INVESTMENT STRATEGY

for science and technology

2021

LAWRENCE LIVERMORE NATIONAL LABORATORY

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Science and Technology on a Mission

Patricia K. Falcone
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, 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.

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 2021 LLNL Investment Strategy for Science and Technology outlines the priorities for this year's LDRD program investments and also informs decisions on other institutional investments including facilities and scientific 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.

I'd like to highlight three items in our investment approach this year. First, as a national resource for the U.S., LLNL is using its science and technology capabilities to help the nation respond to the COVID-19 pandemic; second, we are paying enhanced attention to the White House-identified technologies of the future; and third, we have added hypersonics science and technology as a mission research challenge.

In response to the COVID-19 crisis, LLNL has invested LDRD funds, and other investments, to help the nation better understand the SARS-CoV-2 virus and help find therapeutic solutions. LLNL scientists and engineers quickly brought together LLNL's skills in high-performance computing, simulation, and data science with LLNL's expertise in bioscience and bioengineering to rapidly launch research aimed at developing new therapeutics and medical countermeasures to combat COVID-19. LLNL investigators are combining computational and experimental resources to model, identify, and validate possible antiviral and antibody candidates. They are also applying machine learning tools to existing medical datasets to identify risk factors for COVID-19 patients. More information is available at our COVID-19 website: www.llnl.gov/coronavirus.

Our leadership in mission-critical science and technology can also help accelerate national leadership in areas such as those called out by the White House in the "National Strategy for Critical and Emerging Technologies," which outlines fields that the United States will promote such as artificial intelligence, energy, quantum information science, communication and networking technologies, semiconductors, military, and space technologies. LLNL's investments are already delivering innovations in many of these fields in support of our LLNL and National Nuclear Security Administration (NNSA) missions. By leveraging this work, we will improve the U.S.'s leadership and competitive position.

In recognition of the importance of hypersonics to our national security and our mission, we have expanded our efforts in this area and called out hypersonic science and technology as a new mission research challenge. Advancing hypersonics requires integrating science and technology at the intersection of many of LLNL's programs and disciplines, including weapons, materials science, and space security. 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 accordingly modified and optimized with both high confidence and minimal test opportunities. These demands require an understanding of the physics, chemistry, nonequilibrium thermodynamics, and flight dynamics of both nominal and hostile flight conditions in this unique regime. More about the compelling mission drivers and our investment approach can be found on page 40.

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 R&D priorities that overlap with these areas.

Please enjoy this description of the many opportunities before us, find related information on the Lab's science and technology website, www.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.

> *At LLNL, our work is to diminish the likelihood and impact of war, of terrorism, and of natural and man-made disasters through the innovative application of cutting-edge science and technology.*
>
> — William H. Goldstein, LLNL Director

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 of 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 are 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. Delivering on 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)—for engaging prospective partners and building 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 2020 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

Stockpile Stewardship

All-WMD Threat Reduction

Multi-Domain Deterrence

Energy Security & Climate Resilience

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

- Develop an enhanced understanding of the performance of the nuclear package, including details about manufacturing, build, aging, Stockpile-to-target Sequence (STS), and lifecycle environment.
- Improve S&T to enable the rapid and cost-effective development of weapon design options that meet requirements and enhance safety and security.
- 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 characterize the health of the stockpile without significant destruction of assets.
- Advance and extend the utilization of existing underground test (UGT) data through improved scientific understanding.
- Enable the transformation of the NNSA production enterprise by building S&T tools, developing advanced manufacturing technologies, rapid prototyping, and reimagining processes to improve efficiency.
- Recruit, train, challenge and retain a new generation of stockpile stewards to respond to future challenges.

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

All-WMD Threat Reduction
Counter the weapons of mass destruction (WMD) threat and enhance global security by anticipating security threats and providing unique capabilities, expertise, and innovative solutions to make us safer:

- Evaluate potential emerging threats to guard against technical surprise and anticipate security vulnerabilities.
- Improve capabilities to monitor proliferation, support arms control, detect and respond to terrorist threats, and effectively respond to and manage consequences of WMD incidents.
- Support the Intelligence Community with analyses, data science applications, and sensor capabilities that enhance awareness of evolving threats.
- Advance forensic science and technologies for attribution.
- Advance rapid response to biological and chemical threats and emerging diseases.

Pertinent Mission Research Challenges: Chemical and Biological Countermeasures; Forensic Science; Nuclear Threat Reduction; Quantum S&T; and Space Science and Security.

Multi-Domain Deterrence
As an indispensable partner to our stakeholders, anticipate threats to national security, provide mission support, and develop technologies and systems that enhance deterrence at the earliest possible stage of conflict to prevent further escalation, bolster defense, and enable dominance in long-term competition:

- Use systems analysis, advanced modeling, and foundational research to evaluate enduring, emerging, and prospective challenges facing key national security stakeholders; identify capability gaps; help shape operational requirements; and contribute to developing operational concepts and plans.

- Analyze implications of emergent domains of conflict (including but not limited to space, near-space, undersea, the electromagnetic spectrum, and cyberspace); assess adversary capabilities and strategies; model resilience of U.S. technologies and system architectures; conduct feasibility, trade, and architecture studies; and evaluate approaches for deterring escalation and prevailing in crisis and conflict.

- Develop capabilities supporting advanced military systems (including hypersonic, advanced kinetic and directed energy systems; advanced manufacturing capabilities; and other enabling technologies).

- Provide advanced capabilities for cyber and electronic warfare, autonomous systems, data science, and resiliency against cyberattack.

- Develop verification technologies and 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: Cybersecurity and Cyber-Physical Resilience; Directed Energy; High Explosives Physics, Chemistry, and Material Science; Hypersonics ; Nuclear Threat Reduction; Nuclear Weapon Science; Quantum S&T; and Space Science and Security.

Energy Security and Climate 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 atmospheric carbon dioxide (CO_2), 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.

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

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 33–46.

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 7–12:

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.

Institutional investments aim to strengthen the Laboratory's S&T base and, in particular, focus on a set of seven core competencies that are crucial to mission success.

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 pp. 13–32:

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

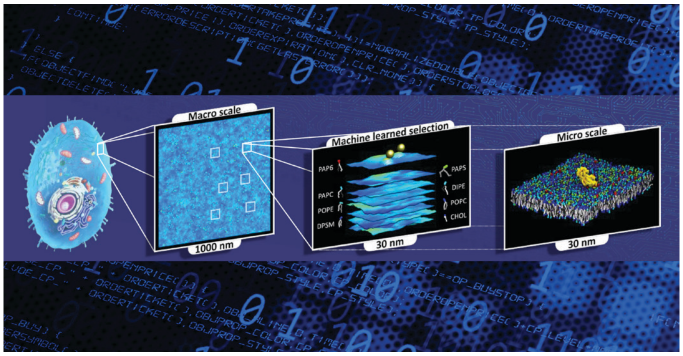
Enabling a new, precision approach to data- and simulation-driven threat characterization, diagnosis, and intervention development.

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.

Today, our capability to respond to evolving and emerging bio-threats is limited. Development of a new therapy or diagnostic can take a decade or more with low probability of success. At the same time, the rapid acceleration of precision biotechnology with low barriers to access is increasing the potential for the emergence of novel, engineered threats. A tested and validated predictive biology framework will enable a new, precise, data-driven, simulation-based approach to threat characterization, diagnosis, and intervention development.

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.



JDACS4C Pilot 2 creates new Multiscale Machine-Learned Modeling Infrastructure (MuMMI) — Wins Best paper at SC2019.

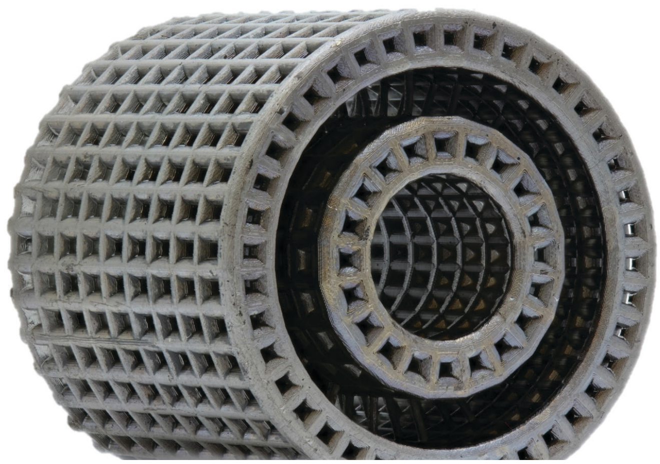
LLNL is developing a world-class capability in engineering biology, building on strengths in microfabrication, advanced manufacturing, and precision experimental biology. Although these technologies fuel advances in predictive biology, the extreme complexity and scale of biological and health data expands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

A public–private partnership approach
Developing an integrated multi-disciplinary 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

Supporting the S&T innovations and partnerships that produce global-scale carbon dioxide removal solutions and unlock climate change mitigation strategies in 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 expectation 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.



Additively manufactured reactor designed to electrochemically convert carbon dioxide into higher value chemicals

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-, thermo-, and biochemical approaches for making fuels and industrial chemicals and feedstocks, such as ethylene (C_2H_4), 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.

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
Defining 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."
- Storing carbon dioxide in existing California oil reservoirs, utilizing the infrastructure and expertise resident across California.

LLNL will work 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 will come from many sources, and LLNL will help create 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.

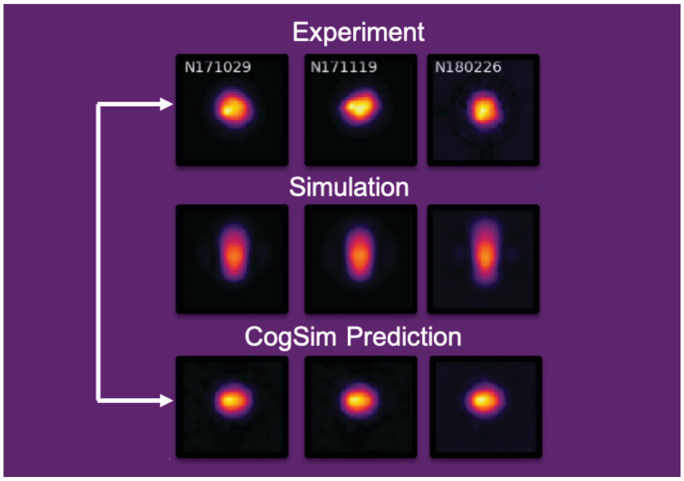
We are exploiting rapid advances in simulation science, artificial intelligence, and high-performance computing (HPC) to transform a broad spectrum of predictive modeling applications. These transformations are enabling new science-driven responses to high priority national challenges ranging from nuclear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

Mission needs to model complex systems
To meet mission needs, our simulation tools to model ever more complicated full-system behaviors and to 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 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 make possible entirely new approaches to assure 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 projects modeling COVID-19 spread and designing COVID-19 drugs leading to new strategies for biodefense.

Improved predictive models
The driver applications are employing cognitive simulation to improve predictions by coupling large ensembles of



Cognitive simulation models use experimental data to correct simulation predictions. Here, a CogSim model ingests image data from past NIF experiments to make predictions of real experiments. The CogSim model is far closer to true experimental observations than simulation alone.

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 AI 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
TThese CogSim models integrate seamlessly with

advanced design optimization loops, allowing for rapid 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 up 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
CogSim will provide improved predictive power, greater computational efficiency, and fast, flexible AI-driven design. It will ultimately provide a framework that combines simulation and experiments to empower scientists to develop a deeper understanding of complex processes and to design optimally effective responses to scientific challenges.

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.

The Space Science and Security Director's Initiative was launched in recognition of the increasing 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. Recent advances at LLNL include innovations in satellite technologies and data analytics make new mission concepts and architectures possible. 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 communications across the military and government
- Intelligence—for indications and warning, threat detection, and technical intelligence
- Civil—for science, earth observation, and climate monitoring
- Commercial—for communications, financial transaction processing, entertainment, and increasingly, for space platform-derived business information.

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 deployment of mega-constellations for commercial communications. The increasing quantity of space objects, both active and inactive is taxing our capacity to monitor space activity. Our adversaries are moving quickly to deploy new space capabilities and some of these threaten our ability to operate in this environment.

LLNL has mobilized to respond to this changing landscape by growing its efforts through the Space Science & Security Program, which is supported by Title 10 and Title 50 Strategic Partnership Program efforts and by LLNL internal investment through the Director's Space Initiative. The effort relies on three mutually supportive elements:

- All-source intelligence analysis—employed to anticipate and respond to emerging threats. LLNL analysts work in multidisciplinary teams to analyze and evaluate technologies, applying their subject matter expertise and modeling tools.
- Advanced modeling and simulation (M&S) tools—used to quickly evaluate and improve potential mission concepts. The Laboratory's scientists and engineers use commercially available, open-source, and custom-written codes to understand the performance of technologies such as sensors, satellites, and system architectures. LLNL excels in applying physics-based M&S tools to complex problems using high-performance computing resources
- Novel hardware—deployed to meet mission requirements with application to small satellite platforms. Small satellite platforms have multiple virtues, including resiliency, faster technology refresh, and lower risk. In addition, constellations of small satellites offer a pathway toward high-cadence observations, which represents a potential game-changing capability for space situational awareness missions. LLNL has pioneered the development of space-based space situational awareness payloads using very small satellites. Our novel hardware efforts also apply to ISR, and missile and hypersonic vehicle detection and tracking.

LLNL optical engineer Brian Bauman, mechanical designers Darrell Carter and Alex Pertica, look over several small space telescopes, three of which have already flown in space.

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, and qualification ecosystem. An integrated approach creates opportunities to reduce cost, infrastructure footprint, and development times. 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, and porous materials needed for our national security stakeholders.

Our R&D priority is to rapidly create and qualify novel materials, structures, and advanced manufacturing methods. Underlying this priority is the need to predictively understand materials processing, structure, property, and 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. Specific R&D thrusts include:

A new 3D printing technique, developed at Lawrence Livermore, could allow scientists to print glass that incorporates different refractive indices in a single flat optic, making finishing cheaper and easier.

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
We have sought to drive advancements in manufacturing through fundamental understanding of the underlying science, which leads to improvement of these processes, as well as invention and development of new processes with capabilities such as 3D micro- and nanoscale features, mixed

material structures, and radically improved throughput. Additionally, inventing and developing processes for bioprinting and other emerging fields will be critical. 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 and computer-assisted design package to provide the sophisticated, nonintuitive designs required by our application space 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 newly established 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.

Advanced and in-situ characterization

The accelerated development and optimization of new materials, processes, and components requires 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. In-situ and operational techniques are also required to probe material properties and performance under 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 and spanning atomistic scale to continuum levels. 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.

Scale-up and qualification

Nonlinear scale-up challenges require in-depth analysis and detailed understanding of processes that affect the transition from bench top 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.

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. Partnerships will be further enabled by 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 and NIF to energy security

High-Energy-Density Science

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

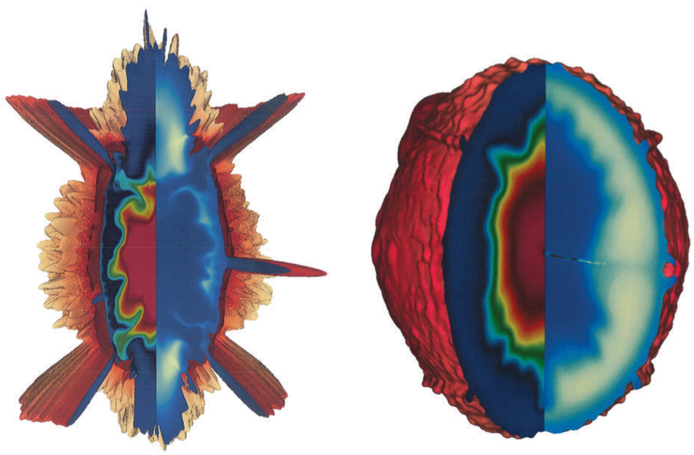
High-energy-density (HED) science is the study of matter and radiation at conditions of high pressure or temperature or under the influence of a strong external perturbation, such as an intense laser, particle beam, pulsed power, or radiation source.

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 the National Ignition Facility (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. 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.

Understanding matter at HED-like conditions is a challenging problem with important applications in Laboratory missions. Producing and controlling burning plasmas in the hot dense matter regime tests our fundamental physics understanding of the complex interplay between hydrodynamics, atomic kinetics, radiation, and particle transport.



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

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.

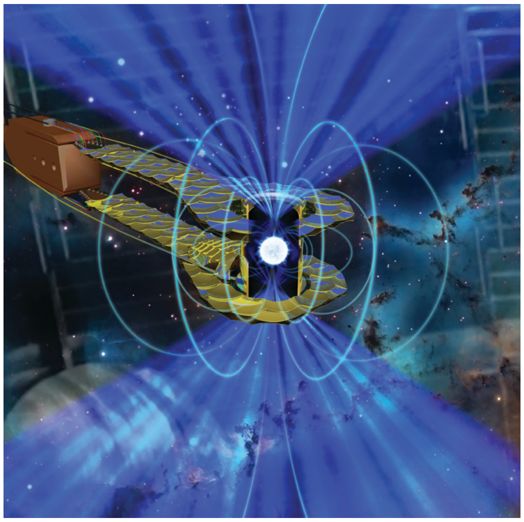
- The Stockpile Stewardship Program (SSP) uses the latest science and technology for qualifying newly manufactured components and assessing an aging nuclear weapons stockpile without relying on nuclear testing. The science responsibilities include developing, validating, and deploying high-fidelity, 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 timescale.

- 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.

R&D Priorities

Properties of materials at extreme conditions
The science and applications include numerous dynamic material phenomena, such as shock-induced chemistry,



NIF can create plasma conditions needed for directly probing the properties of materials in white dwarf stars.

plasticity, and phase transition kinetics; high-strain-rate phenomena; high-pressure and high-temperature synthesis and characterization of novel materials; and properties of matter in the warm dense regime.

- R&D investments in experimental diagnostics are needed for in-situ probes such as high-energy radiography, diffraction, extended x-ray absorption fine structure (EXAFS), and widely applicable temperature diagnostics. Time resolved x-ray diffraction will be an important driver over the next 3 to 10 years.

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

- 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 targetry and diagnostics, data analytics and machine learning, and rapid simulation and feedback control will be required to harness this potential.

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.

In the pursuit of ignition, an understanding of the various heating and cooling mechanisms, and the role that engineering features, such as laser drive, and target and hohlraum design have on capsule performance, are key. Some needs include:

- 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 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 multi-channel spectrometers and proton spectrometers are examples of the latter.

Radiation hydrodynamics
In this branch of hydrodynamics, the moving fluid absorbs and emits electromagnetic radiation, and in so doing modifies its dynamical behavior. 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:

- New experimental platforms, including capsule and hohlraum designs and diagnostics, are a high priority. High energy neutron, x-ray (~1 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.
- 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.

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 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, 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.

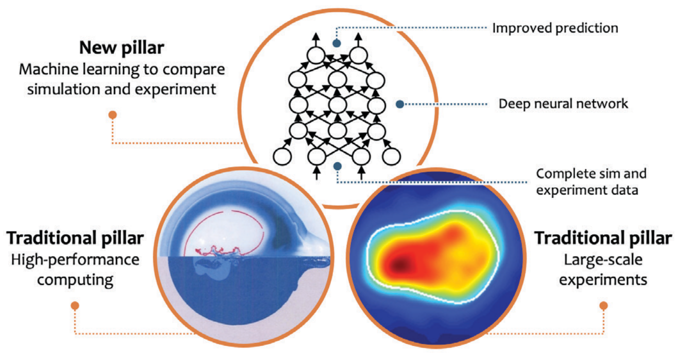
- With the emergence of high-repetition-rate, high-intensity short pulse lasers, HED experiments at high-rep-rate will be transformative for the science of laser–plasma interactions and applications. The integration and development of high-throughput targetry and diagnostics, cognitive simulation with advanced design optimization loops that rapidly integrate empirical data, and feedback control will be required to harness this potential.

High-Performance Computing, Simulation, and Data Science

In support of mission needs, advancing high-performance computing to understand and predict the behavior of complex systems by:

- *Providing leadership in the technically challenging drive toward exascale-class computing.*
- *Developing and applying higher fidelity, realistic, and reliable science and engineering solutions.*
- *Creating scalable capabilities to manage and recognize patterns in big data.*

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 all of the Laboratory's principal mission areas. However, current HPC systems and applications must be improved to predict, with the requisite confidence, the behavior of complex systems, particularly when existing data are sparse or unreliable and actionable information is urgently needed. 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 exascale computing and beyond.



Scientists at LLNL have developed new artificial methods to better integrate experimental data with simulated predictions. This approach, called cognitive simulation, improves physics model predictions.

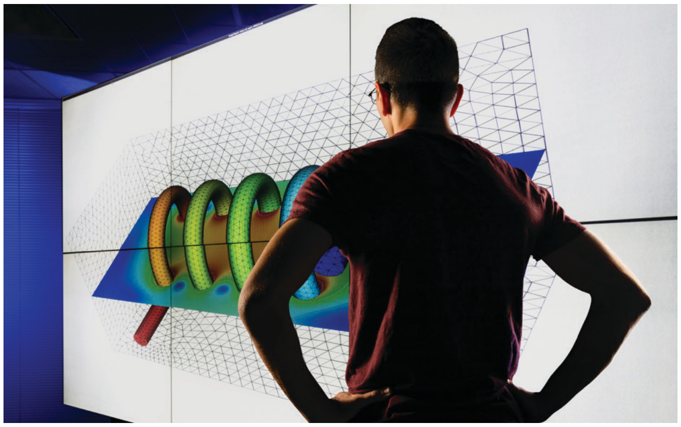
R&D Priorities

High-performance computing (HPC)

LLNL has long been a recognized leader in the deployment, research, and application of HPC to solve complex S&T problems. The Laboratory is able to meet computing challenges through expertise in vertical integration—from leading-edge hardware and foundational software to multiphysics applications and data-science analytics for situational awareness. LLNL is leading the drive toward exascale-class computing, where the development of algorithms for applications that can effectively use massive amounts of parallelism and concurrency while reducing data motion and usage is a major challenge. While large investments by industry in artificial intelligence (AI) technologies have driven computer architectures in directions not necessarily amenable to scientific computing, 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. Simulations are also increasingly leveraging AI and machine learning (ML) techniques, which often have complementary, and sometimes conflicting, requirements that must be addressed. 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.

- **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 through the use of 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, datacentric computing and its confluence with traditional simulation poses new challenges and opportunities for fundamental algorithm and computer science infrastructure development.



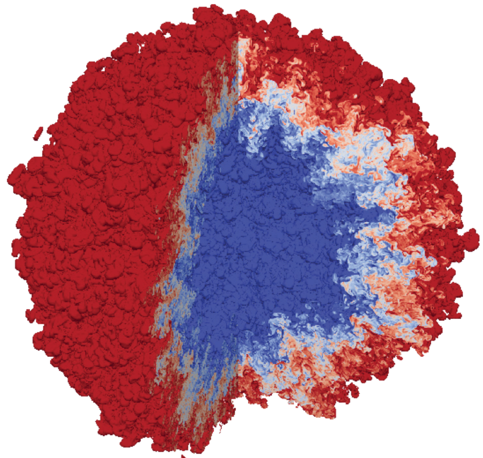
MARBL, used to simulate magnetic diffusion in a coil on a high-order tetrahedral mesh, is a multiphysics code that enables researchers to model complex pulsed-power experiments for high-energy-density science.

- **Multiprogrammatic and Institutional Computing**
The Laboratory's Multiprogrammatic and Institutional Computing (M&IC) Program brings tailored, cost-effective computing services to LLNL. The intent of M&IC is to leave no scientist behind, a key principle made possible by a two-decade sustained partnership between the institution and the weapons program. M&IC's success has followed from adroitly managing two strategies: 1) leveraging weapons program procurements to build clones at very attractive costs and 2) procuring systems to maximize the institution's exploration of the leading edge. Recently, M&IC invested in Ruby (6PF/s), a new unclassified CPU cluster. M&IC users benefited from access to new capabilities funded by other programs: artificial intelligence devices installed on Corona and Lassen. M&IC expanded efforts in cloud computing by deploying an initial HPC-cloud capability and helped users port and test their workflows using it. Efforts in cloud computing will require ongoing research and evolution of our system software stack to support the diverse, rapidly evolving, and growing needs of AI and data science applications. M&IC will continue to identify gaps for institutional users and seek to fill them with systems that build on the Corona procurement model.

- **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). HPC technology roadmaps continue to change rapidly to target expanding markets in cloud computing, AI/ML, and cybersecurity. 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 Sierra and Cerebras CS-1, an innovative new hardware design that was integrated into Lassen, and the SambaNova system for AI applications, integrated into Corona. All these systems will provide a rich testbed for exploring disaggregated system architectures. In the future, LLNL must consider a diverse set of node types, which will 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.

- **Advanced software engineering for high-performance computing**
Software is a key capability for almost every

program at LLNL. Given the increasing need to respond more rapidly to new mission requirements while reducing costs, LLNL must continue to adopt best practices, and, when necessary, innovate our approaches to software development and maintenance. Hardware innovations in computing architectures such as multicore, GPUs, and AI processors require us to rapidly address 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 build systems, and performance analysis and correctness tools. However, bridging the gap between software engineering research tools and production HPC codes remains a challenge. The Weapons 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 are positive steps in this direction.



The Sierra supercomputer makes routine—instead of heroic—high-fidelity calculations such the turbulent fluent mixing in a spherical geometry—part of a simulation of an idealized inertial confinement fusion implosion.

However, with El Capitan looming on the horizon, as well as other architectures under evaluation, progress in the Weapons Program will continue at a rapid pace through focused investments that may leave some innovative approaches behind. Thus, coupling must remain strong across the Laboratory by investing in a common base of foundational scientific computing open-source software with opt-in adoption for both existing and newly developed LLNL applications. The RADIUSS effort will harden research tools and libraries; provide direct assistance to developers; support training to strengthen the workforce; forge a path for defining DevOps (the set of practices combining software development and IT operations) in the context of HPC development; and create a culture around improved research software engineering practices at LLNL. Looking to the future, LLNL must move research tools developed to support performance portability, component-based approaches for application development, and advanced workflow tools into development practice. Finally, best practices in modern software development and DOE policy motivate LLNL programs to exploit and contribute to open-source software, and developers to engage with the open-source community.

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 to efficiently 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 cross sections, 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 need to be made 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 subscale physics and the larger continuum simulation, necessitating that some form of the high-fidelity simulation be run in-situ with the continuum simulation. This combination could be an instantiation of the high-fidelity code, or perhaps an AI/ML capability that replicates the high-fidelity model. Research is necessary into how and when this kind of multiscale coupling needs to occur.

- **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 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 past experience 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 objects like images, spectra, and time series.

- **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 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, enable quantitative consideration of design tradeoffs, and help ensure data manageability, interpretability, and integrity.

Information Systems and Data Science

LLNL creates scalable capabilities to manage and recognize patterns in big data. 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

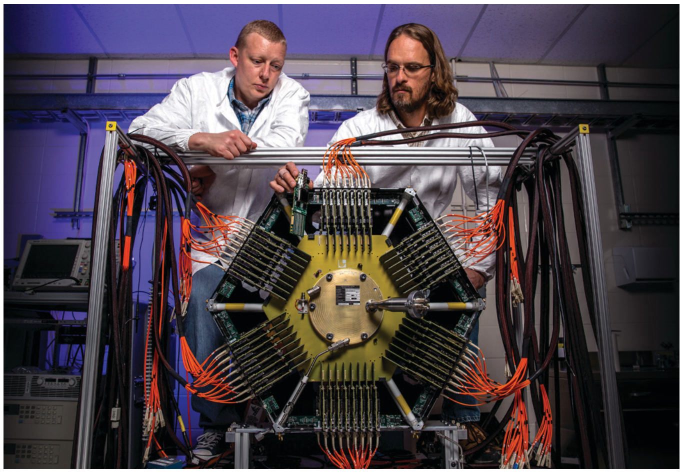
questions. The queries are exceedingly complex, based on subject-matter-expert models, such as a process model for acquiring chemical weapons. This science-based pattern discovery requires new AI/ML algorithms, improved natural language methods, new graph-based methods, and the means to scale efficiently 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. Finally, the design space of AI/ML models is practically limitless, so the ability to rapidly design new 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.

Nuclear, Chemical, and Isotopic S&T

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.

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 and forensic sciences, which support efforts in nuclear and chemical threat assessments, incident response, CBRNE (chemical, biological, radiological, nuclear, and explosive) forensics, and environmental science. These applied capabilities rest on a strong fundamental research foundation aimed at exploring the frontiers of physics and chemistry by advancing our knowledge in nuclear structure and reactions, heavy-element chemistry, cosmochemistry, and physics beyond the standard model.



Nuclear physics experiments probe the properties of nuclei using unique LLNL capabilities, such as this time-projection chamber, which is being used for a precision measurement of fission.

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

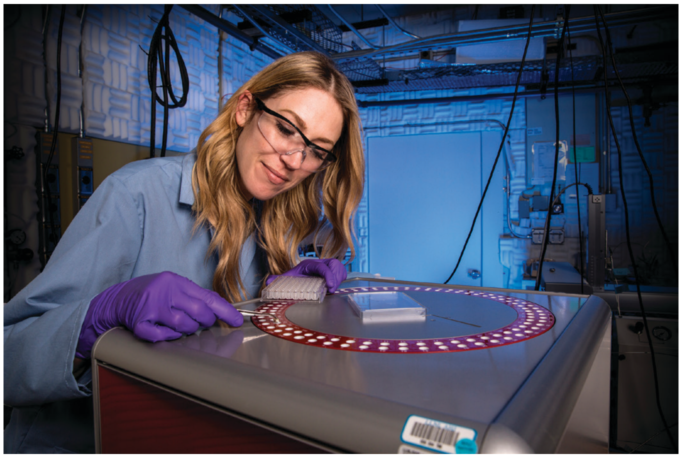
R&D Priorities

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, 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 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 provides an experimental platform to study nuclear reactions and measure basic nuclear data needed for assessing nuclear device performance and understanding stellar nucleosynthesis. Development of innovative chemical separation and automation methods is leading to advanced field-deployable technology for nuclear incident response and enables rapid, one atom-at-a-time separation platforms for exploring the chemical properties of the newly discovered superheavy elements on the periodic table. 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 the stockpile stewardship and technical nuclear forensics applications.



Analytical methods developed at LLNL are applied to several research areas including cosmochemistry, environmental chemistry, hydrology, and biomedicine.

- **Analytical and forensic science**
  Analytical chemistry is the science of determining the composition of a substance, both qualitatively and quantitatively. The development of state-of-the art analytical methods is the foundation for forensic science related to CBRNE 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 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 actinide ultratrace 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.

- **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 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 include: (1) the composition and nature of dark matter; (2) neutrino physics; (3) probing 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.

Facilities

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

Equipment investments will focus on refurbishing workhorse analytical instrumentation while building one-of-a-kind capabilities to maintain our technical edge. A new Secondary Ion Mass Spectrometer and 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 are among the top priorities. The CAMS upgrades include 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 onsite, 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. Of particular importance are investments that will enable greater colocation of personnel and resources, enhanced local capabilities (including a revitalized accelerator complex in B194, renovated radiochemistry laboratories in B151, a refurbished and expanded CAMS facility that includes new ion sources, beamlines, and detectors to address emerging mission needs, and access to DOE neutron, photon, and radioactive beam facilities across the U.S.), shared data acquisition capabilities, and a collaborative information hub. Longer-term investments will focus on establishing the Livermore Nuclear Science Center, a unique and dedicated facility delivering gamma, charged-particle, and pulsed, 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

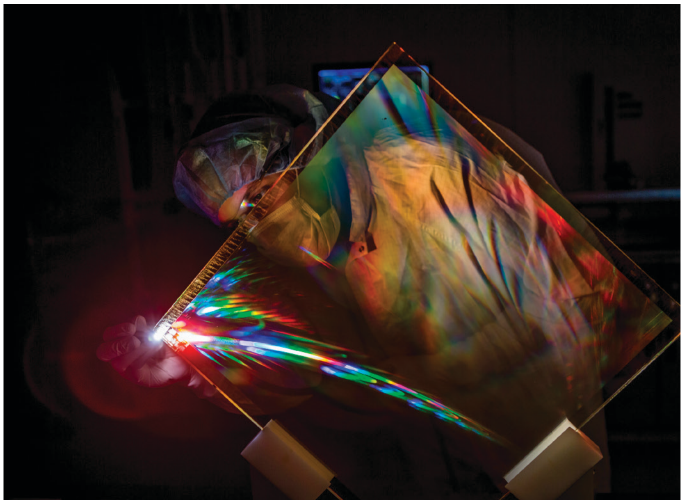
Designing, building, and reliably operating complex laser systems that dramatically advance the state of the art for strategically important applications.

Core competencies in lasers and optical materials (LAOM) science and technology have enabled the Laboratory to design, build, and reliably operate a sequence of large and complex laser facilities that have successively broken world records in laser energy, power, and brightness. These successes reflect longstanding expertise in systems engineering, and laser construction and operation, which are complemented by leadership in photonics science and technology, optical material science, laser–material interaction physics, and laser system modeling and simulations. Together, these LAOM core competencies have enabled innovative advances in laser design and optical material quality, damage resistance, and manufacturing processes.

In support of stockpile stewardship, the National Ignition Facility (NIF) is proving an invaluable tool for exploring high-energy-density (HED) science regimes including conditions relevant to fusion research not accessible by other experimental facilities. NIF experiments provide key insights and data for simulation codes used in weapon-performance assessments and certification. NIF is also an increasingly important resource for weapons effects studies and national nuclear forensics analysis. LAOM core competencies are critical to operating and continuously improving NIF's utility and cost efficiency.

LLNL's advanced laser technologies also have material processing applications that strengthen national security and U.S. economic security. These include selective-laser-melting (SLM) additive manufacturing (AM) for metals; laser-driven mechanical surface treatments; and subtractive manufacturing with short-pulse lasers. AM is important to stockpile stewardship as a simpler, more cost-effective means to manufacture a diverse set of parts for nuclear weapon life-extension and modernization programs.

Directed energy (DE) with high-average-power or pulsed lasers is a potentially disruptive technology for defensive applications. Advanced laser architectures, optical system design, and laser–material interaction science are central to providing timely solutions to existing and emerging threats. Communications, navigation, and sensor systems increasingly employ laser and photonics systems containing LLNL-developed technology and create synergies with other areas of interest to LLNL and DOE. The anti-reflective coating on this grating debris shield restores lost NIF energy and eliminates a source of optics damage. LLNL is well-positioned to participate in the emerging area of ultra-short-pulse lasers, particularly for applications that require high average and/or high peak power. Of growing importance is the use of such lasers to produce secondary radiation 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 stockpile stewardship-relevant radiography applications.



The anti-reflective coating on this grating debris shield restores lost NIF energy and eliminates a source of optics damage.

Investments in the core area of optical material science enhance the damage performance, functionality, and cost effectiveness of optics. New investment in AM could change the way conventional and free-form optics are made, opening new applications that are important to LLNL's core missions. Core strengths in optical fiber design and processing capabilities also continue to provide solutions for national defense challenges.

R&D Priorities

- **High-energy, high-average-power laser technology**
  A principal focus is to sustain LLNL's world leadership in high-energy and high-average-power laser technology. LLNL will explore novel system

architectures, laser materials, and laser components for high energy and high-power lasers through high-risk, high-payoff technology demonstrations. High average power for DE applications can be achieved either by increasing a single laser's output power (e.g., alkali lasers) or by coherently operating many low-power lasers (e.g., fiber lasers). Both approaches require technological advances in an area where LLNL has special expertise. Advances in solid-state laser diode capabilities for high-efficiency pumping are being successfully pursued in partnership with industry.

- **Short-pulse laser technology**
  Although short-pulse laser technology expertise is widespread, a discriminating capability is LLNL's ability to extend short-pulse laser technology to higher per-pulse energy and repetition rates. Investments are needed to extend current capabilities in pulse energy and repetition rate and to develop and demonstrate applications of short-pulse laser-driven radiation sources. These technologies could effect a paradigm shift that accelerates stockpile-stewardship-related HED science and the emergence of laser-driven radiation sources for a host of national security applications.

- **Photonics and enabling materials science**
  Expertise in photonics and enabling materials science is key to innovating and mitigating mission uncertainty risks. Applications range from optical-surface science for advancing optical damage resistance and developing novel optical materials and fiber laser designs, to improved optical manufacturing. Other areas of interest include fundamental understanding and optimization of diode pump technology critical to advanced lasers and development of systems that combine the best of photonic and radiofrequency technologies.

- **Diagnostic science and technology**
  Advanced diagnostics are important to essentially all Laboratory missions and particularly so to NIF and its role in stockpile stewardship. The Stockpile Stewardship Program directly funds much of this work. However, internal R&D resources will support fostering new and high-risk, high-reward ideas in diagnostic science and building our future workforce in this critical area.

- **Systems engineering**
  LLNL's core competency in this aspect of LAOM has enabled, for example, transformation of a laser design for inertial fusion energy into an innovative high-average-power laser architecture for generating short pulses at unprecedented repetition rates. World-leading laser design and construction projects continue to develop and refine LLNL's systems engineering expertise and position LLNL to exploit these technologies for a variety of mission applications.

- **Laser–material interaction 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 DE weaponry, and fundamental science of laser-based material processing. Investments in experimental science and computational modeling will expand applications for lasers in areas important to the Laboratory.

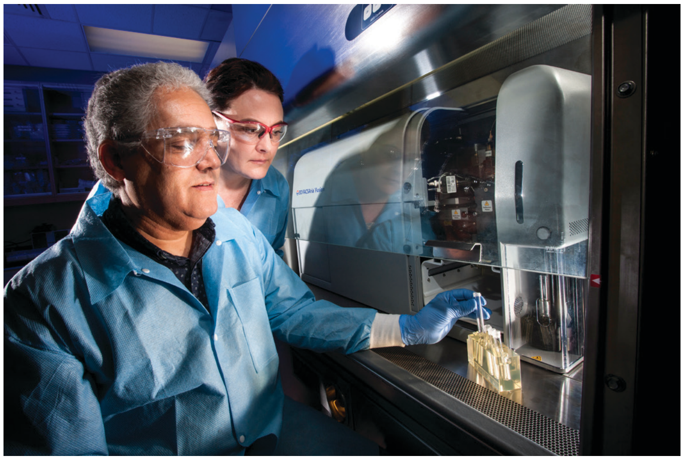
- **Modeling and simulation**
  LLNL's unique capabilities in high-performance computing extend to modeling and simulating advanced laser systems. Laser modeling and simulation investments maintain LLNL's world-leading capabilities, enable the development of new and innovative laser technologies, and reduce the time from concept to working prototype.

- **Industrial and commercial applications**
  LLNL will develop an S&T portfolio targeting commercial applications of lasers and manage the portfolio so that competencies developed also benefit our core national security missions. The Laboratory's presence in laser-based advanced manufacturing can attract the best and brightest and connect us with advances in the global technology community.

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 bioenergy.

The bioscience and bioengineering core competency emphasizes a culture of multidisciplinary research that enables innovation through combined technology development and biological problem solving. The core competency encompassess the expert skills, unique capabilities, and special facilities needed to inspire ground-breaking research that addresses the most pressing problems in health, energy, and environmental security. We rely on a convergence of biology, high-performance computing and precision engineering to understand the properties and predict the trajectories of complex biological systems. We draw on world-class capabilities in genomics, bioinformatics, molecular and cellular simulations, bioengineering, biosensors, additive manufacturing/bioprinting, select agents, toxicology, and bioanalytical science to perform our work.



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

One of the central challenges of our mission is developing the bioscience and biotechnology expertise needed to understand and manipulate complex cellular systems. LLNL is making strategic investments in efforts to develop tools that allow us to characterize biology more robustly, more quantitatively and more precisely; develop a deeper understanding of the complexity of biological systems and communities relevant for health and environmental security; and use these tools and understanding to deliver new technology that will counter emerging threats.

R&D Priorities

We anticipate significant challenges in biosecurity, human health and bioenergy that include rapid response to pandemics and emerging disease, the growing threat of climate change, the need to understand and characterize complex biological systems, and the emerging ability to engineer life and novel materials. New approaches will be needed to detect, understand, and counter health and environmental threats on a time scale that is orders-of-magnitude faster than is now possible. New paradigms will be needed to protect the nation.

To address these challenges, our strategy is to closely integrate computational tools and experimental systems to more thoroughly characterize and predict changes in the behavior of complex biological systems as a result of perturbation. Our researchers are working to understand the mechanisms of injury and disease, engineer microbial communities for health- and environmental-related objectives, and develop bio-derived materials and biological production methods for a wide range of applications. These efforts bolster our ability to fundamentally understand the biological drivers for specific outcomes and translate that understanding into solutions.

We have three strategic thrusts aimed at solving key national security problems defined within three research themes. The strategic thrusts (integrating experimental and computational tools, expanding and testing our understanding of cellular mechanisms, and developing solutions to counter vulnerabilities) provide a framework for solving complex biological problems in our primary research themes (microbiome engineering for health, energy and the environment; rapidly responding to the emergence of novel pathogens; and diagnostics, prognostics and treatments for cognitive impairment). The first research theme, microbiome engineering, is focused on understanding microbial communities, both within the environment and within the human body, with the goal of being able to manipulate/functionalize the communities for different or better outcomes. The second 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 final research theme is focused on understanding human brain function for protecting neurological health. These research themes were chosen to leverage our strengths and expertise in biology, computing and engineering, and to position us to 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, active learning loops 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 models that strive to combine computations and experiments are needed to understand how environmental changes (exposure to toxins, infectious agents, diseases, changing climate) affect the organism and then predict the organism's response. The models need to be human relevant and designed to be modified in a systematically controlled manner to observe and measure responses to differing experimental conditions. 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 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 bio-engineering, 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 and test 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 the national security needs of the country. This knowledge provides the basis for engineering cells and communities to combat disease and develop bio-production methods. Our priorities are to:

  - Understand, design, and engineer microbes and microbial communities for health and energy challenges.
  - Improve our understanding of the molecular basis of disease.
  - Understand the underlying cellular and molecular pathways involved in microbial pathogenesis.

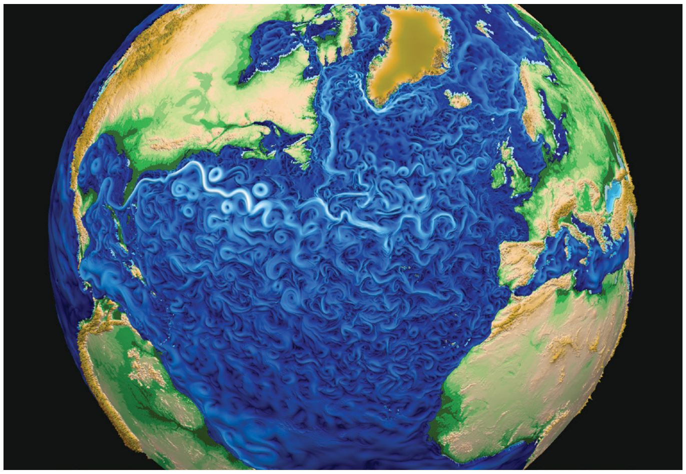
- **Develop solutions to counter current and emerging challenges**
  Combining strengths in interrogatable models with cellular mechanisms and cellular engineering enables a revolutionary, holistic approach to accelerate the development of countermeasures to human exposures and disease. Establishing 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.



This high-resolution ocean simulation uses the Energy Excascale Earth System Model, which divides the globe into a grid do to just 15 kilometers.

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. 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 also produce groundbreaking analyses of the causes of climate change and their potential consequences on the Earth system. LLNL is also one of the lead developers of DOE's 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 subsurface modeling, including shock physics, seismic simulation, fracture mechanics, and geophysical signals associated with hydraulic well stimulation. 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 energy waste; and the management of hydrocarbon, thermal reservoirs, and reservoirs used for storage of carbon dioxide.

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. 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 for model validation and model improvements are required for the stratosphere and higher altitudes.

- **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.

- **National security emergence 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.

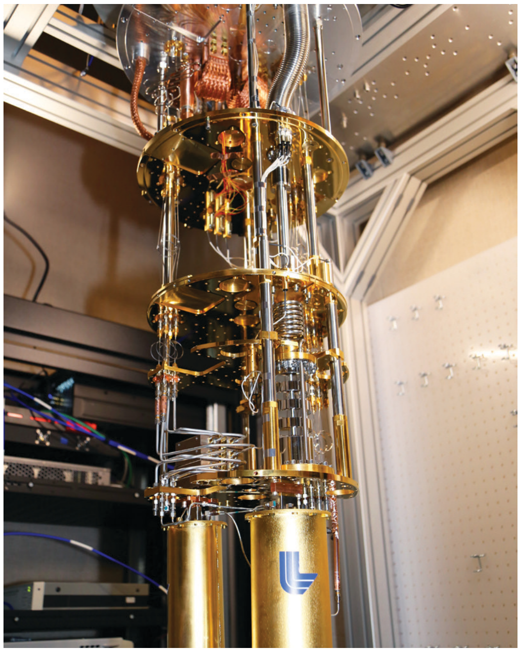
- **Atmospheric modeling for renewable energy**
  Forecasting wind and solar generation requires modeling skills in atmospheric flow, atmospheric physics/microphysics, and integrated computational fluid dynamics modeling that are currently not available. Atmospheric models cannot currently handle the 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.

- **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 have no known efficient classical algorithms. 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 threat reduction.



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

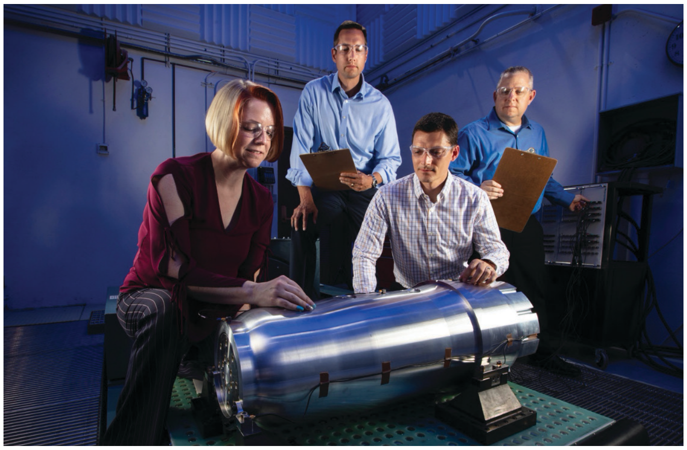
LLNL's quantum science strategy is centered on the use of a multidisciplinary co-design research environment that draws on the Laboratory's deep expertise in physics, chemistry, optics, engineering, materials, and computer science. The challenges associated with realizing the hardware and software approaches 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 both 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 novel 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 of nuclear weapons science has produced tremendous insights into the science and engineering of an operating nuclear weapon. We possess the technical expertise to respond to our adversaries; however, 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.



Vibration experiment to demonstrate that the W80-4 can tolerate the environments that it will encounter.

LLNL must 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.

For a select few areas, nothing short of preeminence is our goal. 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, we offer a legacy of successes to those seeking 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. Some key science focus areas are:

- **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 computer centers has delivered a quantum leap in designer productivity and agility. This capability enables significant advances in assessment and certification methodologies for both the current stockpile, and the modernization efforts. LLNL will continue to invest in R&D associated with state-of-the art numerical methods, computational algorithms, and physics model development, which 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. ML methods present an avenue for incorporating high-fidelity physics in our large, multiphysics simulations. Automated, AI-guided optimization will enable a single expert to consider design attributes across a range of options through AI-assisted execution of simulations with in-situ analysis capabilities, reducing time spent on problem setup and requiring far fewer simulations overall.

- **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, enabling higher-fidelity study than ever before of the conditions salient to weapons, directly informing today's stockpile choices. In the absence of nuclear testing, our enterprise faces two major challenges: the need to make impactful stockpile assessments utilizing HED capabilities on a faster timescale, and the need to achieve ignition and burn, enabling 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 the first 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); the 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.

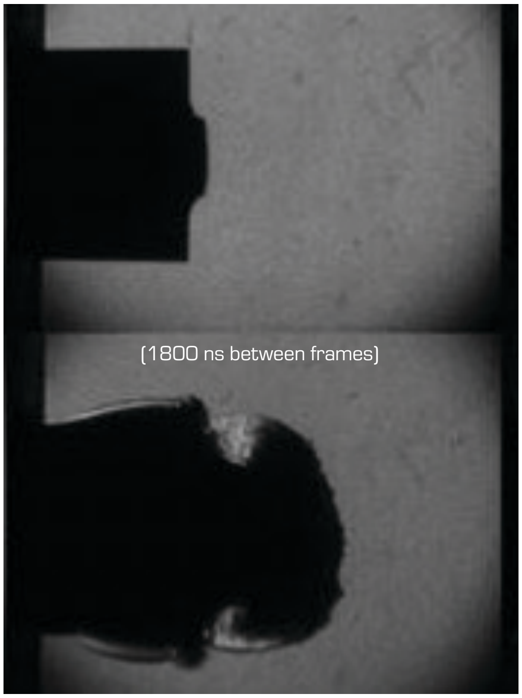
- **Deploying advanced manufacturing technologies**—LLNL is in the process of introducing disruptive techniques that have the potential to revolutionize the future design and manufacturing of nuclear weapons. The nuclear weapons program seeks to reduce the design-to-deployment time for components to three years by utilizing innovative materials and feedstocks; developing new manufacturing platforms; deploying process-aware inverse design methods; and vigorously pursuing technology maturation.

- **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 platforms to support emerging needs in survivability, modern manufacturing, and hypersonics. To fully utilize these science discovery and model validation experiments, the Laboratory also needs to develop advanced diagnostics and radiography concepts to better characterize the experimental conditions achieved.

High Explosive Physics, Chemistry, and Material Science

Improving fundamental understanding and prediction of high-explosive 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 particular 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).



Ultrafast imaging of detonator output after explosive detonation; images taken at LLNL's premiere High Explosives Applications Facility (HEAF).

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 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.

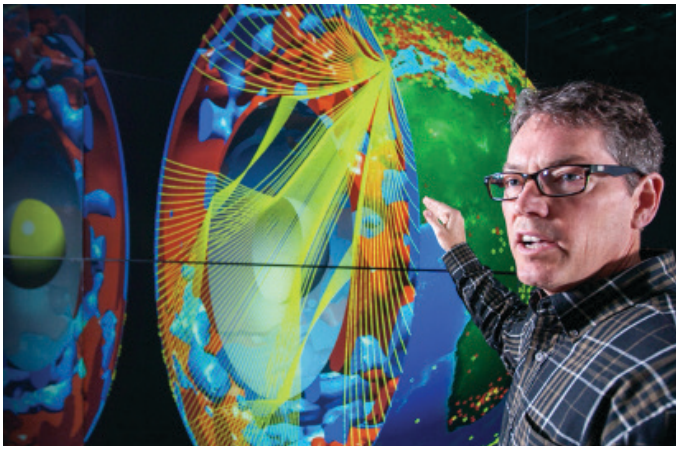
- **Investigating manufacturing methods to enable development of options for an agile nuclear deterrent and promote collaboration with the production agencies through accelerated HE feedstock and component production**—Responsive manufacturing offers opportunities to target key performance uncertainties, develop nonintrusive instrumentation for stockpile monitoring and forensics, pursue innovations in safety and surety, and explore proliferation space. New data science techniques should accelerate materials development, manufacturing, and qualification.

- **Designing, predicting, and qualifying new HE molecules for stockpile use and characterizing home-made 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. Advances in scientific computing should be applied to quantify fluid dynamic characteristics of reactors for predictive resulting feedstock and components. 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 innovative technologies and systems to prevent, detect, counter, and respond to use or threatened use of nuclear weapons or weapons-usable materials.

LLNL provides science-based, intelligence-informed expertise to our national and international partners to: prevent and detect state and non-state actors' development of nuclear or radiological weapons or acquisition of 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 events, or accidental/unintentional incidents. Response includes searching for threat devices, components, and/or materials, by rendering them safe or by managing the consequences.



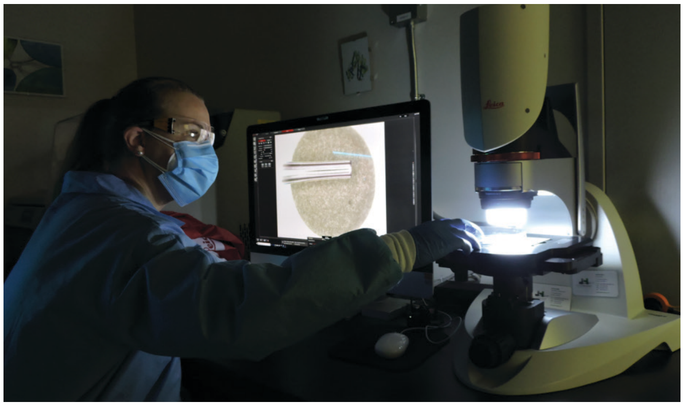
LLNL-G3D enables accurate calculation of seismic-wave travel times from any location in or on Earth to any potential sensor location.

Sponsors of nuclear threat reduction activities seek deployable global and space-based technologies to use flexibly and quickly. Focus areas include:

- **Understanding emerging technologies**—We need validated models of how materials behave, and better understanding of how emerging technical approaches could be deployed to evaluate and disable potential threats by proliferators.
- **Enabling nonproliferation and arms control**—Research, development, and technical solutions are necessary to ensure the continued viability of the nonproliferation regime and to inform and support future arms control initiatives.
- **Strengthening proliferation warning**—We need enhanced data analytics capabilities to extract actionable threat information from massive, heterogeneous data streams for early-stage proliferation detection.
- **Advancing nuclear threat detection and assessment**—Accurate and timely detection of nuclear threats, including proliferative activities, materials, and devices, requires improvements in detection materials and sensors as well as more flexible and intelligent data processing for integrated detection networks. Innovative methods for exploiting threat-relevant signatures and improved experimental and modeling capabilities to assess the full threat spectrum are needed.
- **Improving nuclear test detection**—A better understanding of the signatures of nuclear explosions is needed, including underground, low-yield, and clandestine nuclear tests. New technologies to enhance our ability to identify and characterize nuclear explosions are required.
- **Enabling rapid nuclear incident response**—Fast-running, high fidelity tools for the Nuclear Emergency Support Team (NEST) are required to enable swift and confident technical guidance to response and render safe teams and will provide assessments of potential consequences resulting from a nuclear emergency.
- **Accelerating post-detonation event assessment**—Advanced forensic analyses and data fusion of prompt signals and material collections are needed for rapid and accurate decision support after a nuclear detonation.

Chemical and Biological Countermeasures

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



LLNL scientists use cutting-edge technology to develop and characterize novel detection assays and medical countermeasures that mitigate outbreaks involving chemical and biological agents.

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 S&T work focuses on developing health measures to protect against and aid recovery from illness and injury, including new ways to provide pretreatment prophylaxis that extend opportunities for medical intervention. Our S&T developments are 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.

The best response to crisis is to prevent, disrupt, degrade, or deny the factors that allow a crisis to originate. Through strategic partnerships involving multiple government agencies, LLNL supports established CB security programs and provides a strong foundation for new S&T strategies that respond to increasingly complex threats. Additionally, we study emerging disruptive technologies and Dual Use Research of Concern (DURC) biotechnology products that drive innovation and improve health but can also be misused. Our work promotes a culture of safety and security while providing ethical and responsible research in the life sciences.

- **CB countermeasure development**—Support the development of tools that facilitate response and recovery from traditional/non-traditional chemical warfare agents, synthetic opioids, and biological select agents and toxins. Utilize advances in nanotechnology, and microencapsulation science to develop innovative materials that aid therapeutic countermeasure stability, effectiveness, and delivery.

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

- **Emerging disruptive technology and DURC**—As LLNL scientists develop new approaches, we can inform others about the beneficial use of biology, informatics, and biotechnology; in addition, we assess the misuse of these same technologies and support education of policy experts, medical health professionals, and leading scientists.

- **Detection**—Use advanced methods to detect and characterize new and emerging biological threats. Use S&T advances to develop new model systems that aid in understanding how chemical and biological agents (as well as CB countermeasures) interact within target cells and tissues. Promote new approaches for understanding the role of the microbiome in human health and warfighter protection.

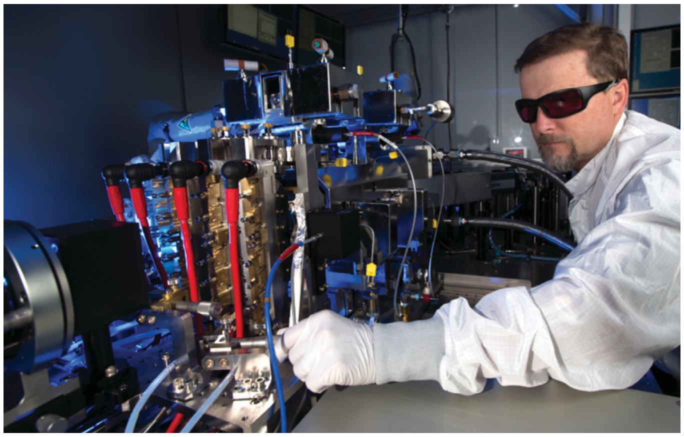
- **Biomarker discovery for early detection, prediction, and prognosis of disease or exposure**—Mitigate the impact of CB incidents by identifying biomarkers that signal health susceptibilities and impairments before the onset of symptoms. Protect health and speed recovery by understanding effects of therapies and medical treatment on human systems including physiological and microbiological (microbiome balance) and finding biomarkers to reconstitute and repair microbiomes and other affected systems.

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 at risk U.S. military assets deployed on land, at sea, airborne, and in space. 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 (DE-MSHORAD). 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 (M^2<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 in order to identify and counter new threats; new countermeasures; or new operational constraints to directed energy.

Forensic Science

Advancing the state of the art in chemical, biological, radiological, nuclear, and explosive (CBRNE) as well as traditional forensic science to support a broad set of national security needs.

Unique technical expertise and experience in forensic science at LLNL is applied across the spectrum of CBRNE and other threats. Many of these efforts are focused on in the Forensic Science Center, a national security resource supporting a broad set of mission areas including the creation of new analytical methodologies, techniques, and materials for use during CBRNE investigations and in support of the warfighter. R&D thrusts include:

Exploiting the signatures of chemical, biological, radiological, nuclear, and explosive materials is the cornerstone of the forensic science mission of the laboratory

- **Collection and Detection Strategies: Predicting, sampling, and detecting 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 hand-held rapid screening tools with sufficient detection limits are needed to prioritize suspect sample collection locations to avoid overtaxing forensic laboratories. Methods to advance detection capabilities in the lab or in the field are desired, including multiplexed and miniaturized techniques, or those that identify the 'unknown-unknown'. These 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.

- **WMD Threat Characterization: Identifying, developing, and validating novel techniques to 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 weapon-related activities. Developing rapid analytical capabilities for accurate measurement of stable and radioactive components plays a vital role for timely response to WMD events. Key focuses are:

  - Understanding how the method or sophistication of a synthesis/production pathway may affect the information that can be gleaned from a sample and the interface between comingled hazards and signatures.

  - Exploiting novel analytical or data science methods to rapidly produce and mine data for signatures of interest or to identify unknown-unknowns. High throughput or multiplexed analysis techniques are also of interest.

  - Developing improved and validated capabilities to measure and predict 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.

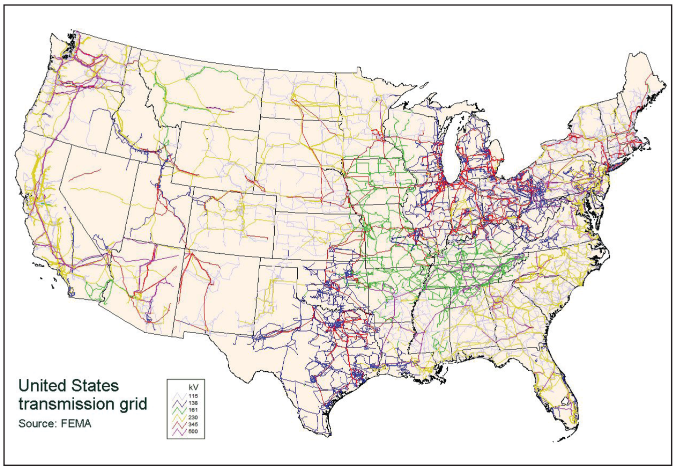
- **Exposure signatures: Understanding the scope and nature of human exposure signatures for current and emerging threats, including chemical weapons, narcotics, and pharmaceutical- based agents, biological agents, and radiological materials**—Developing a robust pharmacokinetic and metabolic understanding 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, that can be used to develop protective countermeasures and therapies. Additionally, applications that push toward clinical or field diagnosis would be valuable, especially when coupled with the administration of potential countermeasures.

- **Advancing traditional forensic science: Reducing reliance on subjective methods and providing statistically relevant objective methods for traditional forensic analyses**—The research focuses are to improve current forensic science, reduce the reliance on subjective human-driven comparisons or bias that may be introduced from computational methods, and 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 will leverage unique capabilities in this mission area, such as expertise in 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.



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

- 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.

- 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. Potential investment areas include: network mapping and situational awareness; network modeling and simulation; graph analytics; machine learning techniques for network behavior and indicators; network-focused uncertainty quantification; and technologies focusing on IT networks or operational technology networks.

- Cybercentric computing and communications innovations—Developing next-generation techniques and technologies requires advances in state-of-the-art computing architectures, algorithms, and electronic communication systems. Research and development areas may include: resource-constrained computing; distributed computing, 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.

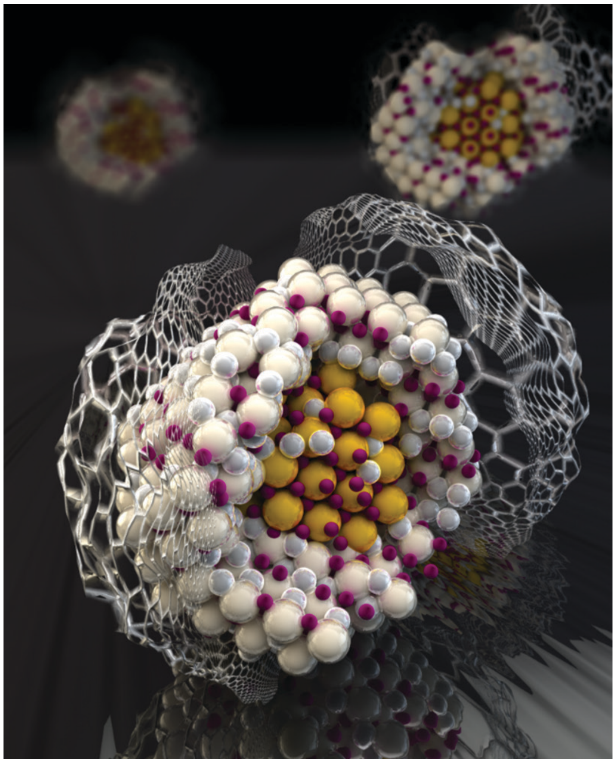
- Cyber-physical resilience—Cyber-physical systems play an integral role in many civilian and military systems. Potential areas for investment include: cyber-physical characterization and measurement; modeling and simulation techniques for mixed hardware–software systems; data fusion and analytics that 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, to include: laboratories to support 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 atomistic and mesoscale models are being developed to diagnose how novel materials like this nanoconfined Li-N-H system can be adapted for compact, low-pressure hydrogen storage in vehicles.

- 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 addressing 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 objectives.

- Negative emissions—Methods and analysis of the effectiveness for 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 cycle life 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 examples include optimization of hydraulic fracturing in unconventional shale oil and gas reservoirs, stimulation of geothermal resources to create enhanced geothermal systems (EGS), and subsurface sequestration of carbon dioxide to reduce impact of carbon-based energy generation.

Hypersonics

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 drive the realignment of Livermore's mission-oriented science, technology, and engineering workforce. Hypersonic vehicles have the potential for unpredictable high-speed 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 accordingly modified 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.

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; and predictive design of novel materials.

- Advanced materials and manufacturing: 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).

• 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/nonequilibrium thermodynamics; 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.

  - 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).

• 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 (RF, EO/IR, visible, ultraviolet).

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