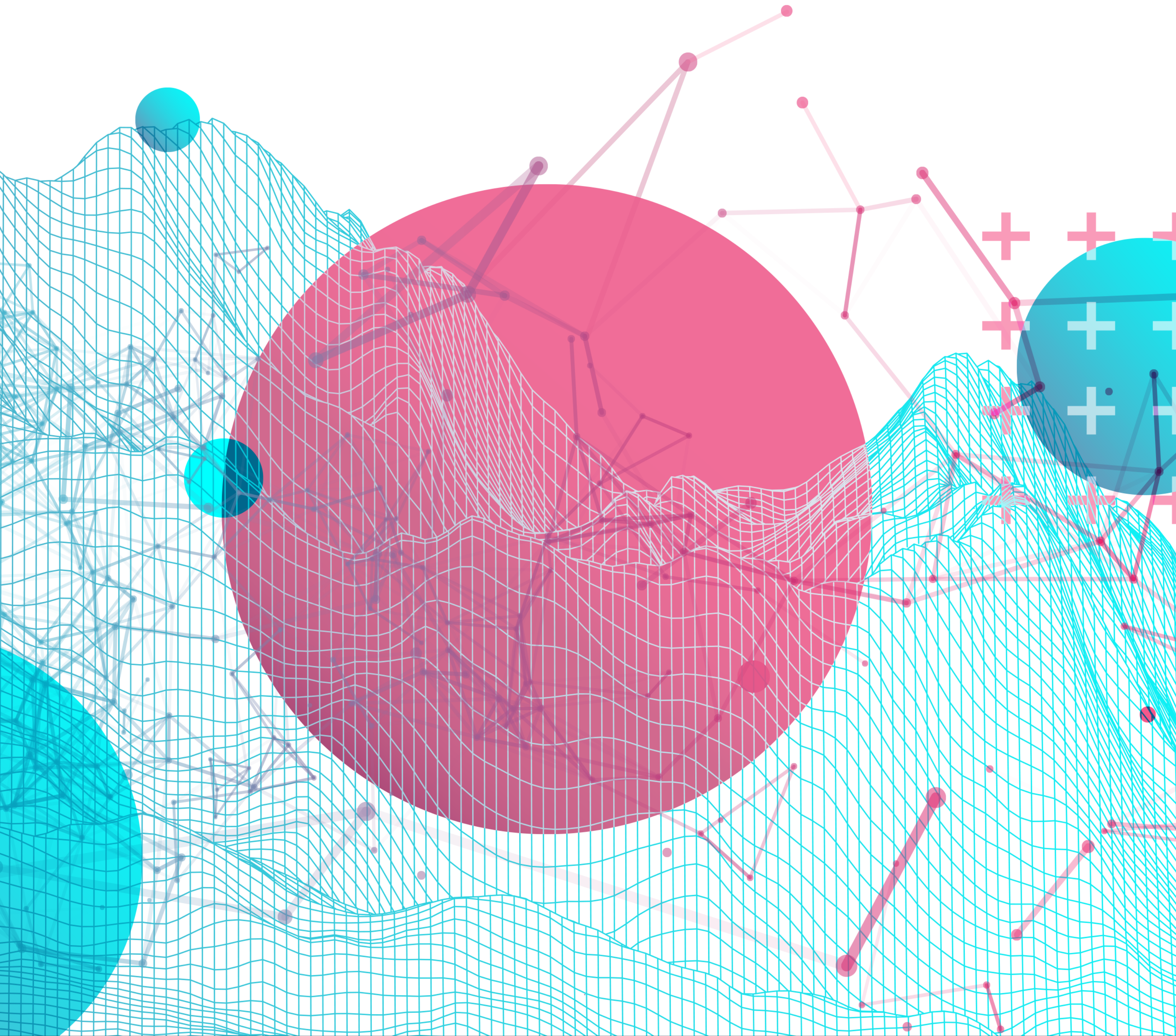
Investment Strategy

for science and technology

2020



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 the future needs of our national security missions. The *2020 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, we are continuing the pilot component of the LDRD program targeting "disruptive research"; second, we are paying enhanced attention to the White House-identified technologies of the future; and third, we have added quantum science and technology as a mission research challenge section.

Last year, we introduced a new element to the LDRD program targeting "disruptive research" (DR) ideas. Laboratory Director Bill Goldstein has called for "out-of-the-box" ideas in the form of "exceptionally innovative and unconventional" DR proposals that may provide long-term impact through order-of-magnitude improvements. We funded nine DR proposals last year. For example, one project proposes to improve wireless technology by three orders of magnitude in speed, power, and bandwidth all while reducing the size to that of a postage stamp. This new element recognizes the risks involved in such disruptive projects and encourages creative, outside-the-box thinkers to pursue exciting and novel ideas.

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 as "industries of the future." These five technologies, advanced manufacturing, artificial intelligence (AI), 5G cellular wireless broadband, synthetic biology, and quantum information science (QIS) are highlighted as having "promise to fuel American prosperity far into the future, while improving the security of our homeland." The Laboratory 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.

In recognition of the importance of the National Quantum Initiative to the nation and to our mission, we have expanded our efforts in this area and called out quantum science and technology as a new mission research challenge. Last year we made investments in understanding potential hardware and software approaches for a new generation of quantum computers, developing new materials with special quantum properties, and probing the ways in which quantum computing, sensing, and information processing can help solve complex problems critical to our mission. Quantum science and technology remains a focal point for us. More about the compelling mission drivers and our investment approach can be found on page 30.

Please enjoy this description of the many opportunities before us, find related information on the Lab's science and technology website, st.llnl.gov, consult with your colleagues, and reach out with any questions. We are grateful for the ability to make strategic investments that sustain Lawrence Livermore National Laboratory as a national resource for innovative solutions to tough, important national security challenges. And we are determined to use these investments to keep the Laboratory an exciting and meaningful place to work for top-flight scientists and engineers.

A Strategy for Science and Technology Investments

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

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

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

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

> *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 views 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 ten 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 a strong partnership 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 2019 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
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 “as delivered” nuclear package, including details about manufacturing, build, aging, and lifecycle environment.
- Enhance the underpinning S&T to enable timely development of weapon design options to cost-effectively meet potential requirements and enhance safety and security.
- Advance the state of the art in simulation capabilities, high performance computing (HPC) platforms, and experimental facilities and diagnostics that—together—enable validated, predictive simulations to support assessments and address future design requirements.
- Enhance surveillance capabilities to understand the health of the stockpile without significant destruction of assets. Enable the transformation of the NNSA production enterprise—building S&T tools, rapid prototyping, and reimagining processes to improve efficiency.
- Recruit, retain, train, and challenge 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; Quantum S&T

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:

- Evaluate potential emerging threats to guard against technical surprise and anticipate security vulnerabilities.
- Improve capabilities to monitor proliferation, detect and respond to terrorist threats, and effectively manage consequences and respond to WMD incidents.
- Support the Intelligence Community with analyses, cognitive big-data tools, and sensor capabilities that enhance awareness of evolving threats.
- Advance forensic science and technologies for attribution.
- Advance rapid development of medical countermeasures to pathogens and emerging diseases.

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

Multi-Domain Deterrence
Anticipate threats to national security, create innovative S&T solutions, and develop technologies and systems that strengthen deterrence, bolster defense, and enable dominance in long-term competition:

- Employ systems analysis and advanced modeling to deconstruct challenges facing key national security stakeholders; and develop novel concepts and solutions in critical defense-related technology areas.

- Explore implications of space as an emergent war-fighting domain; assess adversary capabilities and strategies; model resilience of U.S. technologies and system architectures; and evaluate approaches for deterring conflict.
- Become an indispensable partner in the national effort to develop hypersonic vehicles and associated technologies through expertise in underpinning S&T and leading-edge design of conventional warheads.
- Provide advanced cyber capabilities for threat assessment and analysis, network modeling, and support to national security stakeholders.

Pertinent Mission Research Challenges: Cybersecurity and Cyber-Physical Resilience; Directed Energy; High Explosives Physics, Chemistry, and Material Science; Quantum S&T; Space 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 cyber attacks 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; 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. Using these strengths, the Laboratory develops 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 30–39.

Director's Initiatives

Director's Initiatives 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 7–11:

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

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.

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

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

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

Laboratory Core Competencies

In support of these mission areas and to ensure the continued preeminence and quality of the Laboratory's S&T, institutional investment priorities strengthen LLNL's S&T 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 S&T.

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.

Each core competency is a defining capability or signature expertise in which LLNL is a recognized leader in the field. The core competencies are listed below and further described on pp. 12–29:

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.

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.

Advanced Materials and Manufacturing—meeting NNSA and national needs for the rapid, cost-effective development of advanced materials and manufacturing processes and systems.

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.

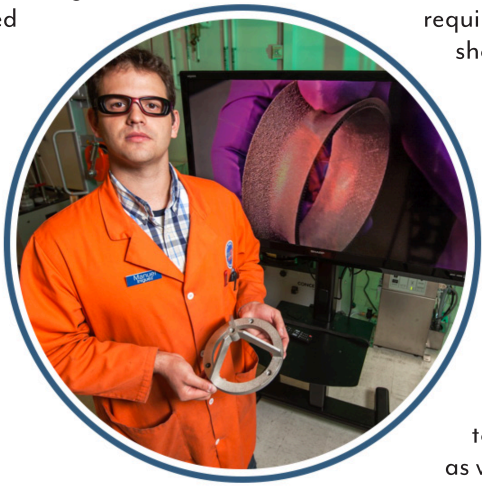
Bioscience and Bioengineering—working at the interface of biology, engineering, and the physical sciences to address national challenges in biosecurity, chemical security, bioenergy, and human health.

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

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 is focused on meeting NNSA's needs and broader national needs for the rapid, cost-effective development of advanced materials and manufacturing processes and systems. This initiative is 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 density, 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.



This highly coupled ecosystem can be broken down into four critical areas of investment:

Optimal design
As materials and manufacturing processes advance 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, non-intuitive 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 and Optimization. Not only will these methods apply to designs of components and material architectures but can also be used for manufacturing process optimization.

Feedstock materials and synthesis
Many of our programmatic applications require unique source materials ranging from nanomaterials with unique morphologies, to functionalized particles, powders, wires, and polymers, to name a few. As such, tailored synthesis or modifications to acquired materials is critical. Expanding into new cutting edge materials, such as those required for bio-printing, are new thrusts that should be pursued.

Advanced manufacturing processes
The past five to ten years have seen rapid advancement in advanced manufacturing capabilities ranging from additive manufacturing to microfluidic assembly and other methods. In this initiative, we have sought to drive these advancements 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, and mixed material structures. Additionally, inventing and developing processes for bio-printing and other emerging fields will be critical. Along with using these processes to create architected materials, this has been the core thrust of the Center for Engineered Materials and Manufacturing. Understanding of the underlying science has been pursued through an integrated modeling and simulation, experimental, and characterization approach.

Qualification
To transition new materials and processes to our programs, we must be able to qualify them in an accelerated fashion. This involves modeling and simulation to understand process limitations, new in-situ diagnostics for defect detection, fast non-destructive evaluation for part inspection, and data fusion and machine learning for process control.

Engineering the Carbon Economy

Supporting the S&T innovations and collaborations that create global-scale carbon dioxide removal and climate change mitigation solutions in the new carbon economy.

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 Engineering the Carbon Economy 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 recognized, and LLNL is acting now because the enormous size of the activity requires us to create technology innovations today.

A new carbon-recycling economy: industrial chemicals from CO_2

Renewable, carbon-free electricity is an important resource for achieving dramatic carbon reductions. It will permit us to make many carbon-based fuels and products not from fossil carbon, but from CO_2 that we have harvested from the atmosphere. LLNL is inventing new electro-, thermal-, and bio-chemical approaches for making fuels and industrial chemicals and feedstocks, such as ethylene (C_2H_4), from CO_2. LLNL 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's imperative that LLNL continue to make significant investments in this fast-growing field.

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

The choices that must be made 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 Engineering the Carbon Economy 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:

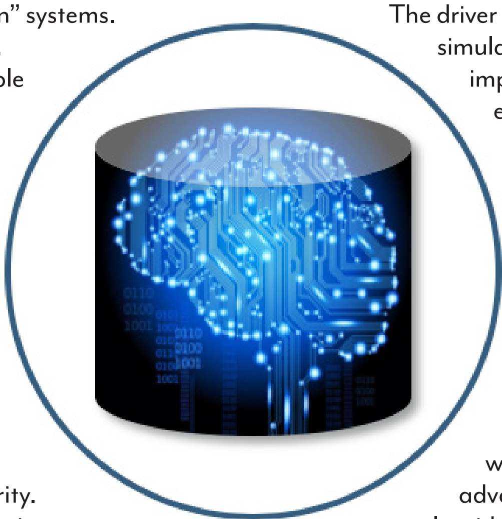
- Additively manufactured 3D reactors that combine structure and materials in unparalleled ways to achieve improved performance for metrics such as productivity, conversion, efficiency, selectivity, and stability.
- Carbon capture from biofuel production to enable negative emissions fuels—fuels that when burned, emit less carbon than was permanently stored during their production.
- 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 machine learning, high-performance simulation, and empirical data to improve prediction for national security applications.

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



Mission needs to model complex systems
LLNL mission priorities are increasingly focused on the performance, resilience, and security of complex systems in a broad spectrum of applications that includes stockpile stewardship, nuclear nonproliferation, critical infrastructure protection, and next-generation biosecurity. Our critical missions challenge 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 require a rethinking of our existing tools and approaches.

Innovative tools for modern problems
We require cognitive simulation models that use advanced machine learning to combine our rapidly expanding simulation capabilities with our precision empirical data sets. These new models are distinguished by their ability to incorporate, adapt to, and guide experimental observation, endowing them with an unparalleled ability to bridge the gap between purely numerical models and real experimental observation. Cognitive simulation systems will enable entirely new approaches to assure our national security, economic growth, and the health of our citizens.

Cognitive Simulation Initiative objectives
The objective of this Director's Initiative is to accelerate R&D in the effective integration of machine learning, high-performance simulation, and empirical data for important national security missions. The Initiative is developing this approach using inertial confinement fusion (ICF) and weapons science as driver applications.

Improved predictive models
The driver applications are employing cognitive simulation to develop models that make improved predictions by coupling large ensembles of simulations with more limited quantities of experimental data. The improved models also deliver better detailed quantification of uncertainty, and quantitative measures of the value of past and future experiments.

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.

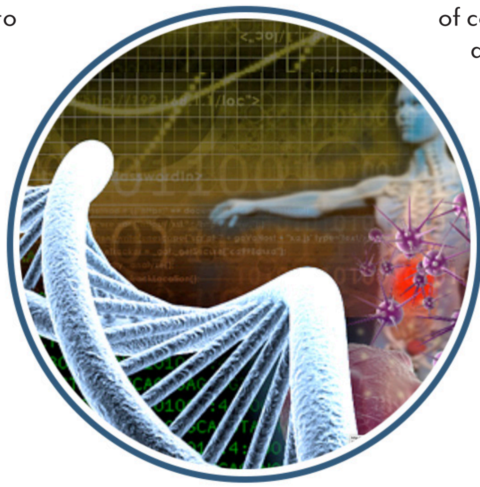
New AI-driven design methods
These new CogSim models integrate seamlessly with advanced design optimization loops allowing for new designs that rapidly integrate empirical data for improved performance and increased confidence. The underlying algorithms and workflows provide a testing ground for developing experimentally validated capabilities that can then be used for other stockpile stewardship applications where design, testing, and validation are more difficult.

Leading advances in scientific approaches
The impact of cognitive simulation will be felt in all aspects of modeling. These new approaches will provide improved predictive power; greater computational efficiency; and fast, flexible AI-driven design. Cognitive simulation will ultimately be a unifying framework that combines theory-based simulation and experimental data to empower scientists to develop deeper understanding of complex processes and to design optimally effective responses to contemporary scientific challenges.

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. 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.

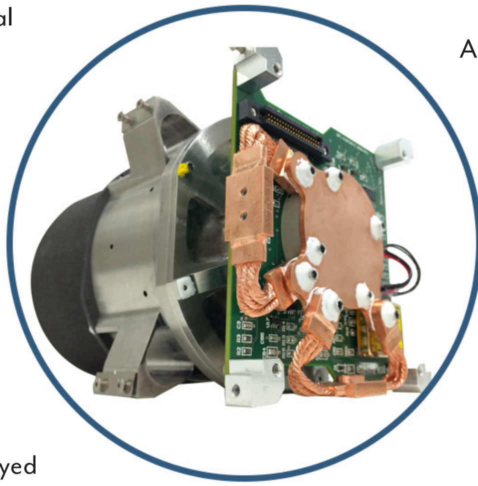
A public–private partnership approach

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.

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 and the Laboratory's long-standing involvement in and many advances to space science. The urgency for LLNL to contribute to this new mission has several drivers, including: increasing commercial competition from international firms; aggressive behavior from countries developing counter-space capabilities; and a more complex global security environment that requires more data to keep decision-makers informed. The initiative is building on deep expertise in space science together with recent advances in manufacturing technologies and data analytics that make new mission concepts and architectures possible. 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 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.

Novel hardware—deployed to meet mission requirements with application to small satellite platforms, as well as physics-based modeling and simulation of distributed space operations. Small satellite platforms have multiple virtues, including resiliency, faster technology refresh, and lower risk. In addition, constellations of small satellites offer a pathway towards high-cadence observations, which represents a potential game-changing capability for missions in: space situational awareness; intelligence, surveillance, and reconnaissance; and missile tracking.

Advances in LLNL core competencies support a broad portfolio of space science and space security projects:

- High resolution x-ray spectroscopy, atomic and nuclear physics, and chemical and isotopic science provide the experimental basis to help scientists better understand astrophysical observations and to analyze sample returns from space missions.
- High-performance computing plays an important role in modeling the performance of instrumentation during the design phase, and the basics physics of astrophysical phenomena. Key to our success in this area is applying methods and techniques from stockpile stewardship to the broadest set of challenges.
- Advanced manufacturing helps Livermore researchers develop new ways of making essential parts and opens pathways for creating the constituents for new detectors and optical elements.
- Laboratory expertise required for the nuclear non-proliferation mission is also used to develop technologies to sense and measure x rays, gamma rays, and other forms of radiation.

High-Energy-Density Science

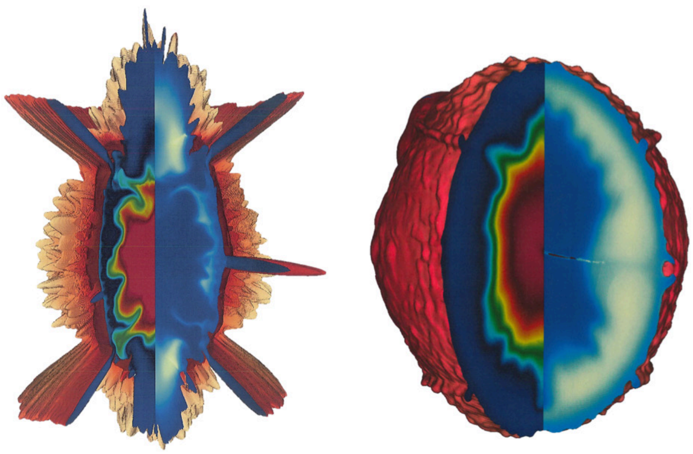
Providing international leadership in studying and controlling matter under extreme conditions of temperature and pressure.

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, 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, where world-leading experimental and simulation capabilities are located, since its founding.

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 and planets, can be attained. This 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, which serve as early testbeds for the higher temperatures and pressures that experiments can reach at NIF, while also enabling physics studies. These testbeds include both large and mid-size facilities such as the Jupiter Laser Facility at LLNL, Omega, 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 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.

- 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. 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 shock-induced materials behavior, plasticity, phase transitions, and chemical reactions; 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.

- The trajectory of HED experiments covers both 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.

- Probes of all forms of energy sinks (plasticity, viscosity, phase transitions, chemical reactions, mixing/demixing) are needed.

Properties of hot dense matter
The atomic, thermonuclear, nuclear and radiative properties of hot matter. They include dense plasma absorption and emission spectroscopy, radiation heating, opacities, spectral line shapes, dense plasma effects and the breakdown of the isolated atom picture, non-equilibrium atomic kinetics and radiation transfer, and detailed x-ray spectra simulations. Plasma transport properties such as electrical and thermal conductivity, viscosity, and charged particle stopping are also included. Properties of hot dense matter also include thermonuclear and nuclear processes in dense plasma environments. The phenomena of interest include plasma screening, non-Maxwellian ion distributions (kinetic effects), nuclear excitation by electron capture, and big-bang nucleosynthesis.

- Integration of reduced-order models into design codes that allow for the incorporation of detailed microphysics in hydrodynamic simulations is needed.

- A better understanding of dense plasma effects on atomic, nuclear, and thermonuclear processes in hot, dense, and high neutron flux environments is needed for both 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
The branch of hydrodynamics in which 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.

- 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 becomes blurry. A metric identifying when kinetic effects matter to a design code will be needed. The incorporation of 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.

- Data analytics and machine learning have recently become useful tools for researchers in HED physics. Large amounts of experimental data and simulation information are generated and must be analyzed to gain understanding and draw conclusions. Extracting useful information out of this multidimensional space using data analytics and machine learning shows great potential.

Laser–plasma interaction and applications
The study and manipulation of laser-produced plasmas in nonrelativistic and relativistic intensity regimes for applications in HED science. At high 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 of being harnessed and applied to other areas of science (e.g., compact electron accelerators and radiation sources).

- A predictive modeling of laser–plasma interactions suitable for hohlraum physics studies and the development of plasma optics. Incorporation into beam-propagation codes of kinetic and nonlinear effects important to NIF laser–plasma interactions as identified in PIC and Vlasov codes is needed, as is coupling of beam propagation codes to rad–hydro codes.

- The interaction of high-intensity and ultrashort (sub-picosecond) laser pulses with tenuous gases or plasmas and with solid-density plasmas. 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 and should be pursued.

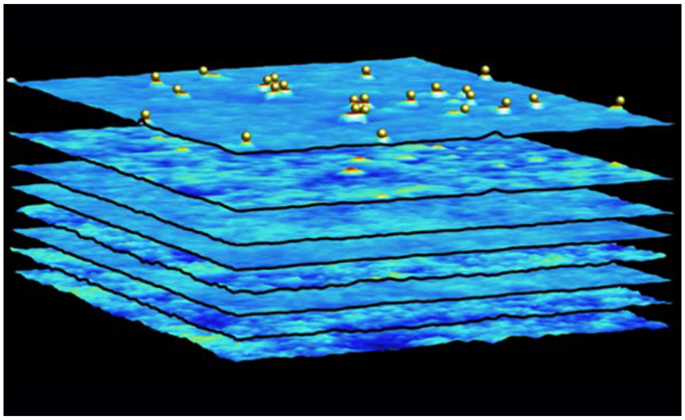
- With the emergence of high-repetition-rate high-intensity short pulse lasers, HED experiments at high-rep-rate will be transformative for the science of laser-plasma interactions and applications. The integration and development of high-throughput targetry and diagnostics, data analytics and machine learning, and rapid simulation 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 simulations.*
- *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.



A machine-learning-guided selection process (MuMMI) is used to choose interesting regions of the macro-model simulation of RAS proteins on a cell membrane to examine with high-resolution micro simulations.

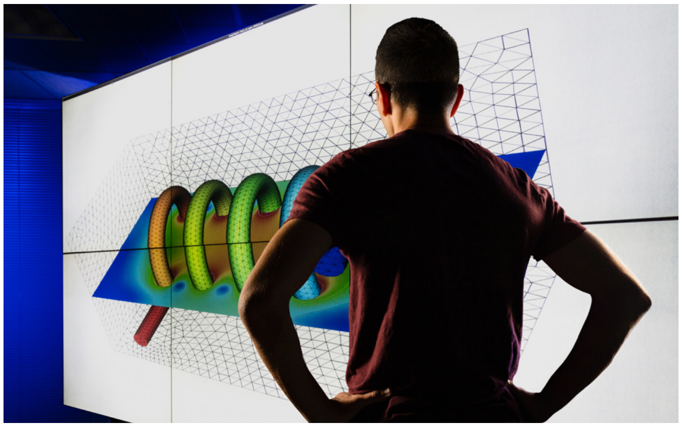
R&D Priorities

High-performance computing (HPC)

- **LLNL provides leadership in the drive toward exascale-class computing**
  The challenge is to develop algorithms for applications that can effectively use massive amounts of parallelism and concurrency while reducing data motion and usage. In addition, simulations are increasingly leveraging techniques from artificial intelligence (AI) and machine learning (ML), which often have complementary requirements that must be addressed. To accomplish this, algorithms must be reimagined in ways similar to the paradigm shift triggered by the emergence of distributed parallel programming. LLNL has long been a recognized leader in the deployment, research, and application of HPC to solve complex S&T problems and is able to meet the computing challenges through expertise in vertical integration—from leading-edge hardware and foundational software to multiphysics applications and data-science analytics for situational awareness.

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

use of programming models, workflow and other productivity tools, system software, power awareness, resilience, and data science techniques. Furthermore, as HPC capabilities evolve, so do the potential uses of HPC, and the rise of large-scale, data-centric computing and its confluence with traditional simulation pose new challenges and opportunities for fundamental algorithm and computer science infrastructure development.

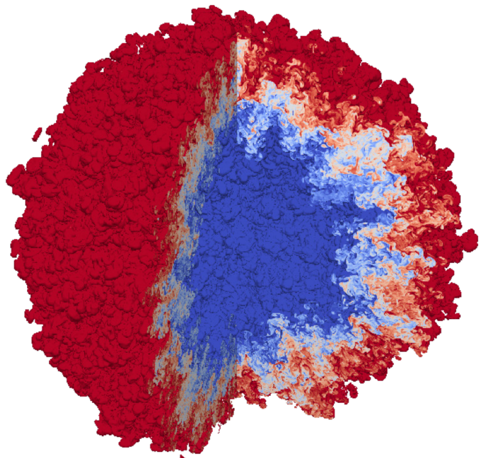


MARBL, used to simulate magnetic diffusion in a coil on a high-order tetrahedral mesh, is a multiphysics code that enables researchers to model complex pulsed-power experiments for high-energy-density science.

- **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. Following these strategies, M&IC deployed two systems in FY19, Lassen and Corona. Lassen is a smaller version of the new Advanced Simulation and Computing (ASC)/SSP system, Sierra. Corona is designed for exploring AI/ML efforts. M&IC has also expanded efforts in cloud computing. In particular, the Workflow Enablement project has purchased hardware and software for production-level HPC-related cloud infrastructure including the support of containers. Efforts in cloud computing will require ongoing research and evolution of our system software stack.

- **Innovative architectures**
  LC systems have provided a fertile research environment for exploring the use of emerging technologies such as processing in memory (PIM), nonvolatile random-access memory (NVRAM), and graphics processing units (GPUs). However, HPC technology roadmaps are rapidly changing to target expanding markets in cloud computing, AI/ML, and cybersecurity. LLNL 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 shift away from traditional HPC simulation. This effort must not only maintain activity on traditional HPC simulation architectures. LLNL must also identify and develop strategies to exploit the innovations that target nontraditional architectures. Ongoing efforts show that simulations clearly benefit from heterogeneous architectures, such as Sierra and Cerebras CS-1, an innovative new hardware design that is being integrated into Lassen and which will provide a rich testbed for exploring heterogeneous system architecture issues. 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 co-design 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 faces a major inflection point in how we develop and maintain software. Hardware innovations in computing architectures such as multi-core, GPUs, and AI processors are outpacing our ability to write software effectively and efficiently. 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,



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.

a "valley of death" with respect to the usability of tools separates the initial innovations from the breadth of LLNL's software developers. Thus, we must implement a strategy to deploy a common base of foundational scientific computing software with opt-in adoption from LLNL applications. This effort will harden research tools and libraries, provide direct assistance to developers, support training to strengthen the workforce, and create a culture around and improve 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 along with DOE policy motivate LLNL programs to exploit and to contribute to open-source software, and developers must engage in 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 sub-scale physics. This physics is 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 extent possible to inform these physical data models, many of the regimes we care about are not easily accessible, or measurable, through experiments. Thus, we are heavily dependent on first principles, or high-fidelity simulations, such as molecular dynamics, to improve our sub-scale physics and, therefore, 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, since the limitation of these models, in many cases, is simply computational resources. In some cases, the dynamic nature of the problem requires tight coupling and concurrency between sub-scale 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. Nevertheless, research into how and when this kind of coupling needs to occur is necessary.

- **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, to create surrogate models that approximate expensive and time-consuming simulations, and to 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 sample solution; and by understanding the mathematical structure of high-dimensional data. New design optimization methods need to be explored, such as gradient-free algorithms, to solve problems with discrete or otherwise non-analytic cost functions. Innovative uses of machine learning can identify unexpected features within ensembles and provide feedback to guide ensemble sampling strategies in solution space. In addition, existing optimization methods need to be extended to highly nonlinear and dynamic regimes. Methodology improvements must be complemented with user workflow enhancements that streamline execution of large ensembles 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) for 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 special to LLNL's mission needs and 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 ultimately be based on strong mathematical foundations that enable deeper understanding of performance impacts due to limited data, uncertainty quantification, and explainability of inferences.

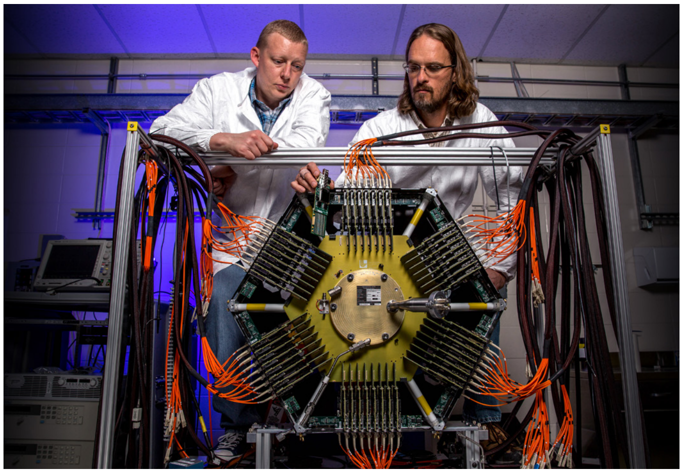
- **Distributed decision making and collaborative autonomy**
  The advent of highly dynamic and distributed platforms, each with a significant degree of autonomy, offers an unprecedented opportunity to deploy "swarms" of multimodal sensors for real-time situational awareness and decision-making in support of multiple mission areas. Progress 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 prevailing conditions, as well as a new generation of algorithms that can collectively fuse multimodal sensor data across the 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.

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.



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.

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 filling technical and knowledge gaps in key nuclear, chemical, and isotopic signatures S&T. Forefront scientific research in these fields is critical for attracting our future workforce and LLNL's ability to extend our capabilities to meet future national security needs.

- **Structure and reactions of nuclei**
  The study of atomic nuclei is essential for understanding the evolution of the universe. It also provides the 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 facilities, such as the Facility for Rare Isotope Beams (FRIB), which offers an unprecedented opportunity to study nuclear properties, especially neutron-rich nuclei near the limits of stability, and (2) high-performance computing, which will enable a more comprehensive and predictive theory for not only how nuclei are assembled, but how they react.

- **Radiochemistry**
  Research in radiochemistry explores nuclear reactions, the limits of nuclear stability, and the properties of the heaviest elements. The ability to recreate the conditions in stars or nuclear weapons in the laboratory at the National Ignition Facility, combined with the development of new chemical separation and automation methods, diagnostics, and experimental platforms, constitutes the foundation for solving exciting fundamental

problems, such as the exploration of nuclear reactions in a plasma, and complex mission challenges, such as the assessment of known or unknown nuclear devices. Research into how radiochemical processes are affected by plasma environments, such as the fractionation of chemical elements and isotopes across a broad range of spatial and temporal scales, will support both the stockpile stewardship and nuclear forensics programs. The development of sensitive, compact, flow-through, deployable platforms will enable nuclear incident response while being synergistic with the development of atom-at-a-time platforms needed to explore the properties of the newest and heaviest elements on the periodic table.

Radiochemistry research at LLNL is focused on experiments to study the properties of radioactive isotopes, develop fast and fieldable separation methods, and apply techniques and knowledge to nuclear forensics scenarios.

- **Analytical and forensic science**
  Analytical chemistry is the art and science of determining what matter is and how much of it exists. The development of state-of-the art analytical methods is foundational for forensic science related to CBRNE threats and pre- and post-detonation nuclear forensics. Another key area is the extraction of unique chemical and/or isotopic signatures to detect and study processes of interest. The same analytical methods also enable ground-breaking 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 ultra-trace isotopic capabilities to earth system processes; 5) biomedicine and human health (including personalized medicine), by utilizing high-throughput carbon-14 measurements coupled to chemical separation instruments for rapid medical analyses; and 6) environmental chemistry, by studying the microbial processing and transport of various forms of organic 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 the acquisition of 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 hand-held detectors for first responders; radiation monitors for border portals; gamma 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 the big bang with ultra-high-energy nuclear collisions; 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 infrastructure, equipment, and workforce development.

Short term infrastructure investments aim to better integrate capabilities and to improve mission delivery. Of particular importance are investments that will enable greater co-location of personnel and resources, enhanced local capabilities (including a revitalized accelerator complex in B194, renovated radiochemistry laboratories in B151, a refurbished CAMS facility infrastructure, 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 the Livermore Nuclear Science Center, a unique and dedicated facility delivering gamma, neutron, and particle beams for nuclear experiments, collocated with radiochemistry and atom and 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 where crucial experimental data are needed.

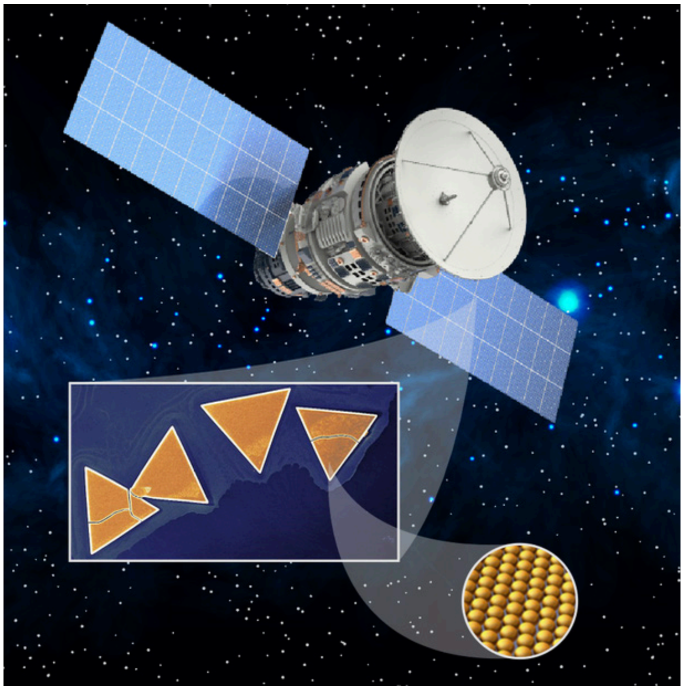
Equipment investments will focus on refurbishing workhorse analytical instrumentation while building one-of-a-kind capabilities to maintain our sharp technical edge. A new high-resolution Nano-Secondary Ion Mass Spectrometer for high-precision isotopic mapping (under construction); new Secondary Ion Mass Spectrometer and Thermal Ionization Mass Spectrometer; a medical cyclotron to produce isotopes of interest locally; and upgrades to CAMS, including actinide AMS and cosmogenic AMS beamlines for improved sensitivity are among the top priorities.

Advanced Materials and Manufacturing

Meeting NNSA and national needs for the rapid, cost-effective development of advanced materials and manufacturing processes and systems.

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. LLNL is pursuing more agile, responsive, and integrated approaches to accelerate material development, manufacturing, and qualification solutions. The concept was demonstrated in the Laboratory's partnership with the Air Force during the BLU-129/B program, in which a composite material and novel high-explosive fill moved from concept to field within 18 months.

The challenge is to integrate design, fundamental understanding, and deployment of new materials and manufacturing processes. Our goal is to deliver materials and components with tailored properties on an accelerated schedule and at reduced cost, with a special focus on the specific needs of our national security stakeholders. Doing so requires advances in our world-class experimental and computational materials and manufacturing science capabilities. Success depends on expanding strategic partnerships to create a mutually beneficial network encompassing NNSA production facilities, national laboratories and other FFRDCs (federally funded research and development centers), academia, and U.S. industry. Our efforts will support U.S. manufacturing competitiveness through workshops, partnerships, collaborations, technology advancements, and the newly constructed collaborative Advanced Manufacturing Laboratory (AML) in the Livermore Valley Open Campus (LVOC). These efforts will also facilitate the recruiting and career development of the next generation of materials scientists, chemists, and engineers at LLNL.



LLNL is developing new techniques to deposit ordered arrays of nanocrystals with applications in nanocrystal-based devices such as solar cells, infrared detectors, and light emitting diodes.

R&D Priorities

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 extend, build on, and integrate foundational capabilities at LLNL for validated predictive simulations, tailored materials synthesis, characterization and testing, and precision and additive manufacturing. Specific R&D thrusts include:

- **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 also a focus.

- **Material design and manufacturing**
  Whether thin films, nanoparticles, or complex 3D nano- to microarchitectures, the next generation of materials will require computational tools that optimize geometry and composition over multiple length scales. New computational methods, such as topology optimization, may be used to drive to nonintuitive material architectures and designs. Additionally, new material feedstocks and the manufacturing methods to assemble them are needed to realize structures with the desired properties and performance. The integration of computationally driven design, novel materials, and state-of-the-art manufacturing methods will enable LLNL researchers to produce components with previously unobtainable combinations of properties.

- **Advanced and in-situ characterization**
  The accelerated development and optimization of new materials requires continued access to and development of state-of-the-art materials characterization equipment and expertise. This will apply to "build time" diagnostics, as well as the ability to rapidly and accurately characterize "as built" components with respect to their dimensions, key features, and material constituency. This would include new capabilities for 3D imaging, spectroscopy, and scattering, where each would have unprecedented sensitivity that span atomic to macroscopic length scales and multiple time scales. Developments in materials characterization are further enhanced by complementary consideration of rapid data analysis and modeling tools. In-situ and operando techniques are also required to probe materials 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.

- **Process-aware performance modeling**
  To achieve rapid development-to-qualification of components, advances are needed in validated predictive material-, component-, and system-level models over a broad range of materials sets and spanning atomistic scales 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 modelling needs to evolve from describing ideal systems to describing real systems.

- **Scale-up**
  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. Advances in our expertise in computational design, material synthesis and qualification, data analytics, and machine learning are required to realize scalable material synthesis (including for feedstock materials) and manufacturing processes.

- **Expanded partnerships**
  Expanding our strategic partnerships with academic institutions, U.S. industry, FFRDCs, NNSA laboratories, and production facilities will benefit LLNL's advanced modeling and manufacturing efforts through the communication of best practices, new ideas, and improved processes. Also such partnerships establish pipelines for new talent to access the laboratory. Acess will be enabled further by the new AML in the LVOC, where LLNL staff can work side-by-side with academic and industry partners on materials and manufacturing projects of joint interest. Important areas of collaboration include design and optimization, materials development, manufacturing process development, and qualification and certification. "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 LLNL programs ranging from stockpile stewardship and NIF to energy security.

Lasers and Optical Science and Technology

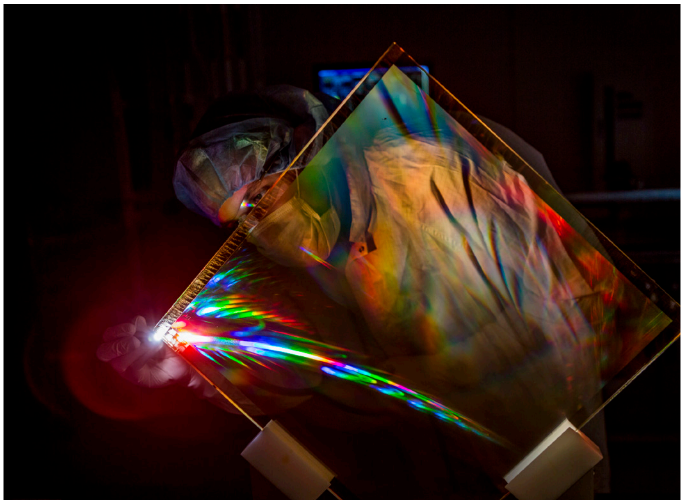
Designing, building, and reliably operating complex laser systems that dramatically advance the state of the art for strategically important applications.

Core competencies in lasers and optical materials (LAOM) 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 induce secondary radiation sources such as x-rays, gamma rays, protons, electrons, and neutrons. The use of laser-induced plasmas to accelerate electrons to many MeV levels in very short distances has been demonstrated.

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 optics 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 for 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. Development of solid-state laser diodes for high-efficiency pumping will be 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 develop short-pulse laser-driven radiation sources. This technology 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, novel optical materials and novel 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 technologies with radio frequency 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 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, the transforming of a laser design for inertial fusion energy into an innovative high-average-power laser architecture for generating short pulses at unprecedented repetition rates. International projects 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.

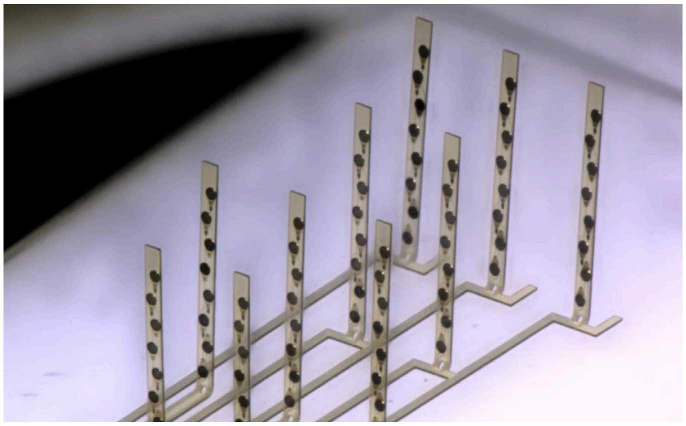
- **Modeling and simulation**
  LLNL's unique capabilities in high-performance computing extend to modeling and simulating advanced laser systems. Laser modeling and simulation investments maintain LLNL's world-leading capabilities, enable the development of new and innovative laser technologies, and 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, bioenergy, and human health.

The biosciences and bioengineering core competency emphasizes a culture of multidisciplinary research that enables innovation through combined technology development and biological problem solving. The core competency supports the expert skills, unique capabilities, and special facilities needed to inspire ground-breaking research that addresses the most pressing problems in health and energy 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, bioprinting, select agents, toxicology, and bioanalytical science to perform our work.



Novel LLNL-fabricated 3D biocompatible microelectrode arrays, consisting of electrodes distributed along vertical polymer probes, are used to evaluate the functioning of neuronal networks (e.g., bursts/min).

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 the biosecurity arena that include rapidly advancing technology, the growing threat of climate change, and the emerging ability to engineer life. 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 develop computational tools and create three-dimensional experimental models that can be integrated to more accurately understand and predict complex biological systems. Through experimentation, researchers are working to understand the mechanisms of disease, engineer microbial communities for health- and environmental-related objectives, and develop 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.

- **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. Our priorities are to:
  - Develop physiologically relevant, high-fidelity in vitro and in silico tools that are validated by comparison to in vivo systems.

- Create computational tools for large-scale, comparative biology challenges.
- 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.

- **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 and energy 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.
    - Engineer bioreactors to produce pharmaceuticals, biofuels, and other products.
    - Improve our understanding of the molecular basis of disease.
    - Understand the underlying cellular and molecular pathways involved in microbial pathogenesis.
    - Understand the disposition of chemicals and biologics at multiple scales (organism to cell).

- **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 solutions to newly identified threats and understand the risk of perceived future security threats. Continued advancement of detection technologies will enable real-time epidemiology, disease forecasting, and the ability to distinguish new, previously unknown threats from known traditional threats. Our priorities are to:
    - Develop multimodal, integrated detector systems for complex surveillance (fieldable and wearable, for use in environmental and clinical applications).
    - Design and engineer the next generation of materials to sense and protect against exposure to chem/bio/radiological agents.
    - Accelerate the development of therapeutics, prophylactics, and vaccines.

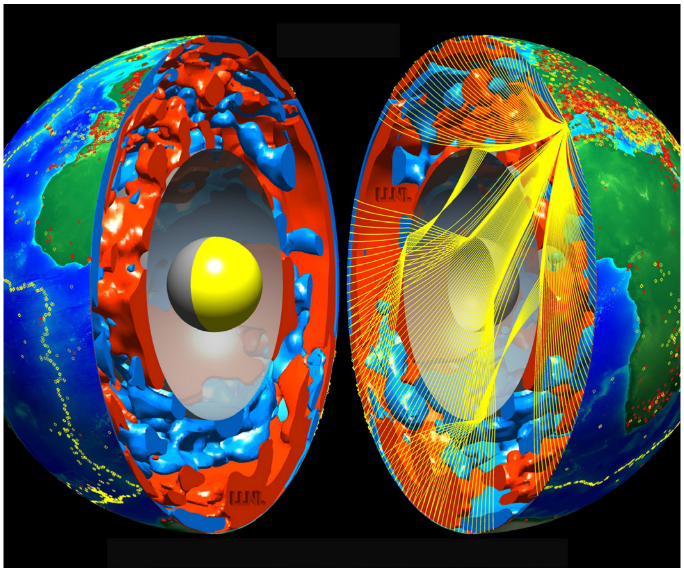
Earth and Atmospheric Science

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 ozone depletion in the upper atmosphere, shale oil and gas, radioactive waste disposal, and the transport of contaminants in groundwater. 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.

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 information to aid emergency preparedness and response efforts in the event of hazardous emissions, such as the Fukushima radioactivity release in 2011. 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.

In Earth science, LLNL has developed world-class capabilities in subsurface modeling, including shock physics, seismic simulation, and fracture mechanics (with advanced tools for modeling fracture networks). 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. These include 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 discovery and management of hydrocarbon and thermal reservoirs.



To advance seismic event monitoring capabilities, LLNL developed a global-scale model (LLNL-G3D-JPS) of seismic velocities (P- and S-wave speeds) in Earth's crust and mantle with regional-scale details.

In addition to solving problems in critical mission areas, these capabilities in Earth and atmospheric science 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, multi-phenomenological 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 development of new defense technologies. Observations for model validation and research into model improvements are required for the stratosphere and higher altitudes.

- **Climate change resilience**
  Higher resolution climate models are needed to provide accurate simulations/projections of climate change and climate change impacts at the local and regional scales. Two especially important climate change 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, model structure, and model parameters.

- **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 are also needed to improve uncertainty estimates associated with NARAC's assessments.

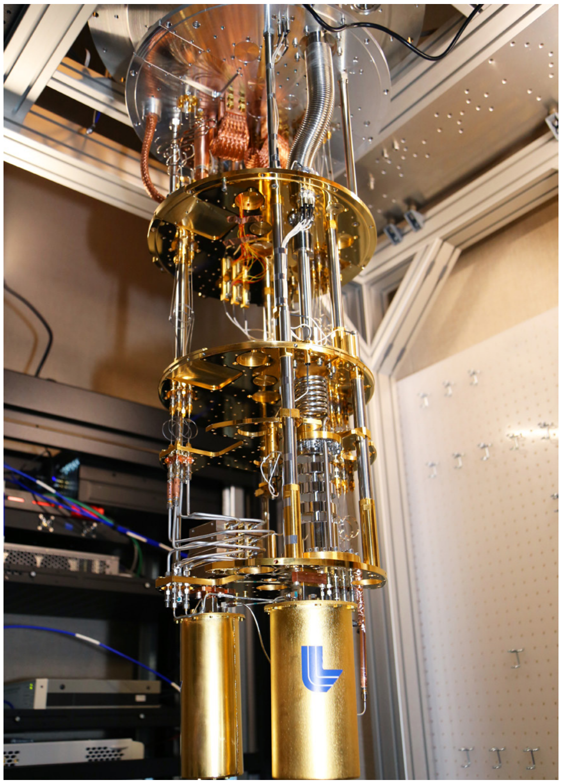
- **Atmospheric modeling for renewable energy**
  Forecasting of wind and solar generation requires modeling skills in atmospheric flow, atmospheric physics/microphysics, and integrated computational fluid dynamics modeling that are currently not available. Atmospheric models cannot handle the complexity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

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.

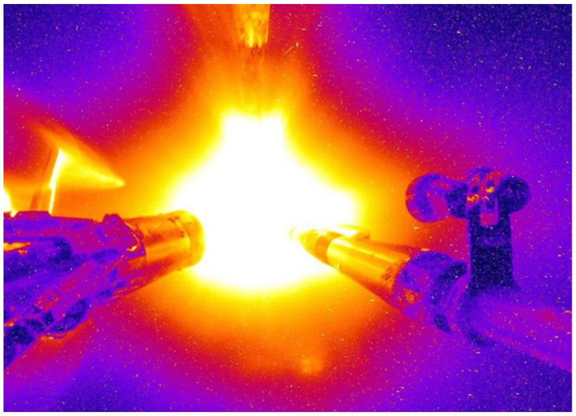
LLNL's quantum science strategy is centered on the use of a multidisciplinary co-design research environment that draws on the Laboratory's deep expertise in physics, chemistry, optics, engineering, and materials science. The challenges associated with realizing the hardware and software approaches needed 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 implementation of near-term usage of quantum computing and simulation will require multidisciplinary teams of physicists, materials scientists, computer scientists, and engineers to design and develop prototype systems and to evaluate new system architectures.
- **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, measurement and processing.

Nuclear Weapons Science

Providing scientific and technological innovation to ensure the safety, security, reliability and effectiveness of our nation's nuclear weapons stockpile, and to readily respond to future national security threats.

Our Laboratory's national security program is anchored in nuclear weapons science. Innovative science and technology impart creative solutions to maintaining and extending the life of the current stockpile and enable timely response to future threats. The inability to perform full system tests of the 21st-century nuclear weapons stockpile accentuates the importance of the Laboratory's mission (as part of NNSA's Stockpile Stewardship Program) to sustain high-level confidence in the nation's nuclear arsenal, which in turn requires workforce excellence. LLNL must continually revitalize and grow the expertise that underpins high-level confidence. The nation relies on the Laboratory to anticipate and be responsive to technical surprise and arising national security challenges.



Experiments at NIF are investigating means for reducing hydrodynamic instabilities and the properties of materials at extreme conditions.

Understanding, predicting, sustaining, and modernizing the stockpile requires underpinning science in many strategic areas that span multiple spatial and temporal scales. The challenge in nuclear weapon science is to capture the crucial physics at all scales. Some key areas of interest are:

- **First-principles understanding of fundamental science**—Validated predictive simulation is a primary objective of stockpile stewardship. To the extent possible, simulation codes are based on physics "first principles" rather than use of parametric models calibrated to data. A key need is therefore improved scientific understanding. Such understanding is achieved through the development of theory, advanced integrated and focused physics experimental platforms, diagnostic capabilities, improved multiscale modeling, efficient model descriptions that adequately capture the microscale physics, and simulation tools that effectively exploit the fastest high-performance computing capabilities. Special focus is on understanding the performance of the weapon "as delivered," including the impact of manufacture as well as aging and lifecycle environment. This need highlights research areas such as lifecycle material properties; high-energy-density science (boost physics, inertial confinement fusion (ICF), radiation-hydrodynamics); energetic material drive (e.g., high explosives); high-fidelity engineering and chemistry models; data science and machine learning; and uncertainty quantification and certification.

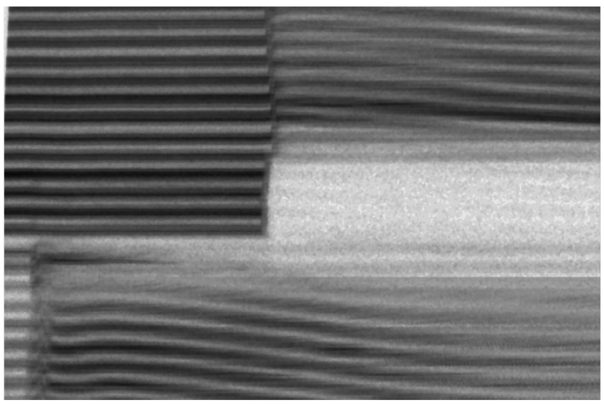
- **High-energy-density (HED) experiments at the National Ignition Facility (NIF)**—Specialized HED facilities such as NIF present opportunities to pursue innovative concepts for platform design, target fabrication, diagnostic techniques, and analysis for application to weapons science. NIF experiments require creativity coupled to disciplined scientific execution, which is important to workforce training in relevant design and engineering skills. ICF on NIF presents the opportunity to explore achieving fusion ignition and gigajoule energies in a laboratory setting, which enable exploration of a whole new range of weapons-related HED experiments.

- **Advanced manufacturing for weapons applications**—Research into new manufacturing techniques offers the potential to tailor material properties beyond those available through traditional techniques. A key aspect of this work is to understand the properties of newly manufactured materials and the impact of changes caused by aging. Capability development is underway to quantify material responses under high-explosive driven conditions in hydrodynamic experiments. The enhanced understanding coming from this research will provide the basis of material and manufacturing solutions that promote an agile, responsive, and survivable stockpile. Equally important, such research will draw the best of the future workforce.

High Explosive Physics, Chemistry, and Material Science

Improving our understanding and prediction of high-explosive behavior to cost-effectively refurbish and enhance the safety of the nation's nuclear deterrent and keep the nation safe from emerging explosives and nuclear proliferation.

LLNL has a mission need to enhance capabilities for understanding and predicting the behavior of high explosives (HE), which are integral to every nuclear weapon system. We provide high confidence in the safety, security, and effectiveness of U.S. deterrent forces and are enabling a transformation to an all-insensitive HE (IHE) nuclear stockpile and the increased use of IHE in conventional munitions. Next-generation weapon systems for the Department of Defense will be exposed to environments that challenge both the tactical lethality and long-term stability of HE materials. Expertise in HE also is crucial for informing and providing solutions to detect, mitigate, and interdict explosive proliferation threats.



A VISAR image shows the laser-driven shock transit through a triaminotrinitrobenzene (TATB) target at the University of Rochester Laboratory for Laser Energetics Omega EP laser facility.

High-resolution, predictive simulations of HE require advances in modeling and algorithms that leverage LLNL's world-class scientific computing resources. Novel diagnostic development, next-generation light sources, and techniques for enhanced chemical and physical characterization of HE materials need to be developed for in-situ and remote applications. New manufacturing methods (i.e., additive manufacturing) and reduced development cycles for feedstock materials are expected to improve the responsiveness of manufacturing HE components. HE R&D priorities include:

- **Making substantial progress toward a unified, 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 ab initio molecular dynamics, mesoscale, and coarse-graining methods for bridging to continuum representations. We are scrutinizing our predictive codes, looking to take advantage of GPU architectures—including applying machine learning as appropriate. LLNL has an ongoing need 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 access to end-stations authorized for HE detonations should continue to be applied.

- **Investigating manufacturing methods to enable development of options for an agile all-IHE next-generation nuclear deterrent through accelerated HE feedstock and component production, to advance surety, and to study improvised nuclear devices**—Responsive manufacturing offers opportunities to target key performance uncertainties, develop non-intrusive instrumentation for stockpile monitoring and forensics, pursue innovations in safety and surety, and explore proliferation space. Continued research in data science techniques are expected to accelerate materials development, manufacturing, and qualification.

- **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 to maintain reproducibility. Advances in scientific computing should be applied to quantify fluid dynamic characteristics of reactors for predictive correlations to 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.

High-explosive experiments and advances in seismic-wave propagation modeling are improving capabilities to detect low-yield nuclear tests.

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-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, and rendering them safe by conducting consequence management actions.

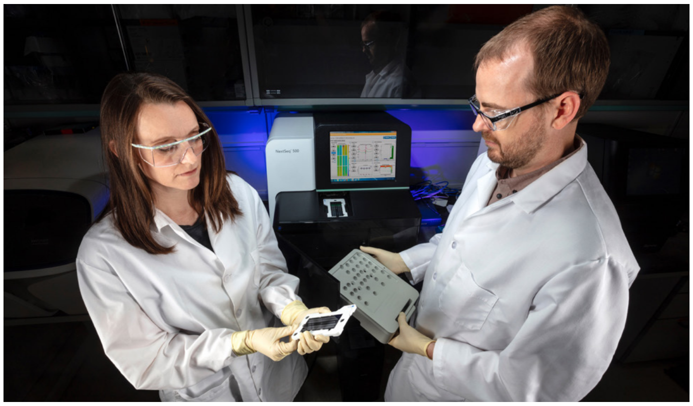
Sponsors of nuclear threat reduction activities seek deployable technologies to use flexibly and quickly. Focus areas include:

- **Understanding emerging technologies**—We need validated models of how unique materials behave and better understanding of how new technical approaches could be used by proliferators in order to evaluate and disable potential threats.
- **Enabling nonproliferation and arms control**—innovative technical approaches are needed to ensure the continued viability of the nonproliferation regime and to prepare for future arms control initiatives.
- **Strengthening proliferation warning**—We need new data analytics capabilities for extracting actionable threat information from massive, heterogeneous data streams to enable early-stage proliferation detection.
- **Advancing nuclear threat detection**—Accurate detection of nuclear threats, including proliferative activities, materials and devices, and requires improvements in detector materials and sensors as well as more flexible and intelligent data processing for sensor networks. Innovative methods for exploiting threat-relevant signatures are also needed.
- **Improving nuclear test detection**—A better scientific understanding of the signatures of nuclear explosions is needed, including underground, low-yield, and evasive nuclear tests. New technologies for enhancing our ability to identify and characterize nuclear explosions are also needed.
- **Accelerating post-detonation forensic analysis**—Advanced radiochemistry techniques for fallout materials and data fusion from all available sensor phenomenologies are needed for rapid and accurate decision support after a nuclear detonation.
- **Enhancing consequence management**—Improved models are needed at the Laboratory's National Atmospheric Release Advisory Center to provide more accurate estimations of the consequences of a nuclear incident and to quantify uncertainties for decision makers.

Chemical and Biological Countermeasures

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

LLNL supports the national mission to defend against chemical or biological (CB) threats and from attack or outbreak. Our work focuses on developing measures to protect against naturally occurring disease as well as the use of chemical or biological weapons. We also seek to better understand the "dual-use" nature of biotechnology and life sciences that drives innovation and improves health but can also be misused in an attack.



Bioscientists reviewing sequence data. Genomic characterization of new and emerging threats is key for developing countermeasures.

Our scientists understand that the best response to crisis is to prevent, disrupt, degrade, or deny the factors that allow a crisis to take place. Through partnerships with numerous government agencies, LLNL is able to support biosecurity programs and to provide a strong foundation for new strategies that prevent and respond to increasingly complex CB threats. Our work supports and promotes a culture of biosafety and biosecurity while providing ethical and responsible research in the life sciences.

- **Risks and appropriate responses**—Understand how advances in the beneficial use of biology, informatics, and biotechnology can enable threats from malicious use and apply that knowledge to develop appropriate scientific methods that assess risk. Address the potential for harm from the development of new engineering technologies that use or modify existing microorganisms to produce reagents or chemicals. Use HPC simulation and modeling to develop platforms that advance experimentation to counter threat and deepen our understanding of biological systems, validate biological models, and improve the development of medical countermeasures.

- **Detection, attribution and biome repair**—Develop capabilities that improve existing detection platforms and use advanced sequencing methods for measuring genomic data to detect and characterize new and emerging biological threats. Promote new approaches for understanding the role of the microbiome in human health and warfighter protection. Microbiomes are important to human immune function and physiology and their relationship with a human host ranges from mutualistic and supportive to pathogenic. A deeper understanding of these interactions will help shape strategies for intervention, repair, and prophylaxis.

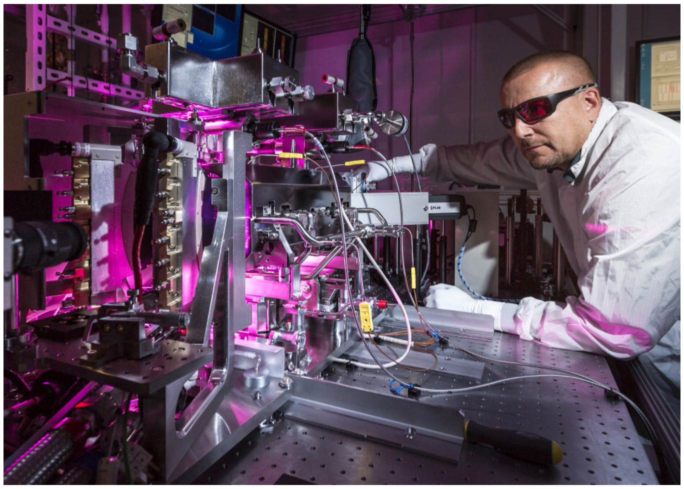
- **Rapid medical response**—Leverage synthetic biology to advance new medical countermeasures, including vaccines that can be produced rapidly when performing real-time research during a response. Characterize biological and chemical threats and support the development of tools that facilitate response and recovery from an incident while preparing new countermeasures for future threats. Use S&T advances to develop new model systems for testing chemical therapeutics that provide neuroprotection and repair.

- **CB countermeasures** —Support the multidisciplinary development of physical, chemical, and biological countermeasures that enhance medical response and mitigate the impact of chemical or bio-incidents. Conduct appropriate research to evaluate disease persistence and the role of secondary transmission of biological contaminants to limit the spread of infection.

Accomplishing these aims will require enduring partnership with other government agencies and institutions, academia, commercial organizations and non-profits. LLNL efforts to support the national security mission and missions in healthcare, agriculture and basic research will continue to identify S&T focus areas that help the nation to actively and effectively prevent, prepare, respond, and recover from accidental, emerging, or deliberate biological or chemical threats.

Directed Energy

Developing compact, robust, efficient high-average-power lasers with high optical quality for a broad range of national security applications.



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

Current and future adversarial weapon systems are increasingly putting at risk U.S. military assets deployed on land, at sea, airborne, and in space. With ongoing advances in the underpinning S&T, interest is growing in future use of directed-energy weapons to counter this threat. Prototype directed energy weapons are beginning to be deployed—for example the demonstration Laser Weapon System (LaWS) on the USS *Ponce*. However, significant technological challenges remain before the directed-energy weapons have a disruptive impact on national security.

Livermore has long provided S&T leadership in the development of high-energy and high-average-power pulsed and continuous wave laser technologies. Robust directed energy with high-average-power or high pulse fluence lasers would find a broad range of tactical and strategic applications for national security. For the directed energy mission, the Laboratory's particular S&T research interests include, but are not limited to:

- **Concepts for generating very high-power laser beams (> 100 kW) with high optical quality (M^2<1.2)**—Important considerations include: efficiency, size, and weight; wavelengths outside the 1–1.1 µm band; high pulse energies (e.g., >100 kJ per pulse for <50-ns pulses); little or no external cooling or thermal management required; materials and components to improve robustness and damage thresholds; and approaches to sub-scale testing for proof of principle and risk reduction.
- **Concepts for beacon illuminator or target illuminator lasers**—Efficiency, size, and weight are important considerations for (what are typically) pulsed, high-repetition-rate laser systems with wavelengths outside the 1–1.1 µm band and high optical quality.
- **Concepts for beam control**—To improve the delivered power density on a distant target, concepts are needed for controlling a high-power laser beam as it propagates through highly turbulent atmospheric conditions.
- **New concepts for laser–matter interaction schemes**— An improved understanding of laser–matter interaction at typical directed energy fluences could reveal ways to create a destructive effect at a target at significantly reduced laser energy and power.
- **Concepts for component improvements**—To overcome severe size, weight, and power constraints, research on improved batteries, cooling systems, and light-weight structures are of high interest.

Forensic Science

Advancing the state of the art in chemical, biological, radiological, nuclear, and explosive (CBRNE) as well as traditional forensics 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 threats. The Forensic Science Center at LLNL is a national security resource that supports a broad set of mission areas, and our scientists create new techniques, materials, and analytical methodologies that are used during CBRNE investigations. R&D thrusts include:

Livermore's Forensic Science Center is helping law enforcement agencies by developing the first-ever protein-based biological identification method.

- **Threat agent characterization, forensics, and defeat**—Identifying, developing, and validating techniques to exploit the signatures of CBRNE and other threats. The goal is to create a capability to identify WMD threat activities, particularly in the material acquisition/production and weapon development/testing phases of the threat pathways. These signatures may be simple indicators of ongoing or historic WMD activity, or more complex, enabling a deeper understanding of weapon-related activities. A key focus is understanding how the method or sophistication of a synthesis/production pathway may affect the forensic information that can be gleaned from a sample, and the interface between chemical and biological hazards and signatures.

- **Unknown–unknown analysis**—Identifying forensic signatures in complex sample sets, which are pertinent to an investigation but are as yet not known. The focus is on developing instrumental and data analysis/integration approaches to identify novel potentially hazardous chem/bio materials without a priori knowledge of their existence. Approaches could include key mass-spectral fragment prediction/recognition, integration of nuclear magnetic resonance methods with chromatography/mass spectrometry, DNA-based methods, key physiological receptor activity, or toxicology assessments.

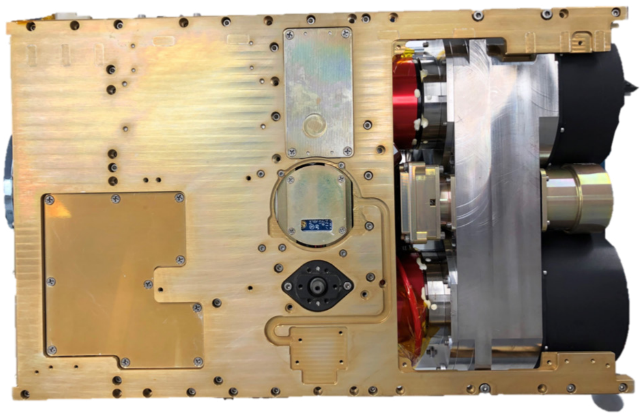
- **Exposure signatures**—Understanding the scope and nature of human exposure signatures for current and emerging threats, including chemical weapons, narcotics, and pharmaceutical-based agents as well as other biological or radiological materials. Developing a robust pharmacokinetic and metabolic understanding of injury and fate of these compounds in the body would enable improved determinations of exposure levels (including chronic low-level), long-term timelines, 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 therapy.

- **Advancing traditional forensic science**—Reducing reliance on subjective methods and providing additional 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.

- **Detection/collection science**—Providing novel approaches to improve the state of the art in detection and collection technologies and materials used in CBRNE forensic applications. Critical challenges include selectivity, and remote/autonomous detection and/or collection.

Space Security

Developing new capabilities to meet national challenges in space situational awareness and intelligence, surveillance, and reconnaissance.



GeoStare, space vehicle #2: Scheduled for launch in early 2020, this is the second nanosatellite developed in partnership between LLNL and Tyvak for space situational awareness.

Recognizing the increasing importance of outer space in the pursuit of U.S. national security, economic, and scientific objectives, LLNL has been making significant internal investments in modeling and simulation, all-source intelligence analysis, and instrumentation design, optimization, and fabrication to help address high-priority national security space issues. LLNL has long supported research in the fields of astrophysics, astronomy, cosmology, and planetary science. These projects have allowed Laboratory scientists to contribute to our understanding of some of the most energetic and exotic phenomena in the Universe, such as the explosion of stars, and to address outstanding questions such as the composition and nature of dark matter and dark energy. The analysis methods, advanced modeling, instrumentation, and measurement techniques developed by LLNL technical staff to work in these disciplines, in turn, support the Laboratory's primary missions in strategic deterrence and national security. X-ray and gamma-ray detectors both enable observations of supernovae and support non-proliferation efforts. The same optical design principles used to make large field-of-view ground-based telescopes are employed to make cost-effective and powerful imaging payloads for small satellites. The analytic methods that provide insight into the composition of our solar system also support forensic studies.

With focused internal investments, LLNL seeks to strengthen and further develop capabilities in the areas of x-ray astronomy, optical astronomy, planetary and solar system studies and astrophysical-based searches for dark matter and dark energy. The most compelling research proposals will couple existing Laboratory facilities with expertise to create new research methods, fundamentally improve instrumentation, or break new theoretical ground. As the Laboratory supports basic science research, it also has an eye on the changing security environment and the way in which the U.S. operates in and derives benefit from sensors in space. Factors include: increasing commercial competition from international firms that are eroding R&D incentives for traditional U.S. providers; aggressive behavior from nation-state actors developing counter-space capabilities; and the changing global security environment that requires new types of measurements to keep decision makers informed.

Importantly, Livermore is building on advances in technologies, manufacturing techniques, and data analytics that have made possible new mission concepts and architectures. LLNL has contributed to significant programmatic achievements by several U.S. government sponsors. It hopes to continue this success by supporting new research projects that look to develop:

- **Small satellite technologies**—The focus is creating and demonstrating technologies at the sensor, payload, and spacecraft level for small satellites (masses of 100 kg or smaller). Such technologies can track missile threats, provide space situational awareness and collect intelligence, surveillance, and reconnaissance at lower cost, higher cadence, or improved resiliency than traditional approaches.

- **Algorithm development and simulation**—Advances and new ideas are needed, focusing on algorithm development and simulation techniques that could help evaluate and improve concepts or better exploit data from existing sensors.

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. Specific research challenges include developing metrics for resilience and assessment methodologies that can merge intelligent adversary threats with probabilistic events. In addition, tools to understand infrastructure interdependencies and cascading impacts are needed. Similar capabilities are also needed at the software and embedded-software system levels to characterize potential vulnerabilities and impacts of cyber attacks.

- **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 are the underpinning of 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, and network-focused uncertainty quantification.

- **Cyber-centric computing and communications innovations**—Developing next-generation techniques and technologies requires mission-specific advances in computing architectures, algorithms, and electronic communication systems. Potential investment areas include: resource-constrained computing, computing-relevant material science and physics, cyber-electronic convergence such as software-defined radio, sensor networks, sensor data exploitation, and software security.

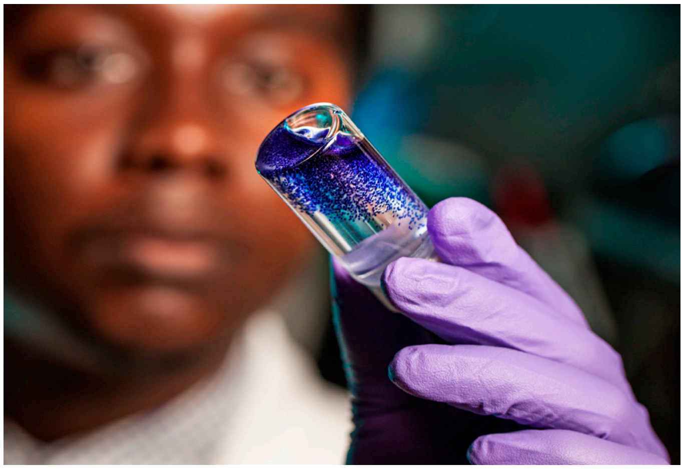
- **Cyber-physical resilience**—Cyber-physical systems play an integral role in many civilian and military systems. Potential areas for investment include: cyber-physical characterization and measurement, modeling and simulation techniques for mixed hardware–software systems, data fusion and analytics that span the cyber and physical environments, dynamic system adaptation, embedded software assurance, and economic incentive modeling and analysis. Additionally, topics concerning the role of humans in cyber-physical resilience are of interest.

- **Experimental infrastructure**—To support the above S&T areas, various equipment and experimental 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; 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. The Laboratory 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:



Novel LLNL microcapsules can be used to capture carbon dioxide from coal or natural gas-fired power plants, as well as industrial processes.

- **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 bio-mimicry 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.

- **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 multi-scale materials simulation, development of innovative manufacturing processes, and numerical optimization. These capabilities are being applied to problems such as developing innovative architected 3D structures for batteries, creating more efficient tailored chemical reactors, and investigating degradation of power generation materials.

- **Water security for adaptation to climate change**—Technologies that help secure resilient sources of clean, fresh water: desalination and selective ion removal, water-treatment technologies, and supporting environmental analysis and infrastructure security. Interests include advanced materials and HPC-based solutions for national, regional, and State of California challenges to water security.

- **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.

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