologies for improving simulation capabilities and big data analysis.*

High-performance computing (HPC) has been a defining strength of the Laboratory since its founding in 1952. Use of the most advanced computers is the integrating element of science-based stockpile stewardship and has been behind breakthroughs in the Laboratory's principal mission areas. However, improvement in our ability to predict the behavior of complex systems with requisite confidence is urgently needed, particularly when existing data are sparse or unreliable. The rapid growth of data science is opening new approaches to prediction and uncertainty quantification workflows that integrate sensor and experimental data with simulation. In short, the continuing expansion in both scale and complexity of mission requirements drives the Laboratory toward both exascale computing and new data-driven and AI-augmented approaches to scientific discovery and engineering design.

A Cerebras CS-1 wafer-scale engine designed for machine learning and artificial intelligence was integrated into Lassen, a top 20 open science HPC platform, enabling new approaches to predictive modeling.

R&D Priorities

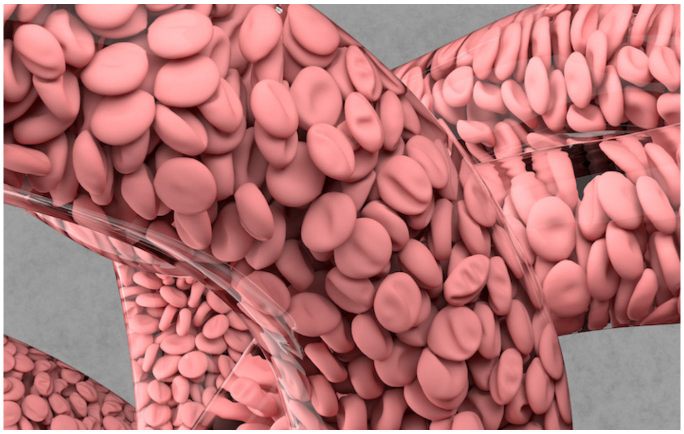
High-performance computing (HPC)

LLNL is leading the drive toward exascale-class computing, where major challenges remain in the development of algorithms for applications that can effectively use massive amounts of parallelism and concurrency while reducing data motion and usage. To move to increasingly heterogeneous HPC architectures, algorithms must be reimagined in ways similar to the paradigm shift triggered by the emergence of distributed parallel programming.

More recent investments by industry in artificial intelligence (AI) technologies have driven computer architectures in directions not always amenable to scientific computing, but those directions do provide significant opportunities if properly leveraged. LLNL must continue to engage with computer vendors to strike a balance between the needs of high-precision scientific computing and low-precision, AI-optimized hardware. Finally, software is a key capability for almost every program at LLNL. Given the increasing need to respond rapidly to new mission requirements while reducing costs, LLNL must continue to adopt community best practices and, when necessary, develop new approaches to software development and maintenance.

- **Computer science and mathematics enabling exascale and beyond**
  The portfolio of LLNL's investments in HPC must be tailored to support and enable the transition to next-generation computing through high-impact R&D in areas such as scalable linear and nonlinear solvers that make effective use of new accelerator technologies; memory-efficient temporal and spatial discretization in complex geometries; asynchronous multiscale and multiphysics methods; verification, validation, and uncertainty quantification; mixed

and variable precision computing techniques; and other analysis methods. Likewise, for efficient data management and end-user workflow, LLNL's computer science capabilities need to bridge domain-specific applications, computational models, and increasingly heterogenous hardware with programming model abstraction layers, workflow and other productivity tools, system software, power management resilience, and data science techniques. Furthermore, as HPC capabilities evolve, so do the potential uses of HPC. The rise of large scale, data-centric computing and its confluence with traditional simulation offers new opportunities for fundamental algorithm and computer science infrastructure development.

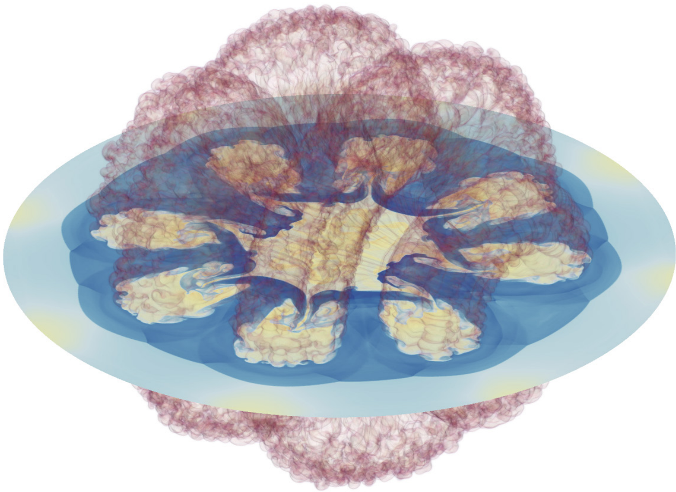


Snapshot of the HARVEY blood flow modeling code simulation showing deformable red blood cells moving through a section of scanned human arterial system.

- **Multiprogrammatic and Institutional Computing**
The Laboratory's Multiprogrammatic and Institutional Computing (M&IC) Program brings tailored, cost-effective computing services to LLNL. M&IC procures and operates some of the most powerful HPC systems in the world and helps to advance software capabilities by procuring and operating test/development systems giving users early access to new technology. M&IC runs the Grand Challenge Program that pushes the envelope of computing with the objective of enabling unprecedented discoveries. M&IC has a thrust in cloud computing designed to support the diverse, rapidly evolving, and growing needs of AI and data science applications and continues to look for ways to improve and advance all aspects of its computational systems and services for institutional users.

- **Innovative architectures**
LLNL provides a fertile research environment for exploring the use of emerging technologies such as processing in memory (PIM), nonvolatile random-access memory (NVRAM), and accelerator technologies (e.g., graphics processing units, GPUs). The Laboratory must work closely with vendors as they develop these technologies to ensure that simulation needs continue to be met efficiently as many vendor R&D innovations are not intended for traditional HPC simulation. The Laboratory must maintain its effort directed toward traditional HPC simulation architectures, as well as identify and develop strategies to exploit the innovations that target nontraditional architectures. Ongoing efforts show that simulations clearly benefit from heterogeneous architectures. Two examples are Cerebras CS-1, an innovative new hardware design that was integrated into Lassen, and the SambaNova system for AI applications, integrated into Corona. These systems are being used for exploring future system architectures, which are likely to include a diverse set of node types and impose challenges for our applications and our system software stack. Thus, large investments are required to develop novel algorithms, programming models, system software, and tools that operate efficiently on these systems in an ongoing codesign process with the vendors. Such leading-edge research will enable us to meet our mission science needs with the full range of possible new technologies, including non-Von Neumann computing technologies such as neuromorphic and quantum computing, building on the initial development of the LLNL Quantum Computing Testbed, which is already being applied to solve mission-relevant problems.

- **Advanced software engineering for high-performance computing**
Hardware innovations in computing architectures such as multicore, GPUs, and AI accelerators require us to rapidly benefit from these new hardware features in software without sacrificing performance, portability, or developer productivity. Enhancing codes to model problems of higher complexity (e.g., multiscale optimal design) is further challenging LLNL software development efforts. The Laboratory has anticipated these challenges with research and innovations in programming models, software builds and dependency management systems, and



The simulation of an ICF-like implosion using the MARBL code on Lassen illustrates the Rayleigh-Taylor and Richtmyer-Meshkov fluid instabilities in a spherically converging geometry.

performance analysis and correctness tools. However, bridging the gap between research and production HPC codes is an ongoing challenge that requires a whole-of-institution approach. The WSC Program, out of mission necessity, has pioneered much of this work and strong coordination is needed to leverage these investments across the Laboratory. Investments in the RADIUSS (Rapid Application Development via an Institutional Universal Software Stack) portfolio of LLNL-developed open-source products are aimed at leveraging these robust programmatic investments across the institution and maximizing the benefits of an open-source community. The RADIUSS effort will harden research tools and libraries; provide direct assistance to developers to build community around their products; support training to strengthen the workforce; forge a path for defining DevOps (best practices for software development and deployment) in the context of HPC development; encourage modern programming styles and practices; and create a culture around improved research software engineering practices at LLNL.

Computational Science and Engineering (CScE)

LLNL develops and applies high-fidelity and reliable simulations in scientific discovery and engineering. To maintain leadership and continue to advance the state of the art, LLNL must create new models to accurately represent physical systems; develop increasingly sophisticated applications, including leveraging AI and machine learning (ML) techniques, to efficiently design and explore more complex, realistic systems; improve our existing models; and assess the predictability of our simulations. We seek to overcome the significant challenges that are imposed by the ongoing revolution in computer architectures by ensuring acceptable levels of performance and efficiency.

- **Improved predictive simulations**
  Uncertainties in simulations are largely dominated by subscale physics. These physical processes are embodied in the continuum simulations through physical data, such as nuclear cross sections, material constitutive properties, and equation-of-state information, along with physical models for unresolved phenomena. While experimental data are used to the greatest extent possible to inform these physical data models, many of the regimes we care about are not easily accessible or measurable through experiment. Thus, we are heavily dependent on high-fidelity models, such as ab initio molecular dynamics, to improve our subscale physics and thereby improve our predictive capabilities. Investments are needed not only to improve the high-fidelity models and codes employed across the Laboratory, but also to enable them to run at scale on next-generation, heterogeneous computer architectures. In some cases, the dynamic nature of the problem requires tight coupling and concurrency between a larger continuum simulation and the subscale physics, necessitating that some form of the high-fidelity simulation be run in situ coupled with the continuum simulation. Promising research is underway to replace or supplement expensive subscale models with machine-learned models trained on thousands or tens of thousands of subscale simulations. Additional research is needed to understand the limits of AI/ML models in these contexts, including how to verify and validate their accuracy and to automatically detect and respond when their behavior is not representative of the high-fidelity simulation.

- **AI and machine-learning techniques incorporated with simulation**
  Simulation capabilities—both discrete and continuous—will be integrated naturally with analytics to produce predictive analysis that brings together data streams and theory-based high-performance simulations. Research is needed to understand the best way to combine data from simulations with machine learning and artificial intelligence techniques to drive experimental design, create surrogate models that approximate

expensive and time-consuming simulations, and improve the robustness and reliability of the simulations themselves. Incorporating machine learning techniques into numerical solution strategies may also enable solution-adaptive acceleration algorithms that can leverage prior solutions to obtain new solutions more rapidly. Integrated learning simulations will provide new and efficient approaches to uncertainty quantification and extend uncertainty estimates to predicting complex data like images, spectra, and time series. A new AI Innovation Center will provide a coordination hub for leveraging the many AI advances occurring across the Programs, industry, and more broadly across the Laboratory. With support from the Institution, as well as the Programs, the AI Innovation Center will establish industrial partner relationships with the many players in AI technologies.

- **Innovative computation for design, optimization, and uncertainty quantification**
  Key questions posed by scientists and engineers typically require exploring highly nonlinear, multiphysics, multiscale simulations of complex systems. More research is needed to develop techniques to quantify uncertainties in the performance of complex systems and to guide the search for their optimal design. Efficacy and efficiency can be improved by developing techniques for more optimal adaptive sampling of ensembles of simulations; by leveraging multi-fidelity models, such as those produced by reduced-order modeling or AI/ML techniques; by amortizing solver costs through concurrent solution of multiple samples; and by understanding the mathematical structure of high-dimensional data. Innovative uses of machine learning can identify unexpected features within ensembles and provide feedback to guide ensemble sampling strategies in solution space. New design optimization methods need to be explored, such as gradient-free algorithms, to solve problems with discrete or otherwise non-analytic cost functions, or where the mathematical formulation makes obtaining exact gradients impractical. In addition, existing gradient-based optimization methods need to be extended to highly nonlinear and dynamic regimes. These methods are the only viable means to explore very high-dimensional design spaces, but they require design gradients; computing these terms could in some cases be added to existing production codes, e.g., using automatic differentiation; in others, appropriately differentiating the numerical constructs poses a fundamental open research question. Methodology improvements must be complemented with user workflow enhancements that streamline execution of large ensembles, promote flexibility in problem formulation, enable quantitative consideration of design trade offs, and help ensure data manageability, interpretability, and integrity. A key workflow challenge is developing a consistent and flexible description of part geometry. In design optimization, representing and modifying part shapes is often the software bottleneck, particularly in full-system design where different simulation codes are used for different system components, or different physics utilize different, and often incompatible, geometric descriptions. Advanced manufacturing machines represent part geometry in still other ways, creating a need for a general, automated, geometry description hand-off from design to simulation to manufacturing.

Information Systems and Data Science

LLNL seeks to leverage machine learning and AI technologies for improving simulation capabilities and big data analysis. Emerging national security priorities in areas such as counterterrorism, nonproliferation of weapons of mass destruction, cybersecurity, and energy security all highlight the need for predictive analysis of the behavior of complex physical and information systems. Data science is also increasingly important in analyzing large data sets for uncertainty quantification (UQ) in nuclear weapons stockpile stewardship, as well as experiments at the National Ignition Facility. LLNL aims to take a leading role in developing capabilities for integrating deep subject-matter expertise into large-scale data analytics. We will build on advances made elsewhere, importing and adapting as much capability as possible and focusing institutional investments on areas that are specific to LLNL's mission needs and that will benefit from the Laboratory's exceptional HPC capabilities.

- **Next-generation AI/ML algorithms and methods**
  Data analytics is driven by questions about systems and the data that they generate. Pattern discovery algorithms are at the core of answering these questions. The queries are exceedingly complex, based on subject-matter-expert models, such as a process model for acquiring or developing weapons of mass destruction. This science-based pattern discovery requires new AI/ML algorithms, improved natural language processing methods, new graph-based methods, and the means to scale efficiently to the largest HPC systems. These methods must be based

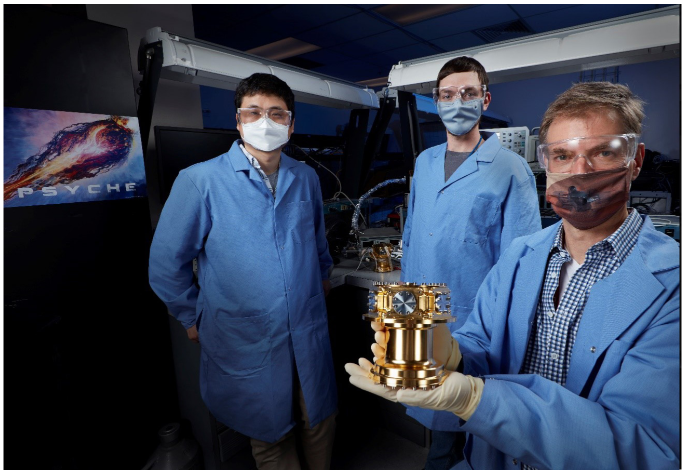
on strong mathematical foundations that enable deeper understanding of performance impacts from real-world requirements and challenges such as limited labeled training data; the need for safe, assured, and interpretable inference; noisy, heterogeneous, multimodal data; and concept drift and the risk of adversarial attacks. New AI/ML algorithms that more easily and faithfully incorporate prior knowledge, such as fundamental physical laws, are also needed, freeing the algorithm to focus on learning and explaining unknown knowledge from data. Finally, the design space of AI/ML models is practically limitless, so developing the theoretical underpinnings to rapidly design new, effective, and efficient model architectures and learning hyperparameters accelerated by HPC resources will be important to the success of next-generation AI/ML algorithms.

- **Distributed decision making and collaborative autonomy**
  The advent of highly dynamic and readily distributed platforms, each with a significant degree of autonomy, offers unprecedented opportunities to deploy "swarms" of multimodal sensors for real-time situational awareness and decision making. Progress in support of multiple mission areas will require extending LLNL capabilities in data science, communications, edge computing, and sensor systems. Information system needs include fundamental architectures for sensor systems that enable real-time collaboration and reconfigurability based on observed conditions. We also need a new generation of algorithms that can collectively fuse multimodal sensor data across a system to construct a real-time "picture" of the operating environment and support actionable decision making. Finally, advancements in reinforcement learning algorithms that defeat human experts in complex games has potential game-changing impacts for complex global security decision making applications (e.g., multi-domain deterrence and defense). Coupled with simulations and HPC acceleration, these techniques if scaled up could integrate large streams of data to learn new strategies and accelerate decision loops, which would help policy makers make better decisions more rapidly.

Nuclear, Chemical, and Isotopic S&T

Advancing fundamental understanding, scientific capabilities, and technologies in nuclear and particle physics, radiochemistry, forensics, analytical chemistry, and isotopic signatures to support LLNL's multifaceted national security mission.

LLNL's capabilities in nuclear S&T are essential for assessing and sustaining the U.S. nuclear weapons stockpile, and integral to reducing the nuclear threat worldwide. In addition, LLNL is an international leader in analytical chemistry and forensic science, supporting efforts in nuclear and chemical threat assessments, incident response, CBRNE (chemical, biological, radiological, nuclear, and explosive) countermeasures and response, and environmental science. These applied capabilities rest on a strong fundamental research foundation aimed at advancing our knowledge in nuclear structure and reactions, heavy-element chemistry, cosmochemistry, and physics beyond the standard model to explore the frontiers of physics and chemistry.



This miniature germanium gamma-ray detector will be part of the mission payload on an upcoming exploration of the asteroid Psyche and will be part of the lander that docks with the asteroid.

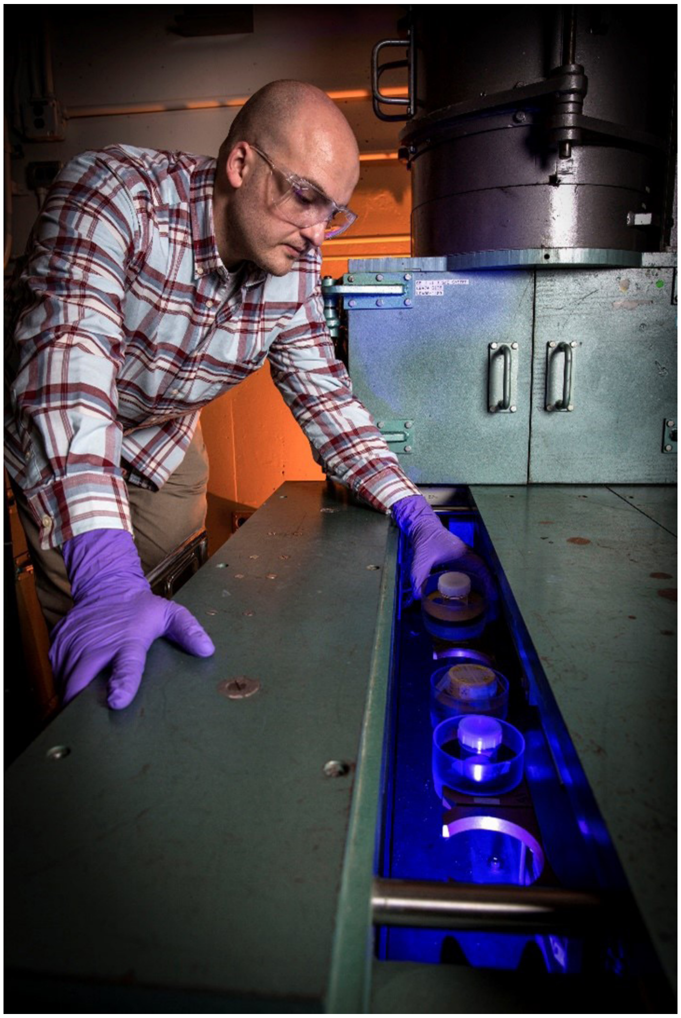
LLNL is currently home to two centers with powerful brand recognition: the Forensic Science Center (FSC) and the Center for Accelerator Mass Spectrometry (CAMS). To enable transformational capabilities in nuclear, chemical, and isotopic S&T, a long-term goal is to establish the Livermore Nuclear Science Center (LiNUS), which will bring all aspects of nuclear science under one roof to meet current and emerging mission needs. This proposed facility will be co-located with a new Forensic Science Center and CAMS to leverage instrumentation investments and domain knowledge to foster collaboration in the development and deployment of new analytical tools and methods.

R&D Priorities

Exploratory research conducted in five principal fields with support from the Laboratory Directed Research and Development Program, NNSA, and the DOE Office of Science enables long-term mission success by supporting technical advances in key nuclear, chemical, and isotopic signatures S&T areas. Forefront scientific research in these fields is critical to attract and retain our future workforce and expand LLNL's capabilities and competencies to meet future national security needs.

- **Nuclear reactions and the structure of nuclei**
  The study of nuclear reactions and the detailed structure of nuclei is essential to understand the evolution of the universe. It also provides the fundamental nuclear data and data infrastructure needed to enhance the predictive capability of weapons simulations and interpret nuclear events. Research into the fundamental properties of nuclei is entering a new era that promises to shed light on many key questions in nuclear physics and chemistry. In this context, combined experimental and theoretical capabilities will be needed to fully unleash the potential of: (1) new national user facilities, such as the Facility for Rare Isotope Beams (FRIB), which offers unprecedented opportunities for harvesting unique and rare isotopes and studying neutron-rich nuclei near the limits of stability; (2) high-performance computing and quantum information science, which will enable a more comprehensive and predictive theory of not only how nuclei are assembled, but how they react; (3) artificial intelligence and machine learning to analyze and identify key uncertainties in nuclear data affecting the national security mission; and (4) new synergistic capabilities combining nuclear astrophysics simulations and nuclear reaction measurements with isotopic measurements of presolar grains and other particles collected from our solar system.

- **Radiochemistry**
Radiochemistry research focuses on establishing new separation and measurement techniques for exploring nuclear reactions relevant to both national security needs and fundamental science, developing platforms for studying the nuclear and chemical properties of materials in a plasma environment, and investigating the limits of nuclear stability and properties of the heaviest elements. The National Ignition Facility (NIF) provides an experimental platform to study nuclear reactions and measure basic nuclear data needed for assessing nuclear device performance and understanding stellar nucleosynthesis. Isotope harvesting at FRIB provides unique opportunities for experimental measurements on unstable nuclei. Development of innovative chemical separation and automated methods is leading to field-deployable technologies for nuclear incident response and enabling rapid, one atom-at-a-time separation platforms for exploring the chemical properties of the superheavy elements. Revitalization of nuclear debris dissolution and measurement techniques sustains mission-critical skills and generates new data to support program needs. Research into radiochemical processes in plasma environments affords insight into mechanisms for chemical fractionation during debris formation and addresses fundamental problems with data interpretation for both stockpile stewardship and technical nuclear forensic applications.



The Nuclear Counting Facility performs radiation detection measurements that support all Laboratory missions, essential science programs, and fundamental research on a wide range of nuclear science and radiochemistry.

- **Analytical chemistry and forensic science**
Analytical chemistry is the art and science of determining the qualitative or quantitative composition of unknown samples. Forensic science at LLNL is associated with the application and deployment of state-of-the art analytical tools and methods related to CBRNE (chemical, biological, radiological, nuclear, and explosive) threats and pre- and post-detonation nuclear forensics while the extraction of unique chemical and/or isotopic signatures is key to detecting and studying many processes in nature and the environment that are of interest. The analytical tools and methods essential to the national security mission also enable groundbreaking research in: (1) cosmochemistry, by exploring the formation and evolution of the solar system; (2) environmental radiochemistry, by studying actinide transport; (3) hydrology, by understanding water cycles in the environment; (4) earth science, by applying unique cosmogenic isotope and ultratrace actinide isotopic capabilities to earth system processes; (5) biomedicine and human health (including personalized medicine), by utilizing high-throughput accelerator or laser-based carbon-14 measurements coupled to chemical separation instruments for rapid medical analyses; and (6) environmental chemistry, by studying the microbial processing, turnover, storage, and transport of various forms of carbon in the ecosystem to understand and ultimately impact the terrestrial carbon cycle, biofuels, and environmental remediation. In the coming years, mission drivers will require continuous improvements in speed and reliability, while fundamental science will continue to push for exquisite sensitivity.

- **Nuclear detection technology and algorithms**
Advanced detector technology forms the basis for acquiring nuclear data, defense against the proliferation of nuclear materials, and scientific discovery. Detector systems relevant to LLNL's mission span a very broad range of sizes and applications. Examples include handheld detectors for first responders, radiation monitors for border portals, gamma-ray detectors for space missions, detectors for dark matter discovery experiments, and neutrino detectors to probe the limits of the standard model, pinpoint supernovae, and locate undeclared nuclear reactors. Advances in detection require robust algorithms to process, analyze, and interpret the data. High-performance computing, big-data architectures, and machine learning will provide a new tool set to fully exploit the trove of data expected from these innovative detector designs. Quantum sensors exploit quantum superposition, entanglement, and squeeze open the opportunity for ultrasensitive threat-detection capabilities.

- **Physics at the frontier**
Understanding the fundamental forces of nature and the properties of the most elementary of constituents of matter and energy drives research at the frontiers of modern physics, which ultimately boosts our ability to develop cutting-edge experimental and theoretical tools and recruit talented researchers to address some of our most complex technical mission challenges for the nation. Only a small fraction (about 5 percent) of the universe is composed of the familiar baryonic matter consisting of protons and neutrons. Indeed, about 25 percent of the universe is composed of an unknown dark matter that only interacts gravitationally, while another 70 percent of the universe is composed of a mysterious dark energy. Furthermore, while the universe seems to have originated with equal amounts of matter and anti-matter, today it is dominated by matter alone. Forefront research areas to explore the makeup of the universe include: (1) the composition and nature of dark matter; (2) neutrino physics and the search for neutrinoless double beta-decay; (3) the physics of quark and gluonic matter at the Large Hadron Collider, the Relativistic Heavy Ion Collider, and the Electron–Ion Collider; and (4) computer simulations of quantum chromodynamics, the strong force that not only binds quarks into mesons and baryons, but also is responsible for the force between nucleons. Physics at the frontier also provides unique opportunities to improve on state-of-the-art detection and analysis techniques, with an emphasis on quantum detectors and machine learning algorithms.

Facilities

To support LLNL missions, nuclear, chemical, and isotopic S&T investments will also target underlying equipment and infrastructure.

Equipment investments focus on refurbishing workhorse analytical instrumentation while building one-of-a-kind capabilities to maintain our technical edge. Top priorities include a new Secondary Ion Mass Spectrometer, Thermal Ionization Mass Spectrometer, a medical cyclotron to produce isotopes of interest locally, a new solenoidal spectrometer to enable direct measurements of neutron-induced reactions on radioactive targets, and upgrades to CAMS. The CAMS upgrades include installation of a gas filled magnet, actinide AMS and cosmogenic AMS beamlines for improved sensitivity, a nuclear science beamline for improved nuclear properties measurements, and a multibeam ion implantation capability for materials studies. These investments expand the experimental capabilities on-site, while providing valuable training for staff and pushing new frontiers in research and development.

Short-term infrastructure investments aim to better integrate capabilities and to improve mission delivery. Priorities include investments that will enable greater colocation of personnel and resources for enhanced capabilities, such as a revitalized accelerator complex in B194, renovated radiochemistry laboratories and dissolver facility in B151, a refurbished and expanded CAMS facility, access to DOE neutron, photon, and radioactive beam facilities across the U.S., and a collaborative information hub. Longer-term investments will focus on establishing the Livermore Nuclear Science (LiNuS) Center, a unique and dedicated facility with a Variable Energy Neutron Source (VeNuS) delivering pulsed, tunable, mono-energetic neutron beams for nuclear experiments, collocated with radiochemistry and atom and nuclear decay counting capabilities. Such a facility will have reconfigurable laboratory space, make use of high-sensitivity, precision instrumentation, and have the capability to produce targets of short-lived radioisotopes for crucial experimental data needs.

Lasers and Optical Science and Technology

Designing, building, and reliably operating complex laser systems that dramatically advance the state of the art for strategically important LLNL missions.

Core competencies in lasers and optical materials have enabled LLNL to design, build, and reliably operate a series of large and complex laser facilities for basic and applied science driven by national security. These lasers have successively broken world records in laser energy, power, and brightness, and have enabled world-leading science, including recent near-ignition fusion experiments on the National Ignition Facility (NIF). These successes reflect longstanding expertise in systems engineering, laser construction and operation, and building collaborations and tech transfer with commercial partners, which are complemented by leadership in photonics, high energy density (HED) science, optical materials, laser–material interaction physics, and laser system modeling and simulations. Sustained investments in these core competencies will continue to enable innovative advances in laser design and capabilities, and support DOE, Department of Defense (DOD), and broader national security missions.

Innovative laser architectures and components, and the underpinning laser and optical materials science, all come together to enable next-generation laser systems for LLNL missions.

For the core mission of stockpile stewardship, the NIF continues to be an invaluable tool for exploring HED regimes not accessible by other facilities, including conditions relevant to burning plasmas and ignition. The NIF provides key insights and data for simulation codes used in weapon-performance assessments and certification and is also an increasingly important resource for weapons effects studies and national nuclear forensics analysis. Sustainment of our core competencies is critical to operating and continuously improving NIF's accuracy, performance and cost efficiency as stewardship leverages new accessible regimes on the NIF.

LLNL is also leading the design and build of next generation ultrashort-pulse lasers, particularly for DOE-relevant HEDS applications that require high average and/or high peak power. Of growing importance is laser-driven secondary sources such as x-rays, gamma rays, protons, electrons, and neutrons. The use of laser-induced plasmas to accelerate electrons to many-million electron volt (MeV) levels in very short distances has been demonstrated and used for MeV x-ray production with potential for SSP and other radiography applications.

In addition to DOE applications, LLNL continues to develop lasers and optics for strategic DOD needs as high-average-power or pulsed lasers remains a disruptive technology for defense. Advanced laser architectures, optical system design, and laser–material interaction science are central to providing timely solutions to existing and emerging threats. DOD communications, navigation, and sensor systems also increasingly employ laser and photonics systems containing LLNL technologies and create synergies with broader LLNL and DOE interests.

Longer-term, recent successes on the NIF motivate emerging needs for next-generation laser systems and optics S&T that can cost-effectively achieve the vision of a high-yield fusion facility for stockpile stewardship as well as the foundations for inertial fusion energy.

R&D Priorities

- **Advanced Laser Architectures and Technologies**
  A principal focus is to sustain LLNL's world leadership in high energy, high peak power, and high average power laser technology. Targeting these focus areas, LLNL will explore novel laser system architectures, new gain media or other optical energy storage or harmonic conversion schemes, and laser components or subsystem demonstrations. Investments are particularly needed to extend current capabilities

in pulse energy, wavelength, repetition rate, peak power, efficiency, beam quality, laser precision, and cost-per-delivered-energy in scalable high energy laser systems. Additionally, focused investments are needed to develop and demonstrate applications of laser-driven particle or radiation sources relevant to HED science, stockpile stewardship, and/or critical national security or national competitiveness needs.

- **Laser System Engineering and Performance Modeling Codes**
  One of LLNL's strengths is the multidisciplinary, system engineering approach to understand the requirements and risks of complex laser systems through their entire lifecycle. Such an approach leverages unique capabilities, a long track-record of physics models-based systems design and optimization, and the use of TOP500 high-performance computers (HPC) with hybrid CPU–GPU architectures. Such tools enable the development of innovative architectures with a shorter development cycle, reducing risks and costs, and ensuring safe operations of the lasers running at their full potential. The areas of focus for continued development to obtain more efficient and precise numerical schemes and capture more detailed physics are resonator simulations, beam propagation, adaptive optics emulation, pumping and laser amplification, nonlinear effects, birefringence effects in heated and stressed media, and thermo-mechanical codes in isotropic and anisotropic situations.

- **Laser–Material Interaction (LMI) Science**
  Understanding and controlling matter–light interactions is an LLNL core competency that extends well below laser conditions typically associated with HED science to include optical material damage in advanced laser systems, laser effects in directed energy (DE) weaponry, and fundamental science of laser-based material processing. Investments in experimental LMI science and computational modeling will expand applications for lasers in areas important to the Laboratory.

- **Optical Diagnostics and Photonics Technologies**
  Optical diagnostics and photonics technologies play a key role in supporting experimental science platforms at LLNL, delivering high precision data to the stockpile stewardship program, providing key measurements for understanding ICF target performance and certifying precision laser pulse shaping on the NIF. High-risk, high-reward ideas and innovations in this focus area are needed to support future laser architectures, control of precision shaped beams and pulsed waveforms, advanced velocimetry, broad spectrum plasma probing, plasma photonics, and RF photonics. Spinoff technologies to address national security challenges include remote sensing, electromagnetic dominance, covert signals intelligence, and secure wireless communication. Continued investments in these technologies will maintain world-class expertise, build our future workforce, and play a central role in developing novel, mission-relevant capabilities.

- **Optics and Optics Manufacturing Technologies**
  This area concentrates on developing novel optic designs and fabrication processes to increase their functionality, lifetime, and yield enabling the performance of high power and energy lasers and imaging systems. This includes continued development of: laser damage resistant optics and coatings; optics with unique functionality (e.g., diffractive, polarization and phase control); paradigm-shifting fabrication methods (e.g., additively manufactured, meta-surface, and freeform optics); customized fiber gain media structures; new materials (e.g., gain media, optical filters, and transparent conductors); methods to recycle optics (damage repair, light blocking); and optical fabrication processes to improve quality and yield with our vendor partners.

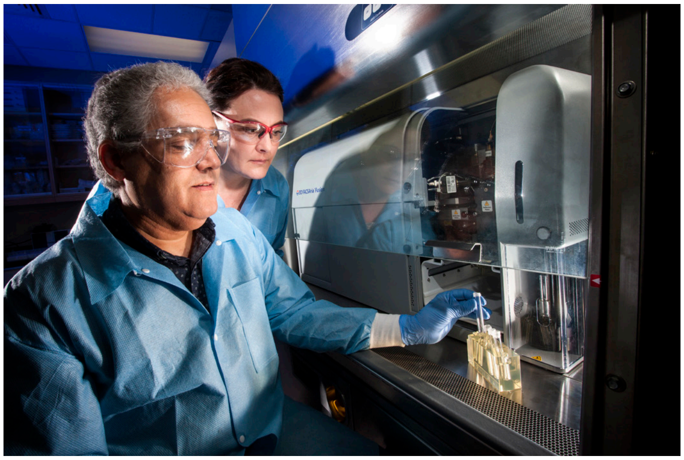
- **Pumping Technologies: Diodes, Pulsed Power, and Energy Storage**
  Advances in pump diode technologies will enable new laser architectures that are both more compact and more efficient. These advances drive the need for novel energy storage and delivery technologies to power high efficiency pump diodes, including new pulsed power technologies to drive pulsed laser systems. Investments in the fundamental understanding, optimization, and integration of pump diodes and driver technologies will expand applications for advanced laser systems and strengthen LLNL's position as a leader in diode-pumped laser S&T. Specific areas of interest include semiconductor laser materials and devices, integrated thermal and optical solutions, energy storage technologies, and pulsed power technologies.

- **Beam and Pulse Shaping Technologies**
  Advanced technologies for the precision adjustment of laser beam profiles, wavefronts, waveforms, and spectra are critical to Laboratory missions. These ensure reliable operation of experimental laser facilities, optimization of laser–target interactions, and high beam quality directed energy. Innovations in this focus area are needed to support high fluence beam shaping at larger apertures; high bandwidth adaptive optics for gas lasers; long stroke, high reflectivity deformable mirrors for high average power lasers; wavefront sensing techniques with improved accuracy; spatially varying birefringent optics; structured light with angular momentum; picosecond pulse shaping over long record lengths; and novel techniques for spectral encoding to mitigate undesirable laser-matter interactions. Continued investments in this focus area will maintain existing competencies and give rise to unforeseen control capabilities.

Bioscience and Bioengineering

Working at the interface of biology, engineering, and the physical sciences to address national challenges in biosecurity, chemical security, human health, and bioeconomy.

The biosciences and bioengineering core competency emphasizes a culture of multidisciplinary research that fosters innovative biological problem solving through integrated technology development. The core competency combines in-house expertise, cutting-edge capabilities, and special facilities needed for groundbreaking research that addresses pressing issues in health, energy, and environmental security. We rely on a convergence of fundamental biology, high-performance computing, precision measurement, and engineering to understand and predict the behaviors and evolutionary trajectories of complex biological systems. We draw on world-class capabilities in genomics, immunology, bionanomaterials, bioengineering, and advanced manufacturing to perform our work.



High precision measurements of in vitro systems are key to integrating world-class computational resources with targeted experiments.

Our main mission focus is developing and maintaining the biosciences and biotechnology expertise needed to understand and manipulate complex cellular systems. We make strategic investments in developing tools and technologies that enable more robust and quantitative biological characterizations; develop a deeper understanding of the complexity of biological systems and communities relevant for health and environmental security; and employ these tools and understanding to deliver solutions for countering emerging threats.

R&D Priorities

Significant challenges exist in rapid response to pandemics and emerging disease and in developing effective biomanufacturing strategies that require transformational response strategies. New approaches are needed to detect, understand, and counter health and environmental threats on an exponentially faster time scale. Cost-effective and environmentally sustainable solutions are needed for biomanufacturing of materials for national security and for supporting a robust supply chain. To address these challenges, we engage in research activities within three strategic thrusts that focus on integrating experimental and computational tools, expanding our understanding of cellular mechanisms, and developing solutions to counter vulnerabilities. We closely integrate computational tools and experimental measurements to characterize and predict changes in the behavior of complex biological systems and understand how they respond to environmental perturbation. Our researchers are working to understand the mechanisms of injury and disease, engineer microbial communities for health-related and environmental objectives, and develop biomaterials and bioprocesses for the bioeconomy. These efforts bolster our ability to fundamentally understand the biological drivers for specific outcomes and translate that understanding into tangible science-driven solutions.

We focus on solving key national security problems within four research themes: 1) rapidly responding to the emergence of novel pathogens; 2) microbiome engineering for health, energy, and the environment; 3) diagnostics, prognostics, and treatments for cognitive impairment; and 4) biomaterials and biomanufacturing for bioeconomy and supply chain security. The primary goal of the first research theme is to enhance our ability to rapidly respond to the emergence of novel pathogens and build a flexible response strategy that can more quickly detect and treat infections. The second research theme, microbiome engineering, is focused on understanding microbial communities within the environment and within the human body with the goal of comprehending and manipulating those communities for desired, beneficial outcomes. The third research theme is focused on understanding human brain function for protecting neurological health. The final research theme is developing bio-based materials and processes to address sustainability and supply-chain security. These research themes were chosen to leverage our strengths and expertise in biology, computing, and engineering, and to position us to effectively address key national needs in the coming decade.

Strategic Thrusts:

- **Integrate experimental and computational tools to enable quantitative descriptions of complex biological systems**—We aim to create rapid design, build, test, and learn (DBTL) cycles that couple world-class computational resources with targeted experiments to enable a deeper understanding of complex biological systems. This approach allows us to predict how these systems respond to manipulation, stress, and countermeasures. Interrogatable biological and computational models are needed that can be modified in a systematically controlled manner to measure responses to differing experimental conditions. These models will allow us to understand how environmental changes (exposure to toxins, infectious agents, diseases, changing climate) affect the organism and then predict the organism's response. These tools will be applied to create a more comprehensive understanding of microbial communities, the human immune system, and the human nervous system. Our priorities are to:

    - Develop physiologically relevant, high-fidelity in vitro and in silico tools that are validated by comparison to the in vivo system.

    - Create computational tools for large-scale, predictive, and comparative biology challenges to understand, predict, treat, and prevent diseases of national health security concern.

    - Develop and use state-of-the-art bioengineering, additive manufacturing, and bioprinting technologies to create human-relevant 3D experimental models that incorporate precision real-time measurement.

    - Develop and improve animal models that recapitulate human phenotypes. Develop novel high-resolution, high-density two-way interfaces between biological and physical worlds.

- **Expand our understanding of cellular mechanisms**—Understanding cellular mechanisms and the interaction among cells, both within tissues and within communities, is essential to developing our response to our national security needs. This knowledge provides the basis for engineering cells and communities to combat disease and develop bioproduction methods. Our priorities are to:

    - Understand, design, and engineer microbes and microbial communities for health, clean energy, and the environment

    - Improve our understanding of the molecular basis of disease and microbial ecology within the natural environment and the host

    - Understand the correlation between genotype and phenotype in organisms involved in pathogenesis and biomanufacturing

    - Improve our ability in gene editing and biosystems engineering including massively parallel genome engineering coupled with evolution

- **Develop solutions to counter current and emerging challenges**—Combining strengths in interrogatable models with cellular mechanisms and cellular engineering enables a revolutionary, holistic approach to accelerate the development of countermeasures to human exposures and disease. Establishing a predictive framework for cellular system identity and function will allow us to create capabilities for engineering microbes and communities for disease prevention, ecosystem sustainability and security, and biomanufacturing. Our priorities are to:

    - Exploit our integrated in vitro, in vivo, and in silico models to predict human phenotypic outcomes of naturally, chemically, and biologically induced neurodegeneration.

    - Design and engineer nanostructured materials and advanced characterization tools for national security applications.

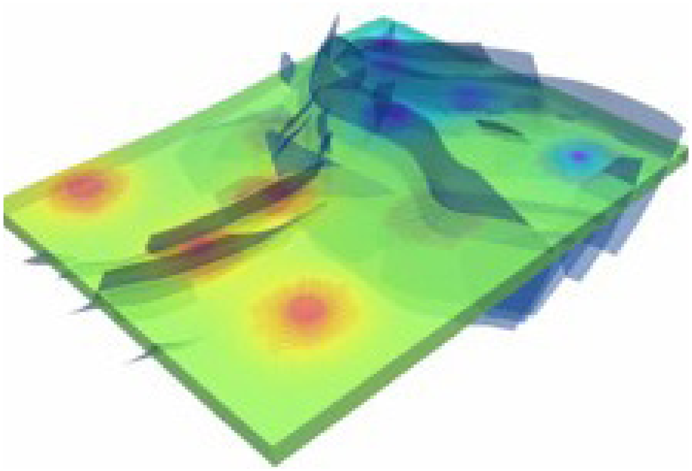
    - Accelerate the development of therapeutics, prophylactics, and next generation vaccines; develop next-generation diagnostic and surveillance systems.

    - Develop platform technologies to leverage biological systems to manufacture novel, critical, and strategic materials.

Earth and Atmospheric Science

Advancing the frontier in Earth and atmospheric sciences to develop innovative capabilities that drive LLNL's energy and national security missions.

The origins of Earth and atmospheric science at LLNL can be traced to the Laboratory's nuclear test activities, atmospheric fallout prediction, and later, geological containment of underground nuclear tests and test-ban treaty verification. Over time, interest expanded to address pressing national environmental and energy challenges such as radioactive waste disposal, geologic storage of carbon dioxide, energy resources such as geothermal energy and shale oil and gas, ozone depletion in the upper atmosphere, and the transport of contaminants in groundwater and the atmosphere. The Laboratory's core competency in Earth and atmospheric science has been closely tied to long-term leadership in high-performance computing (HPC) and data sciences. The validated simulation models developed by LLNL scientists have provided predictive capabilities that find wide-ranging energy, environmental, and national security applications.



Simulation of geologic carbon storage in a faulted region of a potential storage reservoir in the Gulf of Mexico. The simulation was performed using LLNL's exascale reservoir simulation code, GEOSX.

LLNL's longstanding leadership in atmospheric science is central to climate change, renewable energy systems, and atmospheric chemistry, transport, and dispersion modeling. The National Atmospheric Release Advisory Center (NARAC) and Earth system modeling and analysis represent major areas of longstanding LLNL leadership.

NARAC modeling capabilities provide timely and accurate efforts in the event of hazardous emissions, such as the Fukushima radioactivity release in 2011 and the Chernobyl fires in 2020, and have also been used in observation-to-source inversion to determine the location of airborne radionuclide releases. The LLNL Climate Program's Earth system modeling research advances coupled model development on cutting-edge computers, cloud parameterization, tool development for model diagnosis and intercomparison, and management of "big data" for climate research. Importantly, LLNL researchers have also produce groundbreaking analyses of rigorously fingerprinting the causes of "unequivocal" influence of human activities on climate change and their potential consequences on the Earth system. LLNL is also one of the lead developers of DOE's multi-institutional Energy Exascale Earth System Model (E3SM), which enables predictions of climate evolution with unprecedented spatial and temporal resolution.

In Earth science, LLNL has developed world-class capabilities in modeling subsurface modeling phenomena, including shock physics, seismic simulation, fracture mechanics, and other geophysical signals associated hydraulic well stimulation with both natural and anthropogenic activities. The behavior of rocks under loading, the propagation of seismic energy, and the movement and reaction of subsurface fluids underlie many important national security and energy applications. Among these are the detection of clandestine nuclear tests; the vulnerability of underground structures to attack; the hazard earthquakes pose to critical structures; the safe disposal of waste products produced in energy waste generation; and the management of hydrocarbon, thermal reservoirs, and reservoirs used for storage of carbon dioxide and hydrogen.

In addition to solving problems in critical mission areas, these capabilities provide the basis for worldwide collaborations with leading academic groups, industrial partners, and other national laboratories. Our state-of-the-art research and world-class scientific capabilities, including leadership-class HPC facilities, have enabled LLNL to attract and retain a diverse and talented workforce positioning the Earth and atmospheric sciences discipline at LLNL among the leading geosciences institutions worldwide.

R&D Priorities

Research priorities are driven by mission needs and include:

- **Nuclear nonproliferation and stockpile stewardship**
Earth science is critical to both the detection of nuclear events and long-term performance of the nuclear stockpile. The current successful, empirically based nuclear-explosion-monitoring capability depends critically upon seismic data analysis. Similarly, ensuring effectiveness of the nuclear stockpile depends on detailed understanding of material degradation, compatibility, and reactive transport, an area of research expertise that is critical in predicting the evolution of geologic systems as well as multicomponent engineered systems. New capabilities based on advanced data analytics, multiphenomenological data fusion, and machine learning techniques, coupled with multiphysics high fidelity modeling and experimental observations are needed to improve monitoring of low yield events in new locations and ensure the effectiveness of the nuclear stockpile.

- **Defense and homeland security**
A wide range of defense and homeland security applications would benefit from fast and accurate modeling and simulation tools for assessing the response of geologic media to strong shock waves (and the interaction of those waves with underground structures). Examples include defeating hard and deeply buried targets and assessing the vulnerability of infrastructure to terrorist attack.

- **Whole atmosphere characterization**
Improved characterization of the atmosphere from the Earth's surface to space is needed for the national security mission in space science and for developing new defense technologies, e.g., hypersonic weapons. Observations to support climate model validation and improvement are required for the stratosphere and higher altitudes parameterization. Satellite and earth-based observations play an important role in informing climate models by both enhancing our understanding of fundamental atmospheric processes and in supporting model improvements.

- **Climate change resilience**
Higher-resolution earth system models, both spatial and temporal, are needed to provide accurate simulations/projections of climate change and its impacts at the local and regional scales. Two especially important impacts are changes to precipitation and the occurrence of extreme weather events, both of which are difficult to predict with current models. In addition, remaining technical gaps in Earth system models at the interface of the atmosphere and land/subsurface systems, and subsurface hydrology impede the ability of the models to accurately project key climate variables. At Livermore, we continue to improve climate simulations with an ongoing and comprehensive characterization of model uncertainties, including those in model formulation, structure, and parameters such as those embodied in the E3SM Earth System model. Artificial intelligence holds promise for improving model performance, downscaling, and bias correction that are needed to address regional/local climate impacts.

- **National security emergency response**
NARAC needs next-generation multiscale atmospheric transport and dispersion models as well as inverse modeling tools to attribute measured contaminant concentrations to their sources. Novel tools and modeling capabilities including machine learning are also needed to improve the efficiency and uncertainty estimates associated with NARAC's assessments.

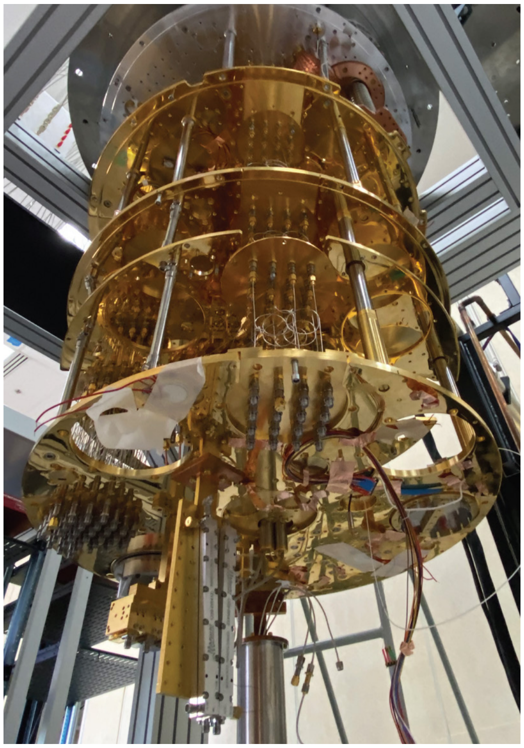
- **Atmospheric modeling for renewable energy**
Forecasting wind and solar generation requires modeling skills in atmospheric flow, atmospheric physics/microphysics, and integrated computational fluid dynamics modeling that are currently not available. Atmospheric models cannot currently handle the complexity of real wind farm topologies and provide accurate predictions of wind patterns. Likewise, atmospheric models representing clouds, water vapor, and aerosol physics and movement are not accurate enough to fully represent time-evolving atmospheric photon transport to solar collectors. Many of these developments may also be applied to constrain the consequences of wildfire, geoengineering, and the potential atmospheric consequences of a nuclear exchange, nuclear winter.

- **Sustainable energy production**
The nation needs advances in subsurface S&T to help enable a safe and secure energy future in the United States. These S&T advances include a better understanding of subsurface stress and the potential for induced seismicity; coupled processes like flow, chemistry, and mechanics; and novel monitoring technologies and data management—all directed at minimizing the environmental impacts of energy production, distribution, and utilization. Included among these concerns is the geologic storage of carbon dioxide, which in California alone may require the subsurface injection of greater than 100 million metric tons of carbon dioxide annually.

Quantum Science and Technology

Harnessing the power of quantum physics to enable new capabilities in sensing, imaging, and computing that address emerging national security needs.

Quantum coherent devices offer the potential for unprecedented precision in sensing and the ability to directly simulate complex quantum phenomena that cannot be described efficiently with classical computing approaches. The continued development and implementation of quantum technologies is expected to have a significant impact on addressing some of the most complex and challenging problems of importance to the Laboratory's missions, particularly in the areas of stockpile stewardship and nuclear threat reduction.



An inside view of a cryogenic refrigerator that houses one of LLNL's prototype quantum computing systems.

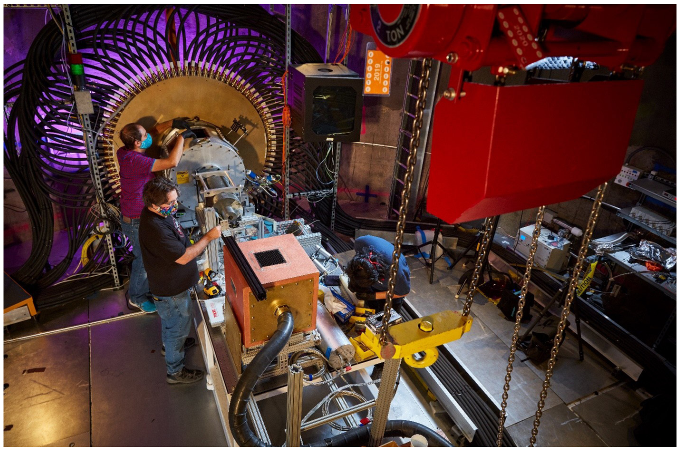
LLNL's quantum science and technology efforts are centered on the use of a multidisciplinary co-design strategy that draws on the Laboratory's deep expertise in physics, chemistry, optics, engineering, materials, and computer science. The challenges associated with realizing the hardware and software approaches needed for a new generation of quantum computers are significant and include synthesis and characterization of materials with special quantum properties; developing a fundamental understanding and control of the sources of noise and decoherence in quantum systems; and careful engineering of the interface between quantum and classical control, sensing, and computing elements. The quantum science R&D priorities at LLNL include:

- **Sensing and detection**—Exploiting phenomena such as entanglement, Bose-Einstein statistics, and wave-particle duality has the potential to enable new sensors and imaging capabilities that far exceed what is possible with today's technology.
- **Quantum coherent device physics**—The building blocks of quantum systems include highly specialized components such as superconducting qubits and resonators that need to be fabricated with high precision under controlled environments. State-of-the-art research laboratories are required to enable the complete design, fabrication, and characterization of quantum devices.
- **Quantum materials**—The performance of a quantum device is often limited by resonant couplings to low-energy states in the materials and interfaces that make up the device (i.e., materials-based sources of noise). Overcoming this limitation requires that subtle forms of noise from decoherence in these systems be understood and controlled.
- **Computing and simulation**—The use of quantum computing and simulation will require multidisciplinary teams of physicists, materials scientists, computer scientists, and engineers working together in a co-design effort to develop mission-relevant algorithms for the quantum computer and to design specialized prototype systems to run those algorithms.
- **Quantum–classical interfaces**—Quantum computers require a classical interface to achieve control and measurement of the quantum device, which requires the development and optimization of scalable quantum–classical interfaces that are capable of low-noise, high fidelity qubit control, and measurement and processing.

Nuclear Weapons Science

Assuring the safety, security, and effectiveness of the nation's nuclear weapons stockpile by providing the science, technology, and engineering (ST&E) capabilities and experts required to support U.S. strategic deterrence in the face of a rapidly changing world and uncertain future.

LLNL's technical excellence in theory, experiments, and modeling has produced tremendous insights into the science and engineering of nuclear weapon operation. We possess the technical expertise to respond to our adversaries today. The nuclear weapons program must pursue a fundamentally new approach to support a more agile nuclear weapons complex of the future and ensure long-term success in deterrence.



Scientists adjust the MJOLNIR (MegaJOuLe Neutron Imaging Radiography) Dense Plasma Focus neutron source and accompanying diagnostics.

LLNL will use a paradigm of anticipation and innovation. The weapons program strives to re-engineer the entire lifecycle of nuclear weapons, from initial concept through design, engineering, production, deployment, surveillance, maintenance, and dismantlement with a focus on agility and sustainability of the system. Most importantly, LLNL must continue to drive ST&E innovation and nurture an exceptional workforce to provide resilience in the face of an uncertain future.

The science that we conduct in support of our nuclear weapons mission is itself a component of our strategic deterrence. In high-performance computing (HPC) and high-energy-density (HED) science, we are not only leaders but pioneers, shaping the international landscape with our work. In the development of next-generation experimental technologies and energetic materials, legacy of successes underscores our capabilities and expertise. We also continuously explore emerging technologies and embrace those that drive game-changing advances for our mission, such as additive and advanced manufacturing.

Our investments, progress, and scientific preeminence will assure adversaries and allies alike of our commitment to ensure the nation can continue to meet the deterrent demands of the future.

Some key science focus areas include:

- **Insightful modeling and simulation methods integrating multiphysics models, cognitive simulation, multiscale modeling, and advanced computing architectures**—LLNL's strategy of fostering tightly integrated codes, platforms, and facilities has continued to deliver major advances in designer productivity and agility. The deployment of Sierra and GPU-enabled simulation tools contribute to this by delivering an order of magnitude improvement in capability. This capability enables significant advances in design, assessment, and certification methodologies for both the current and future stockpile. LLNL will continue to invest in R&D associated with state-of-the art numerical methods, computational algorithms, and physics model development that are fundamental to supporting all advances in predictive science. The enormous advances expected in machine learning (ML) and artificial intelligence (AI) will be a force multiplier for our stewardship mission. Subscale physics can be captured by embedding ML methods in our multiphysics simulation tools, providing major advances in predictive capability. These models, however, will still require large sets of training data, generated by our nuclear weapons science codes running at scale on our latest computer platforms. Automated optimization and AI-assisted execution of simulations will enable a single expert to consider design-innovative attributes efficiently across a range of options.

- **High-energy-density physics and the pursuit of ignition**—The National Ignition Facility and other HED facilities produce unprecedented pressures, densities, and temperatures in a laboratory. This enables higher-fidelity study than ever before of the conditions salient to weapons, directly informing today's stockpile decisions. In the absence of nuclear testing, our enterprise must make impactful stockpile assessments utilizing HED capabilities on a faster timescale and must expand our understanding of burning plasma physics. The ability to achieve megajoule yields at the NIF significantly expands the range of experiments that can be conducted, presenting exciting challenges in laser-target design, fabrication, and diagnostics. Exploration of weapons science questions at HED facilities enable enhanced support to future weapon assessments and design options.

- **Creation and application of tailored energetic materials**—LLNL has delivered first-of-a-kind explosive materials, developed premier reactive flow and thermochemical explosive models, and pioneered the use of additive manufacturing for explosive components. Meeting performance and schedule requirements for future systems will necessitate innovation in four major areas: production, where there is a need to accelerate the timeline; the development of new and tailorable explosives to enable new options for the Department of Defense (DOD); development of highly predictive physics and engineering high explosives (HE) models that are transferable to different scales in order to reduce the schedule and cost of certification; and improved understanding of HE safety to increase efficiency of safe work practices at the national laboratories, Pantex, and DOD sites.

- **Deploying advanced manufacturing technologies**—LLNL is in the process of introducing disruptive techniques that have the potential to revolutionize the future design and manufacturing of nuclear weapons. The nuclear weapons program seeks to reduce the design-to-deployment time for components to three years by utilizing innovative materials and feedstocks; developing new manufacturing platforms; deploying process-aware inverse design methods; and vigorously pursuing technology maturation. This requires close partnerships with our Production Agencies, who need to implement these technologies at a production scale.

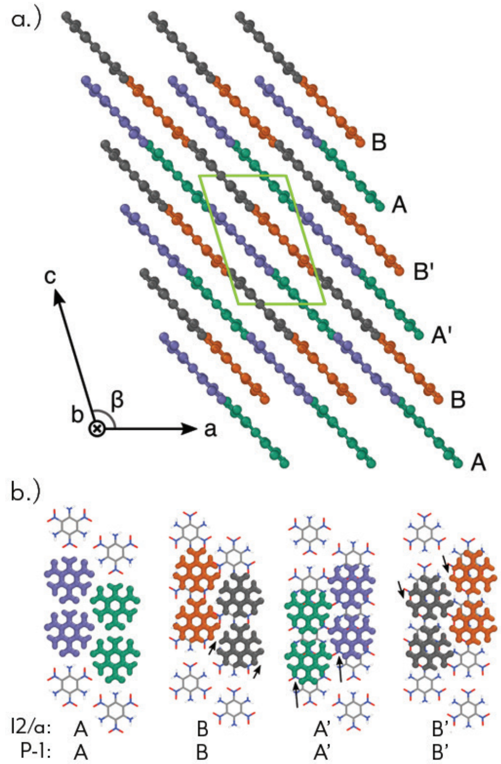
- **Revolutionary experimental platforms, drivers, and diagnostics**—LLNL has long pursued high-risk high-reward technologies to enable an agile and sustainable weapon lifecycle, and to accelerate the delivery of designs, certifications, and qualifications to provide options for our strategic deterrent. The Laboratory must develop new experimental platforms and advanced diagnostics to support evolving needs in survivability, component aging, modern manufacturing, and a changing threat environment. To fully utilize these science discovery and model validation experiments, the Laboratory also needs to develop advanced analysis methods to make the most effective use of data collected.

- **Development and certification of new materials**—LLNL's growing capabilities in advanced manufacturing inspire and enable development of specialized new materials for our modern stockpile. The Laboratory must pursue creative synthesis of materials with the properties required for a myriad of functions critical to nuclear weapon operation. However, certifying that these new materials are compatible and will perform as intended for the entire lifetime of the weapon can delay their adoption significantly. LLNL must pursue automated screening methods for compatibility testing, research into materials degradation, and development of generalized predictive lifetime models that can rapidly assess the viability of new materials.

High Explosive (HE) Physics, Chemistry, and Material Science

Improving fundamental understanding and prediction of HE behavior for the nuclear deterrent and keeping the nation safe from emerging explosives and nuclear proliferation.

One of LLNL's mission needs is to create and apply energetic materials uniquely tuned to specific applications. We must ensure with high confidence the safety, security, and effectiveness of the U.S. nuclear deterrent, bring agility and responsiveness to NNSA for delivering stockpile options for the future deterrent, provide next-generation weapon systems for the Department of Defense, and support U.S. responses to emerging explosive proliferation threats. To meet these needs, the Laboratory must enhance capabilities for understanding and predicting the behavior of high explosives (HE).



(a) The new *I2/a* high-pressure TATB phase showing its ABA'B' layer stacking motif and (b) how the layers are shifted relative to the original *P*-1 phase

High-resolution, predictive simulations of HE require advances in modeling and algorithms that leverage LLNL's world-class scientific computing resources. The Laboratory must also develop novel diagnostics, next-generation light sources, and techniques to enhance chemical and physical characterization of HE materials. New manufacturing methods and faster development of feedstock materials are expected to improve the responsiveness of manufacturing HE components. HE R&D priorities include:

- **Making substantial progress toward a transferable, predictive computational model for HE initiation, detonation performance, mechanical response, safety, aging, and compatibility**—Materials scientists study a reacting material at length and time scales not previously possible. Advances in computing enable improved runtimes for methods bridging from atomistic to continuum representations. We are looking to take advantage of graphics processing unit (GPU) architectures in our codes and applying machine learning and data science. LLNL needs to develop new diagnostics that can measure the temperature and product set of chemical reactions in-situ at nanosecond resolution and micron length scale. Advanced light sources with end-stations authorized for HE detonations should continue to be applied in parallel with efforts to add capabilities at the High Explosives Applications Facility and Site 300.

- **Investigating manufacturing methods and automation with well-characterized understanding linking chemical synthesis, microstructural characteristics, and energetic performance to enable development of options for an agile nuclear deterrent and promote collaboration with the production agencies through accelerated HE feedstock and component production**—Responsive manufacturing offers opportunities to target key performance uncertainties, develop nonintrusive instrumentation for stockpile monitoring and forensics, pursue innovations in safety and surety, and explore proliferation space. In-situ monitoring should be adopted to reduce lot-to-lot variability. Data science techniques with QA/QC measurements accelerate material development, manufacturing, and qualification.

- **Designing, predicting, and qualifying new HE molecules for stockpile use and characterizing homemade explosives**—Efficient and timely evaluation of prospective energetic molecules, formulations, and simulants requires scalable manufacturing processes including kilo-scale batch and continuous flow reactors with specific and tailorable flow characteristics. Continued development in computational chemistry is needed with a target to directly enable the discovery of designer molecules and synthesis routes.

Nuclear Threat Reduction

Developing and delivering enduring science-based, intelligence-informed expertise and capabilities to overcome nuclear threats world-wide.

The threat of nuclear and radiological weapons is an enduring global challenge that requires new technical approaches grounded in a deep understanding of adversary capabilities and integrated deterrence. LLNL combines multidisciplinary science and technology (S&T) with an understanding of existing and future adversary capabilities to: deter, detect, and prevent state and non-state actors' development of nuclear or radiological weapons or acquisition of weapons-usable nuclear materials, equipment, technology, and expertise; counter efforts to steal, acquire, develop, disseminate, transport, or deliver the materials, expertise, or components of nuclear or radiological devices; and respond to nuclear or radiological threats, events, or accidental incidents.

LLNL developed a virtual reality prototype that uses a radiation transport calculation methods to simulate real-time gamma and neutron exposure readings in the virtual environment for more realistic responder training.

Our nuclear threat reduction priorities include:

- **Understanding adversary capabilities and foreign nuclear technologies**—We need validated models for materials and systems that are not represented in the U.S. nuclear stockpile and analytic frameworks to understand long-range future capabilities of state and non-state actors.

- **Characterizing emerging technologies**—We need to better understand the intersection points between nuclear S&T and emerging technologies for data, applications, and innovations that strengthen our early warning proliferation detection capability and assess how they can enable adversaries to improve or conceal their nuclear weapon related activities.

- **Enabling new approaches to nonproliferation and arms control treaty compliance**—We need to improve detection of nuclear proliferation activities by developing new technologies and methodologies, informed by policy needs and operational constraints, to facilitate future international safeguards approaches and arms control initiatives.

- **Advancing nuclear threat detection and assessment**—We need improvements in detector materials and sensors, and more comprehensive and intelligent diagnostic data processing for integrated detection networks to detect nuclear and radiological materials in a timely and accurate manner.

- **Improving nuclear test detection**—We need new technologies to enhance our ability to identify and characterize nuclear explosions above and below the ground, and the ability to fuse and analyze data across modalities.

- **Enabling rapid nuclear incident response**—We need to provide timely and high-confidence assessments with seamless interaction and situational awareness across the whole-of-government. This requires investing in validated, fast-running tools, advanced diagnostics, artificial intelligence, and augmented/virtual reality.

- **Accelerating post-detonation event assessment**—We need advanced technical forensic assessments that use state-of-the-art science, first principles modeling, and experimental approaches combined with data fusion of prompt and material signatures to provide rapid and accurate decision support after a nuclear detonation in realistic environments.

Biological and Chemical Countermeasures

Develop solutions that counter vulnerabilities related to biological and chemical threats and emerging infectious diseases; and advancing the application of biotechnology and related informatics with an emphasis on intelligence-informed, science-based discovery.

Researchers test the efficacy of medical countermeasures on emerging viruses and other biological threats in the LLNL Biosafety Level 3 Select Agent Facility.

LLNL supports U.S. policy, centered within the national security mission, to respond to naturally occurring outbreaks and attacks involving chemical or biological (CB) agents. Our work focuses on developing methods to protect against and aid recovery from illness, chemical exposure, and injury, including new ways to provide pretreatment prophylaxis. Our science is informed and supported by intelligence assessments that help us focus our efforts and drive innovation, which signals preparedness to our adversaries. This is a key deterrence mechanism.

LLNL uses research outcomes and global intelligence to inform the development of tools that better anticipate threats; detect and assess the occurrence of threats; respond to threats with accelerated countermeasure discovery; and contribute to attribution efforts through forensic approaches.

- **Novel CB countermeasure development**—Development of CB countermeasures, including small molecule prophylactics, therapeutics, and vaccines in order to facilitate response and recovery from traditional/non-traditional chemical warfare agents, synthetic opioids, biological select agents and toxins, and biothreat and human-health pathogens. Support the development of tools that facilitate response and recovery from traditional/nontraditional chemical warfare agents, synthetic opioids, novel and emerging pathogens and toxins. Furthermore, employ new model systems (in silico and experimental) that aid in understanding how chemical and biological agents (as well as CB countermeasures) interact within target cells and tissues. In addition to developing agent/pathogen-specific countermeasures, support threat-agnostic approaches based on advances in nanotechnology, synthetic biology, and microencapsulation science to develop innovative materials that aid countermeasure stability, effectiveness, and delivery.

- **Model development and biomarker discovery to accelerate prediction and prognosis of disease or exposure**—Understand the impact of CB on human tissue and organ systems to inform countermeasure development and testing. Mitigate the impact of CB incidents by identifying biomarkers that signal health susceptibilities and impairments before the onset of symptoms so that countermeasures could more rapidly be administered. Protect health and speed recovery by understanding effects of therapies and medical treatment on human systems including physiological and microbiological (microbiome balance) and finding biomarkers to reconstitute and repair microbiomes.

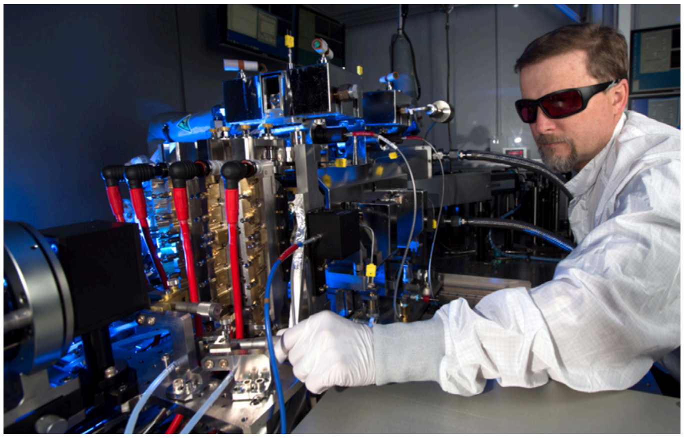
- **High-performance computing simulations and data science to support the CB countermeasure mission and inform response**—Use modeling and machine learning to develop platforms that inform and advance experimentation to counter threats, deepen our understanding of biological systems, and validate biological models to accelerate the development of vaccines, antibodies, and novel types of medical countermeasures for infection or chemical exposure.

Accomplishing these aims will require enduring partnership with other government agencies and institutions, academia, commercial entities, and non-profit organizations.

Directed Energy

Developing compact, robust, efficient high-average-power lasers, high-power microwave technology, and a better understanding of electromagnetic radiation–matter interactions to support national security needs.

Adversarial weapon systems are increasingly putting U.S. military assets deployed on land, at sea, airborne, and in space at risk. Ongoing advances in foundational S&T are driving U.S. interest in developing directed-energy (DE) weapons to counter these threats. Prototype DE weapons are already beginning to be deployed—for example, the Navy's High Energy Laser and Integrated Optical-dazzler with Surveillance (HELIOS) and the Army's Directed Energy- Maneuver Short Range Air Defense Capability (DEMSHORAD). Additionally, prototype High Power Microwave (HPM) systems are also being developed. Although these prototype systems show promise, significant technological challenges remain before DE weapons will have a disruptive impact on national security.



Researchers are exploring concepts for energy-efficient compact systems that generate high optical quality, high-energy, high-power laser beams.

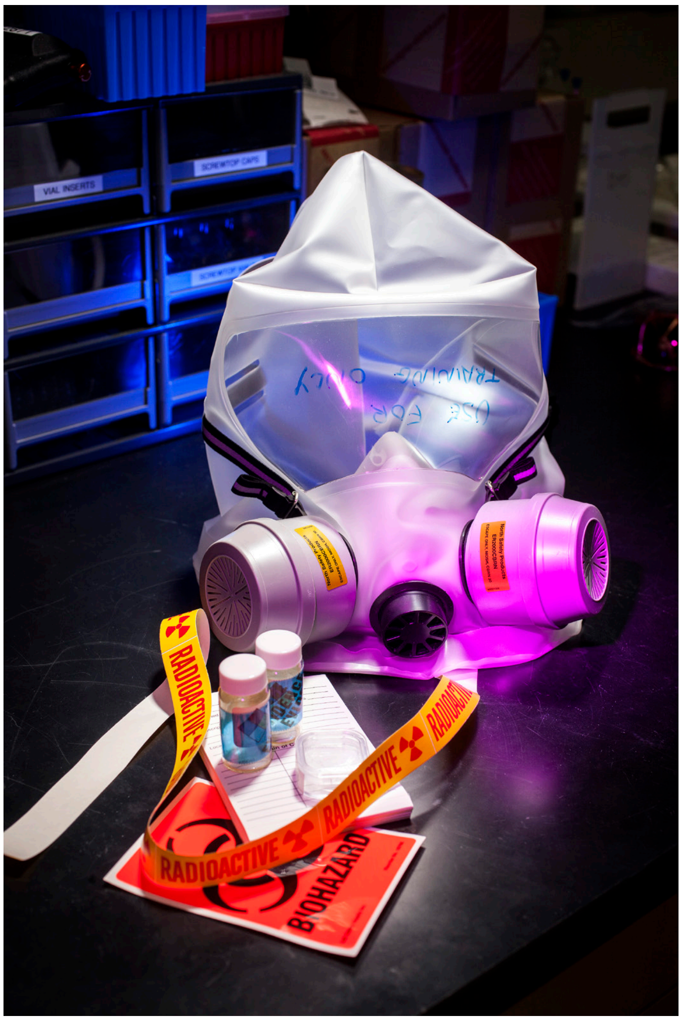
Livermore seeks to meet this challenge by continuing its S&T leadership in developing high-energy, high-average-power pulsed and continuous wave lasers and tunable narrow band and ultrawide band high-power microwave technologies, with a goal of supporting a broad range of tactical and strategic national security applications. Our specific S&T research interests include developing concepts for:

- **Generating very high-power laser beams (> 100 kilowatts) with high optical quality (M2<1.2)**—Key considerations include: efficiency, size, and weight; wavelengths outside the 1–1.1 micrometer (μm) band; lasers with high pulse energies (e.g., >100 kilojoule (kJ) per pulse for <50-nanosecond (ns) pulses); minimizing requirements for external cooling and thermal management; developing materials and components to improve operational robustness and damage thresholds; and developing innovative approaches to subscale testing for proof of principle and risk reduction.
- **High-peak-power microwave technology with frequency agility, high repetition rates, and compact form factors**—Frequencies of interest span 500 megahertz (MHz) – 10 gigahertz (GHz), pulse durations from 1 ns – 1 μs and potential to scale power levels to >100 MW. Topics of interest include high-voltage materials, novel -device concepts, amplifier-based sources, distributed source concepts, wide band antennae, and targeting algorithms.
- **Laser beam control**—Improving delivered power density on a distant target, through innovative concepts for controlling a high-power laser beam as it propagates through turbulent atmospheric conditions.
- **Laser–matter interaction schemes**—Developing a fundamental understanding of laser–matter interaction to improve confidence in lethality and to enhance destructive effects with reduced laser energy and power.
- **Component improvements**—Overcoming severe size, weight, and power constraints, research on improved batteries, cooling systems, and lightweight structures.
- **Improved modeling and simulation**—To better assess target vulnerability, weapon lethality, and system effectiveness with advanced simulation methods and multiphysics modeling tools.
- **Understanding and addressing emerging threats**—Maintaining responsiveness to identify and counter new threats; new countermeasures; or new operational constraints to directed energy.

Forensic Science

Advancing the state of the art in both traditional forensic science and the chemical, biological, radiological, nuclear, and explosive (CBRNE) threat space in direct support of national security and intelligence needs.

New forensic methods, technologies, and multidisciplinary approaches are required that anticipate, prevent, detect, and respond to known and emerging threats and which power readiness across the entire proliferation and use timeline. R&D thrusts include:



LLNL is one of the few institutions with expertise and facilities capable of forensic analysis of threats ranging from biological and chemical to nuclear and explosive.

- **Predicting, sampling, and preserving CBRNE and other signatures—** Collection and preservation of potentially unstable forensic signatures for transport from the field to the laboratory is needed and could include mechanical or chemical methods. Advanced portable rapid screening tools with appropriate detection limits are needed to prioritize suspect sample collection locations to avoid overtaxing forensic laboratories. Other activities can include studies or modeling of the urban or remote environment and how it can affect post-event response and recovery, sample collection location determination, and targeted signatures.

- **Developing and validating novel techniques to detect and exploit the signatures of CBRNE and other threats—**The goal is to create capabilities to identify WMD threat activities, from material acquisition/production and weapon development/testing phases (pre-event) to incident response and forensic analysis (post-event). These signatures may be simple indicators of ongoing or historic WMD activity or may be more complex, enabling a deeper understanding of near- and long-term weapons-related activities. Developing rapid analytical capabilities for accurate measurement of stable and radioactive components plays a vital role for timely response to WMD events. Areas of focus include:

  - New or enhanced tools and technologies for both laboratory- and field-based detection and threat assessment, including multiplexed and miniaturized techniques, "omics"-based approaches to bioforensics, and those that identify the "unknown-unknown" in complex samples.

  - Machine learning-based approaches to data analysis and interpretation and near-real-time threat identification and classification of known and emergent threats.

  - Leveraging nuclear weapons expertise to improve and validate the measurement and prediction of low concentration forensic signatures in pre- and post-detonation nuclear scenarios. Expanding experimental methods and understanding of isotopic fractionation caused by both natural and man-made processes through measurements of stable elements in nuclear materials is needed.

   - Uncovering and understanding the method or sophistication of a synthesis/production pathway by leveraging forensic signatures and their potential interface with comingled hazards.

- **Developing innovating approaches to threat neutralization and defeat**—New approaches are required that both protect people and environments from a wide variety of threats and that accelerate recovery timelines by rapidly responding post-event. This could include material science-, biology-, or chemistry-based defeat or decontamination technologies, medical countermeasures, or force protective equipment.

- **Understanding the scope and nature of human exposure signatures for current and emerging threats**—Develop a robust pharmacokinetic and metabolic understanding of injury caused by and fate of these compounds in the body would enable improved determinations of exposure levels (including chronic low-level), physiological persistence, and metabolic signatures. A key focus is the identification of novel biomarkers indicative of CBRNE exposure and recovery, either at the macro or epigenetic level. Additionally, applications that push toward clinical or field diagnosis would be valuable, especially when coupled with the administration of potential countermeasures.

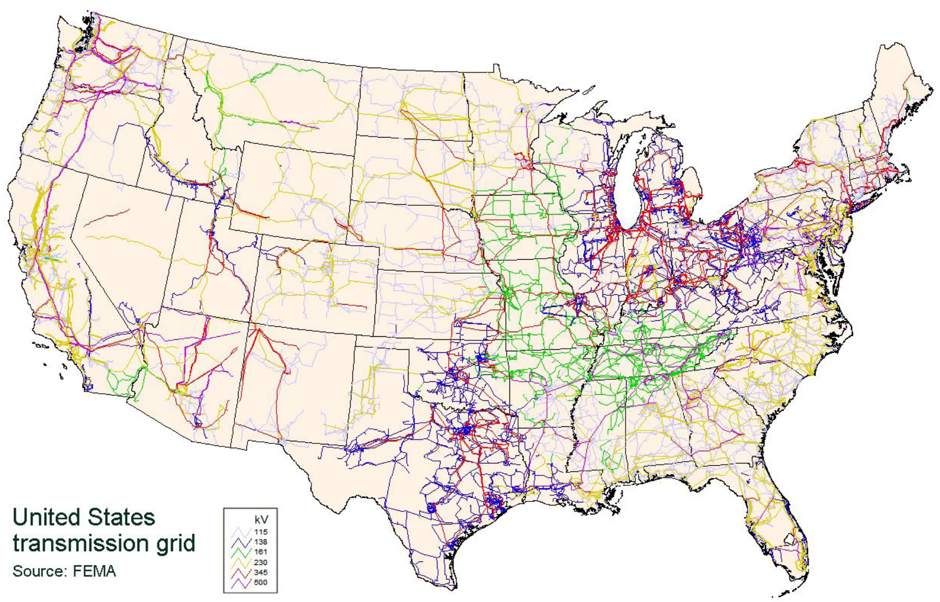
- **Providing statistically relevant objective methods for traditional forensic analyses**—Goals are to improve current forensic science techniques, to reduce the reliance on subjective human-driven comparisons or bias that may be introduced from computational methods, and to bridge the gap between cutting-edge technology and law enforcement applications.

Cybersecurity and Cyber–Physical Resilience

Advancing cyber and network science to support U.S. cyber superiority and ensure the resilience of the complex cyber–physical systems throughout the nation's critical infrastructure.

Ensuring the security and resilience of cyber and cyber-physical systems is integral to national security, domestic security, and both military and civilian infrastructure operations. LLNL is addressing this modern cyber challenge by developing an integrated layered defense approach that leverages numerous unique Laboratory capabilities in this mission area. The layered approach will ultimately be composed of four self-reinforcing pillars of advanced capabilities:

- Understanding our computing systems and supporting network environments
- Keeping adversaries out of our systems
- Detecting and responding to intrusions
- Operating through compromise



The nation's energy grid is an example of critical infrastructure systems requiring cyber-physical resilience to protect against disruptions.

Developing the required capabilities needed to deliver this state-of-the-art layered defense will require building upon many innovative capabilities that are unique to LLNL, such as expertise in high-fidelity modeling and simulation, novel computing architectures, data analytics, software assurance, intelligence-informed risk analysis, sensors, and network science to develop technologies and strategies in support of a broad set of cyber-related missions.

R&D Thrust Areas

- **Measuring, characterizing, and modeling cyber and cyber-physical resilience**—Current approaches to improve resilience rely on general guidelines and best practices, and are unable to quantify security or resilience. Challenges include developing metrics for resilience and assessment methodologies that merge intelligent adversary threats with probabilistic events; tools to understand infrastructure interdependencies and cascading impacts; and software and embedded software capabilities to characterize potential vulnerabilities and impacts of cyberattacks.
- **Machine learning, network, and data sciences**—Characterizing and simulating complex networked system behaviors are fundamental for understanding, designing, and securing the computing, communications, and control networks that underpin many civilian and government activities. Areas of research include large-scale network mapping; network modeling and simulation; graph analytics; machine learning techniques for understanding network behavior and indicators of compromise; network-focused uncertainty quantification; and technologies focusing on improving the security of operational technology networks.
- **Innovations in computing architectures and systems**—Developing next-generation techniques and technologies requires advances in state-of-the-art

computing architectures, algorithms, and electronic communication systems. Research and development focus areas include resource-constrained computing; distributed computing, application isolation, higher security operating systems, edge computing architectures; computing-relevant material science and physics; cyber-electronic convergence such as software-defined radio; sensor networks, sensor data exploitation; and software security.

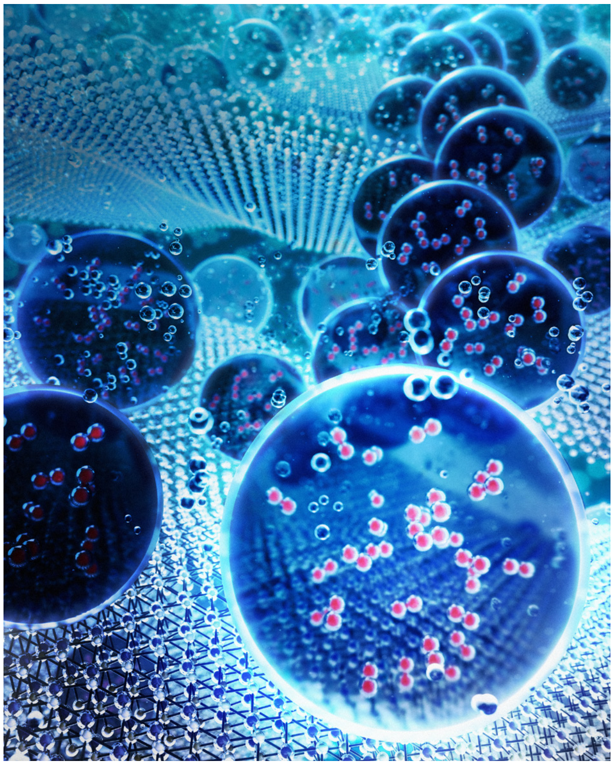
- **Cyber-physical analysis**—Cyber-physical systems play an integral role in many civilian and military systems. Potential areas for investment include cyber-physical characterization and measurement; modeling and simulation techniques for mixed hardware–software systems; data fusion and analytics that span the cyber and physical environments; dynamic system adaptation; embedded software assurance; and economic incentive modeling and analysis. Of specific interest are technologies enabling scalable software/firmware assurance (e.g., the ability to ensure the integrity of all devices going into critical systems, not just a sample); techniques for creating trusted systems out of untrusted components; and systems that are designed to continue to operate even when compromised.

- **Experimental infrastructure**—To support the above S&T areas, various capabilities are desired including Laboratory support of materials science explorations relevant to novel computing architecture; "hardware" in the loop modeling, simulation, and emulation capabilities that integrate high-performance computing; access to commercial cloud environments; data-centric computing; and real-world critical infrastructure systems.

Energy and Resource Security

Applying innovative cross-cutting energy technologies and climate change adaptation to assure national energy and resource security.

Achieving energy security while avoiding the severe impacts of climate change is an important national security challenge. The Laboratory delivers transformational S&T for secure, abundant, low cost, reliable and sustainable energy resources and energy and water systems resilient to climate change. LLNL also provides solutions for improving the security of the nation's energy and water delivery systems and increasing the resilience of these systems to potential cyber and physical attacks and natural hazards. Researchers draw on the Laboratory's S&T strengths in geoscience, atmospheric science, chemistry and chemical engineering, physics, bioscience, materials science and engineering, advanced manufacturing, systems analysis and optimization, uncertainty quantification, and high-performance computing. R&D thrusts include:



Advanced computational models guided the discovery and demonstration of more efficient and less expensive materials for renewable hydrogen production via electrolysis

- **Materials for energy applications**—Advanced materials and manufacturing processes for improved energy efficiency and energy system security and resilience. A major focus is on advancing energy materials science and technology by utilizing core capabilities in multiscale materials simulation, development of innovative manufacturing processes, and numerical optimization. Topics of interest include developing innovative architected 3D structures for batteries, hydrogen production and storage, and more efficient tailored chemical reactors.

- **Increasing resiliency to climate change**—Develop mitigation and adaptation strategies and technologies necessary for effectively responding to climate change. Interests include materials for resilient infrastructure, high-resolution climate modeling and model evaluation, and risk/threat analysis applied to address climate-driven threats to critical infrastructure and national security. Also of interest are strategies and technologies for operating, upgrading, hardening, constructing, moving, and abandoning critical infrastructure assets in an era of changing climate and weather extremes.

- **HPC applied to energy innovation**—Develop simulation tools to assist industry and consortia to advance state-of-the-art manufacturing processes, product design, and product optimization to improve energy efficiency and industrial competitiveness. Applications span industrial challenges; market sectors and products across materials; manufacturing; electrical grid; and transportation including the seven most energy-intensive industrial sectors.

- **Cyber- and physically secure energy and water delivery systems**—Develop new hardware, software, and simulation tools to enhance the security of the nation's energy and water delivery systems and increase their resilience to cyber and physical attack. Objectives include providing advanced tools for use in industry to reach security and resilience goals.

- **Negative emissions**—Methods and analysis of the effectiveness of removing carbon dioxide from the atmosphere, including technology-demonstration partnerships of effective negative-emissions solutions. Objectives include (1) developing cost-efficient carbon capture and decarbonization technologies applicable to natural gas, refineries, cement plants, steel mills, biofuel production facilities, and other major industrial sources of carbon; (2) advancing for manufacturing processes the use of biomimicry catalysts and novel materials that convert carbon dioxide into value-added products; and (3) quantifying and engineering soil systems that store carbon in agriculture and natural ecosystems.

- **Degradation of energy infrastructure**—Develop new understanding, advanced predictive models, and mitigation strategies to prevent degradation of key energy production and delivery infrastructure components. Topics of interest include predicting fouling, scaling, and corrosion of pipelines; developing thermally resistant power turbines; and extending the lifecycle of industrial catalysts.

- **Responsible utilization of subsurface resources**—Develop simulation, monitoring, and control capabilities that enable efficient management of subsurface energy with minimal environmental footprint. Specific applications include optimization of hydraulic fracturing in unconventional shale oil and gas reservoirs, stimulation of geothermal resources to create enhanced geothermal systems (EGS), subsurface sequestration of carbon dioxide to reduce impact of carbon-based energy generation, and mineral extraction for clean energy technologies.

Science of Materials in Hypersonic Regime Conditions

Emergent hypersonic weapons and their associated flight regimes pose new and distinct technical challenges for both offensive and defensive systems.

Detonation of LLNL "purpose-built" hypersonic payload (Holloman High Speed Test Track).

Demand for hypersonic delivery systems is disrupting national defense investment strategies here and abroad. Hypersonic vehicles raise daunting technological challenges that align with Livermore's mission-oriented science, technology, and engineering workforce. Hypersonic vehicles have the potential for unpredictable highspeed maneuverability to evade typical defensive missile warning and tracking systems. The flight profile of hypersonic vehicles differs dramatically from conventional ballistic systems, subjecting the vehicle to extreme, sustained aerodynamic and aerothermal conditions. This extreme flight environment demands that the vehicle and payload be designed accordingly and optimized with both high confidence and minimal test opportunities. A comprehensive understanding of these challenges is critical to designing reliable payloads, assessing coupled vehicle/payload performance, and developing effective defenses. These issues require a detailed understanding of the physics, chemistry, nonequilibrium thermodynamics, and flight dynamics of both nominal and hostile flight conditions in this unique regime. Recognizing the increasing importance of hypersonic vehicle technology and its associated ST&E challenges in the pursuit of U.S. national security objectives, LLNL is making significant internal investments in three key hypersonics mission areas:

- Weapon Systems
- Survivability and Defense
- Space Architecture

The Weapon Systems mission area advances the development of payloads for hypersonic vehicle delivery platforms, with system-level assessments of a given payload and platform as a synergistic combination. Payloads have a broad swath of potential effects on the platforms, and specific constraints imposed by the hypersonic vehicle must account for those effects. A mix of ongoing, near-term, and longer-term concepts is required to maximize the return on national investment into hypersonic vehicle capabilities.

The Survivability and Defense mission areas advance the development of reliable offensive systems and effective defensive measures through an improved understanding of system performance margins under both nominal and hostile conditions. These mission areas are complementary in nature with a common focus on the precise characterization of system performance and uncertainty quantification under the extreme conditions of hypersonic flight in a range of environments.

The Space Architecture mission area advances development of space-based sensors for hypersonic vehicle detection, tracking, and targeting. Spaced-based methods and sensors are essential to understand and characterize the near-space environment in which hypersonic vehicles operate and to conduct mission planning. Space-based diagnostics are vital to test and evaluate hypersonic vehicle performance in the relevant environment under all weather conditions. Livermore has a unique set of technical capabilities and expertise that we are leveraging to achieve programmatic deliverables in partnership with U.S. government hypersonic vehicle sponsors. We aim to continue this success by supporting new research projects that develop:

- **Weapon Systems**—Developing payloads for hypersonic weapon platforms with system-level awareness of payload and platform as a synergistic combination requires critical investment in the following S&T areas:

- **Modeling and simulation:** High-explosive reactive flow models given unprecedented thermal gradients; hypersonic shock/blast interactions and effects across large physical and temporal domains; optimized coupling of effects on targets; and predictive design of novel materials. Numerical methods that efficiently scale on exascale platforms. Workflows that enable rapid, automated creation of fast-running models from general categories of full multiphysics simulations.

- **Advanced manufacturing:** Highly scalable methods, integrated means of process and quality control; concepts to greatly accelerate throughput.

- **Advanced materials:** Multifunctional integrated structures and high explosives (HE); hybrid HE, metalized explosive, and reactive designs; hardware designs for new thermal requirements; additively manufactured HE, fragment packs, and cases; and energy storage that enables longer run times and novel functionality.

- **Diagnostics and sensors**: Laboratory diagnostics to probe hypersonic flow and blast phenomena: spatiotemporal thermal protection system boundary-layer characteristics (temperature, flow, chemistry). Highly automated field diagnostics to gain maximum data collection during the terminal phase of large-scale testing.

- System-level improvements in propulsion technology, based on advanced structural materials, significantly improved energetics, or novel manufacturing capabilities.

• **Survivability and Defense**—Understanding emerging hypersonic flight regimes is central to ensuring reliable offensive systems and developing effective defense measures requiring critical investment in the following S&T areas:

- **Modeling and simulation**: Hypersonic flight environmental physics/chemistry/aerothermal and aerodynamics /nonequilibrium thermodynamics; trajectory modeling; two-way coupling between payload and flight environments; atmospheric modeling; mass and thermal transport; hypersonic fluid-structure interactions under hostile environments; and control margins and signatures.

- **Advanced materials and manufacturing**: High-temperature leading edges and control surfaces, sensor windows, advanced composites designed for performance, manufacturability, and cost; and thermal transport (passive, active) management coupled with an understanding of the response of new materials to a range of environmental conditions.

- **Diagnostics and sensors**: LLNL Independent Diagnostic Scoring System (LIDSS) for hypersonics (LIDAR [light detection and ranging]; radiofrequency (RF); acoustics; electro-optical/infrared [EO/IE]; and thermal imaging), in-situ response detection from materials and subcomponents exposed to a range of environmental conditions.

• **Space Architecture**—Developing critical space-based capabilities for near-space atmosphere characterization, hypersonic vehicle detection, tracking, targeting, and performance measurements requiring critical investment in the following S&T areas:

- **Modeling and simulation**: Predictive upper atmosphere models ("now" and "near-future").

- **Diagnostics and sensors**: Spectral–temporal light occultation; low-earth orbit space sensors for atmospheric characterization and surveillance/tracking systems; and multispectral sensors technology (radiofrequency, electro-optical/infrared, visible, ultraviolet).

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