Investment Strategy
for Science and Technology

FY19

LAWRENCE LIVERMORE NATIONAL LABORATORY

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Science and Technology on a Mission

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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 FY 2019 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.

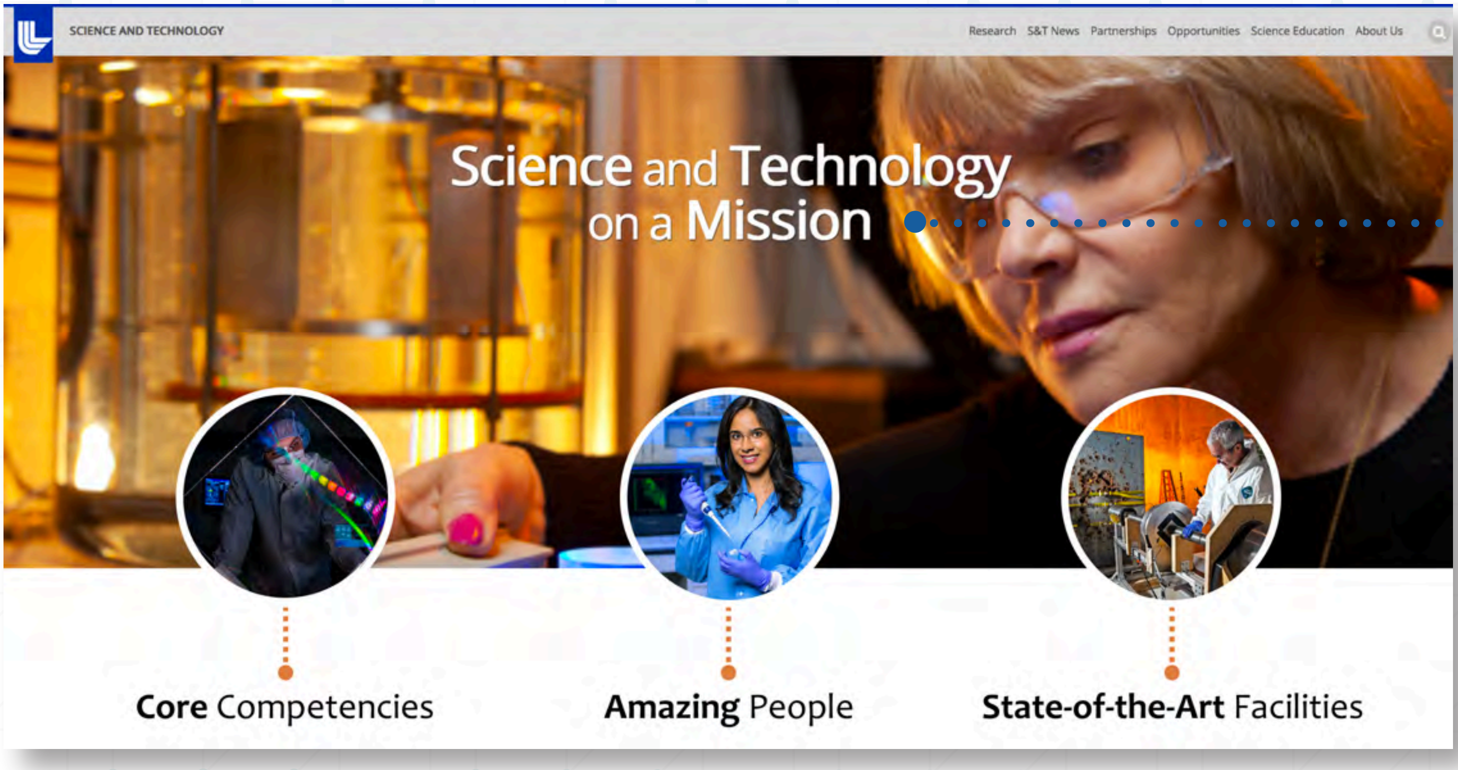
I'd like to highlight three items in our investment approach this year. First, we have a new Director's Initiative in Cognitive Simulation, second, a new pilot component of the LDRD program targeting "disruptive research," and third, enhanced attention to the field of quantum information science.

The Cognitive Simulation Director's Initiative grew out of successes in earlier Director's Initiatives in Data Science and in BAASiC or Biological Applications of Advanced Stategic Computing. Cognitive Simulation builds on the outcomes of those efforts and addresses the use of machine learning and artificial intelligence to guide experiments, digest data from simulations and experiments, and quantify uncertainties. Through greatly enhanced predictions, we believe we can accelerate the process of moving concepts to products-out-the-door for complex systems ranging from nuclear weapons, to new pharmaceuticals, to comprehensive understanding of high-energy-density science. Developing predictive science requires fundamental scientific understanding and draws on our exceptional high-performance computing, state-of-the-art experimentation, and precision engineering.

In the LDRD program this year, in a new process, we are targeting "disruptive research" (DR) ideas. Lab Director Bill Goldstein, in his announcement on December 4, 2018 of the DR pilot, 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. This pilot activity recognizes the risks involved in such disruptive projects. We embrace that risk.

Just last month, the new National Quantum Initiative was signed into law. "Quantum information science represents the next frontier in the Information Age," says U.S. Secretary of Energy Rick Perry. "At a time of fierce international competition, these investments will ensure sustained American leadership in a field likely to shape the long-term future of information processing and yield multiple new technologies that benefit our economy and society." The Laboratory places a high priority on engaging in this national endeavor; we wish to invest in understanding novel phenomena of relevance, potential hardware and software approaches for a new generation of quantum computers, synthesis and characterization of new materials with special quantum properties, and probing the ways in which quantum computing and information processing can provide insights solving extremely complex problems of importance to our mission. While not called out directly as a section in the investment strategy, we are enthusiastic about ideas to meet the challenges at this frontier.

Please enjoy this description of the many opportunities before us, find related information on the Lab's S&T 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 nine 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, 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
Provide the leadership and science and technology for a responsive, efficient weapons complex:

- Assure the continued safety, security, and reliability of the current stockpile.
- Integrate the design, engineering development, material science, and production of the W80-4 and W87-1 replacement warhead programs to increase efficiency and reduce costs.
- Advance the state of the art in simulation and experimental capabilities to address future threats and meet weapon design and certification requirements.
- Develop time-urgent manufacturing solutions for NNSA particularly for plutonium and uranium.
- Progress inertial confinement fusion (ICF) technology to support weapons program needs using the national Ignition Facility (NIF), Z, and Omega facilities.
- Advance computational physics and software developments to more efficiently and effectively utilize future computational resources.

Pertinent mission research challenges: nuclear weapons science; high explosives physics, chemistry, and material science; forensic science

Threat Reduction
Counter the weapons of mass destruction (WMD) threat and enhance global security by providing unique capabilities, expertise, and innovative solutions:

- 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 counter-measures to pathogens and emerging diseases.

Pertinent mission research challenges: chemical and biological countermeasures; forensic science; nuclear threat reduction

Multi-Domain Deterrence
Anticipate threats to national security, innovate, and develop technologies and systems that strengthen U.S. deterrence and defense:

- Enhance space security and situational awareness by assessing adversary capabilities and strategies, applying novel technologies, and modeling of space system architectures for resilience against attack.
- Provide systems analysis and technology development for conventional prompt strike, missile defense, novel directed energy weapons, hypersonics, advanced conventional munitions and sensors, and deterrence modeling support.
- Provide advanced cyber capabilities for threat assessment and analysis, network modeling, and support to national-security stakeholders including the Department of Defense and the Intelligence Community.

Pertinent mission research challenges: cybersecurity and cyber-physical resilience; directed energy; high explosives physics, chemistry, and material science; space security

Energy and Climate Security
Leverage LLNL's unique S&T capabilities to provide the nation affordable, clean, and secure sources of energy:

- Strengthen energy security with S&T breakthroughs that enable diverse domestic sources of energy together with efficient, reliable energy storage and delivery systems resilient to physical and cyberattacks as well as natural hazards.

- Lead in the science, methods, and technologies that reduce atmospheric carbon dioxide (CO_2), capture and recycle CO_2 into fuels, chemicals, and other innovative products, and indefinitely store CO_2 in terrestrial, soil, and geologic systems.

- Enhance our understanding of the Earth system through improved simulations and data gathering, and assessments of energy–climate risks and possible mitigation strategies.

Pertinent mission research challenges: cybersecurity and cyber-physical resilience; energy and resource security

Altogether, these nine mission research challenges reflect the mission pull perspective. They address urgent national security needs for which LLNL has special S&T strengths. Using them, the Laboratory develops the breakthroughs that will "make a difference." The goal is to create new capabilities and game changing advances in our national security programs. These challenges and associated research and development (R&D) thrusts are described on pp. 24–32.

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 seven core competencies that are crucial to mission success. These competencies are essential to the Laboratory's many outstanding achievements—and are vital to the

Core Competencies

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.

continued support of its missions and the advance of S&T. Each core competency is a defining capability or signature expertise in which LLNL is a recognized leader in the field. The core competencies listed below are further described on pp. 11–27:

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

- **High-Performance Computing (HPC)**: Providing leadership in the technically challenging drive toward exascale-class computing.
- **Computational Science and Engineering:** Developing and applying higher fidelity, realistic, and reliable science and engineering simulations.
- **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 responsive, 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 to meet 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.

Director's Initiatives

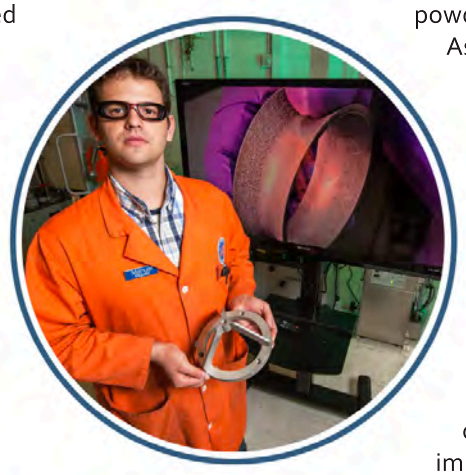
Director's Initiatives focus on identified research areas that merit special attention. They position the Laboratory to address an important emerging national need. These selected multi-year activities strengthen specific science, technology and engineering capabilities through institutional investments in research, workforce development, and infrastructure. Initiatives target new missions and opportunities and build new core competencies. The DI leader provides strategic vision and guidance, and integrates the portfolio of work. The current Director's Initiatives listed below are described further on pp. 6–10:

- **Accelerated Materials and Manufacturing**—creating a more agile, responsive, and integrated material development, manufacturing, and qualification ecosystem to meet NNSA and national needs.
- **Carbon**—preparing solutions for the next major phase of climate change mitigation by creating the S&T and collaborations to support global-scale CO_2 removal.
- **Cognitive Simulation**—accelerating the integration of machine learning, high-performance simulation, and empirical data for national security applications.
- **Predictive Biology**—enabling a new, precise, data-driven, simulation-based approach to 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.

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 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.

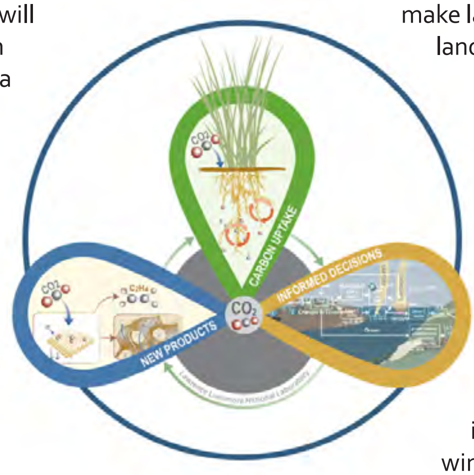
Advanced manufacturing processes
The past five to ten years have seen rapid advancement in advanced manufacturing capabilities ranging from additive manufacturing to microfluidic assembly and other methods. In this initiative, we have sought to drive these advancements through fundamental understanding 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. 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.

Carbon

Preparing solutions for the next major phase of climate change mitigation by creating the S&T and collaborations to support global-scale CO_2 removal.

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



A new carbon-recycling economy: industrial chemicals from CO_2
Carbon-free electricity is an important tool for achieving dramatic carbon reductions. It will permit us to make many carbon-based products not from fossil carbon, but from CO_2 that we have harvested from the atmosphere, either using plants or by direct engineered extraction. LLNL is developing new electro-chemical approaches for making industrial chemicals such as ethylene (C_2H_4), lubricants, and polymers directly from CO_2 and water.

Enhancing our soil by returning carbon to the Earth
The majority 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. By understanding the science that caused the highly productive carbon-rich soils of the central U.S. plains to form originally, we hope to be able to engineer agricultural and agronomic approaches that will return carbon to soil in long-lived forms. This can improve the atmosphere, and make land more productive, allowing marginal land to be returned to a natural condition.

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

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

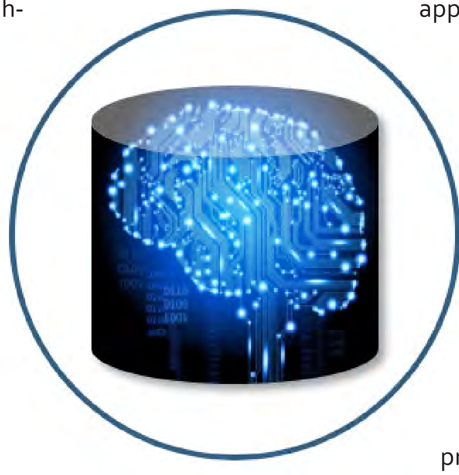
- Carbon capture from biofuel production to enable negative emissions fuels—fuels that when burned, emit less carbon than was permanently stored during their production.
- Storing carbon dioxide in existing California oil reservoirs, utilizing the infrastructure and expertise resident in Central California.

LLNL will work with industry, academia, and other national resources to develop visions like this and turn them into reality in time to meet climate goals. Technology will come from many sources, and will help create the partnerships and industries required to implement these new technologies.

Cognitive Simulation

Accelerating the integration of machine learning, high-performance simulation, and empirical data for national security applications.

The integration of rapid advances in simulation science, machine learning, and high-performance computing is poised to transform a broad spectrum of predictive modeling applications that will enable new science-driven responses to high priority national challenges ranging from nuclear security to precision health care. The centerpiece for this integration will be the development of data-driven "cognitive simulation" systems that bring together high-performance computing, machine learning, 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.Today, our capability to model these complex system behaviors and to predict their response to changes and perturbations is very limited. Developing such predictive capabilities will require new analysis and computing technologies that combine machine learning and simulation into more powerful cognitive simulation models. These models will be distinguished by their ability to incorporate and adapt to experimental observation, endowing them with an unparalleled ability to bridge the gap between purely numerical models and real experimental observation. These new cognitive simulation systems will enable entirely new approaches to assuring our national security, economic growth, and the health of our citizens.

Cognitive Simulation Initiative objectives

The objectives of this Director's Initiative are to accelerate R&D in the integration of machine learning, high-performance simulation, and empirical data and to demonstrate applications to important national security missions. The Initiative is developing this approach using inertial confinement fusion (ICF) and weapons applications as a prototypical examples.

These applications are exploring cognitive simulation for integrating large ensembles of simulations with more limited quantities of experimental data to produce models with improved prediction performance. They are developing new learning algorithms and computational workflows that push today's most advanced high-performance computers to their limits. These algorithms and workflows will provide a testing ground for developing experimentally validated capabilities that can then be used for other stockpile stewardship applications where testing and validation are more difficult.

The impact of cognitive simulation will be felt in all aspects of modeling. These new approaches will provide improved predictive power and greater computational efficiency. They will enable navigation of complex design spaces and ultimately empower scientists to develop deeper understanding of complex processes. Cognitive simulation will ultimately be a unifying framework for combining theory-based simulation and experimental data to empower and amplify our capabilities.

Predictive Biology

Enabling a new, precise, data-driven, simulation-based approach to 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.

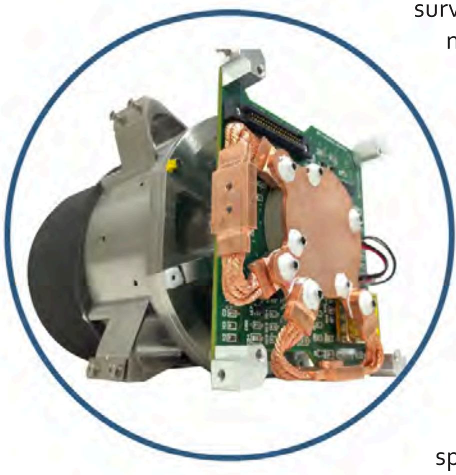
A public–private partnership approach

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 both space domain awareness and intelligence, surveillance, and reconnaissance (ISR) missions.

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 up the design space and possibilities for new materials and applications.
- 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

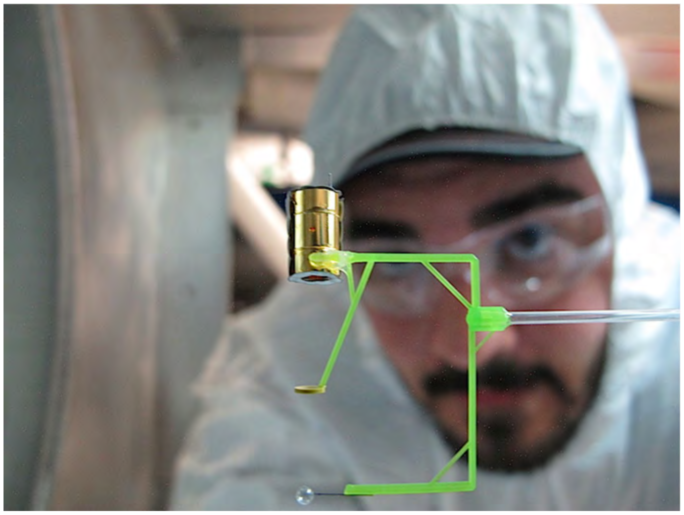
Providing international leadership in studying and controlling matter under extreme conditions of temperature and pressure.

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 scientific 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.



A senior technician holds an assembled cryogenic target for an experiment in the campaign at NIF to demonstrate fusion ignition and burn.

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. 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.

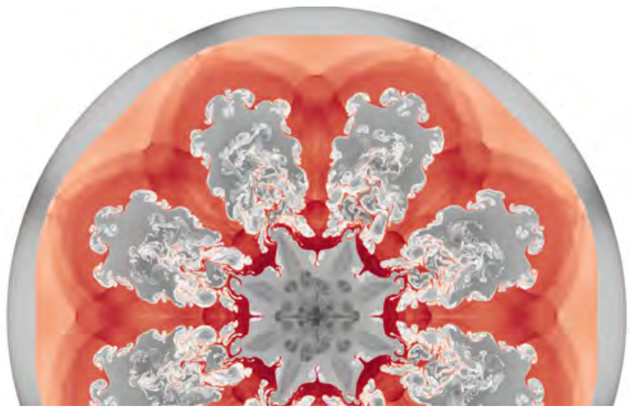
- Secondary sources of particles and photons based on laser–plasma interactions have potential for HED- relevant applications and diagnostics and could be pursued.

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 is 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.



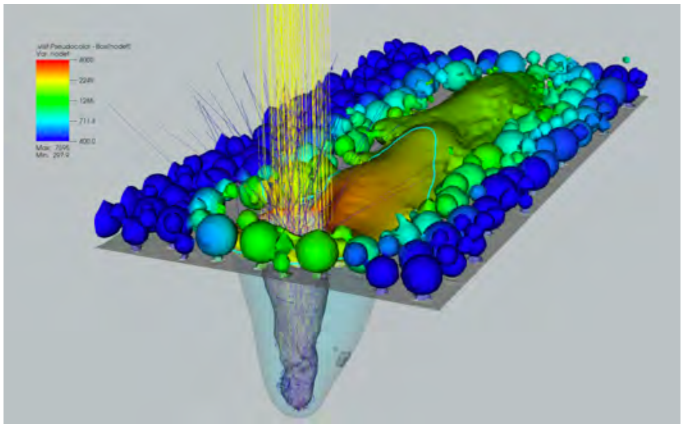
LLNL's BLAST code simulates a cylindrical inertial fusion implosion using discrete "high-order" finite elements, a powerful technique that is well-suited to the architectures of next-generation, massively-parallel supercomputers.

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. 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. LLNL is able to meet the computing challenges with 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 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; multiscale and multiphysics methods; verification, validation, uncertainty quantification; 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.

- **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



Simulations of the laser melted powder in an additively manufactured metal powder process are used to understand and minimize void defects, a critical component to the manufacture of high quality parts.

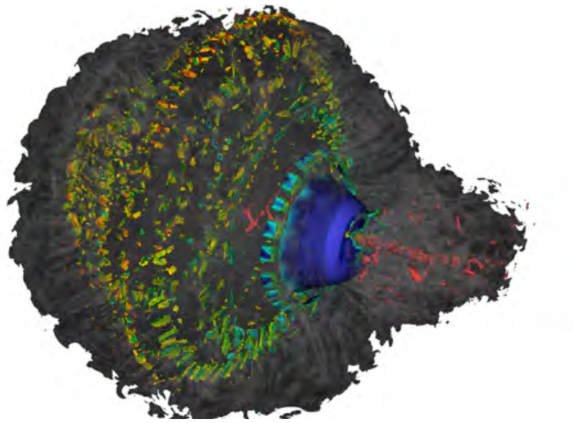
between the institution and the weapons program. M&IC's success has followed from adroitly managing two strategies: 1) leveraging weapons program procurements to build clones at very attractive costs and 2) procuring systems to maximize the institution's exploration of the leading edge. Following these strategies, M&IC is deploying two systems planned for acceptance early in FY19, Lassen and Corona. Lassen is a smaller version of the new weapons program system, Sierra. Corona was designed for exploring cognitive simulation efforts. Once accepted, the Laboratory will have two leading systems for running challenging simulation workloads, offering state-of-the-art artificial intelligence/machine learning capabilities, and supporting emerging complex workflows.

- **Innovative architectures**
  HPC vendor technology roadmaps are rapidly changing to take advantage of expanding markets in cloud computing, machine learning, and cyber security. It is essential that LLNL work closely with vendors as they develop these technologies to assure that simulation needs continue to be met efficiently as the preponderance of vendor R&D investments are shifting away from traditional HPC simulation. In addition, LLNL must take advantage of vendor advances in these nontraditional areas to explore, for example, the cooperation of artificial intelligence (AI) and simulation in complex workflows, sometimes called cognitive simulation. Heterogeneous architectures provide the possibility of improving the quality of simulations while avoiding systems that are too expensive to procure and operate. Nonetheless, the shift to highly heterogeneous architectures, including those that may incorporate novel co-processors, imposes major challenges for our applications. Consequently, 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. Leading edge research is needed to understand how our mission science needs will be met with new technologies such as processing in memory, integration of nonvolatile memory, and integration of graphics processing units (GPUs) and 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 more rapidly respond to new mission requirements while reducing costs, the Laboratory is facing 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 effectively write software. 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, performance analysis tools, etc. That said, there exists a "valley of death" with respect to the usability of tools across the breadth of the Laboratory's software developers. To address this, 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 include hardening research tools and libraries, providing direct assistance for developers, and supporting training to improve the software engineer practices at LLNL. Looking to the future, the Laboratory will be moving research tools developed to supporting 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 are motivating Laboratory programs to exploit and contribute to open-source software, and developers must engage in the open-source community.

Computational science and engineering (CScE)
LLNL develops and applies higher fidelity and more 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.



Grenade detonation simulation created using ALE3D demonstrates a new embedded-mesh coupling technology. The foreground mesh tracks casing fragments, while high explosive is modeled in the background mesh.

- **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 is 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 to not only improve the high-fidelity models and codes employed across the Laboratory, but also enable them to run at scale on next-generation computer architectures, such as Sierra, since the limitations of these models, in many cases, is simply computational resources. In some cases, the dynamic nature of the problem requires tight coupling between sub-scale physics and the larger continuum simulation, necessitating some form of the high-fidelity simulation be run in-situ with the continuum simulation. This could be an instantiation of the high-fidelity code, or perhaps a machine-learned capability that replicates the high-fidelity model. Nevertheless, research into how and when this kind of tight coupling needs to occur is necessary.

- **Machine-learning techniques incorporated with simulation**
  Simulation capabilities—both discrete and continuous—will be naturally integrated with analytics to produce predictive analysis that integrates 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 prediction of 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 exploration of highly nonlinear, multiphysics, multiscale simulations of complex systems. Increasing emphasis is needed to quantify uncertainties in performance of complex systems or 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; leveraging multi-fidelity models, such as those produced by reduced-order modeling; amortizing solver costs through concurrent sample solution; and 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 machine-learning 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 machine learning algorithms, improved natural language methods, new graph-based methods, and the means for efficiently scaling 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 re-configurability 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.

LLNL's automated ion chromatography fraction collection system, which can chemically separate up to 12 samples simultaneously.

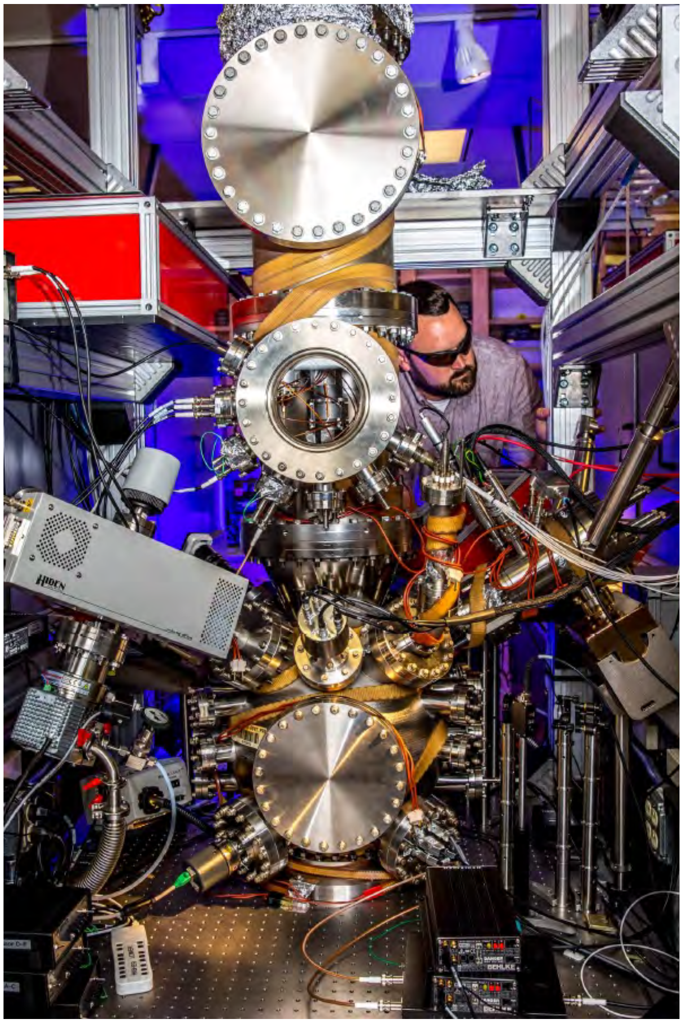
R&D Priorities

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 to understand the evolution of the universe, provide nuclear data 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.



The LION (Laser Ionization of Neutrals) capability at LLNL uses resonance ionization mass spectrometry (RIMS) to perform nuclear forensics and cosmochemistry measurements.

- **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 analyzes; 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, 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 radio-isotopes where crucial experimental data are needed.

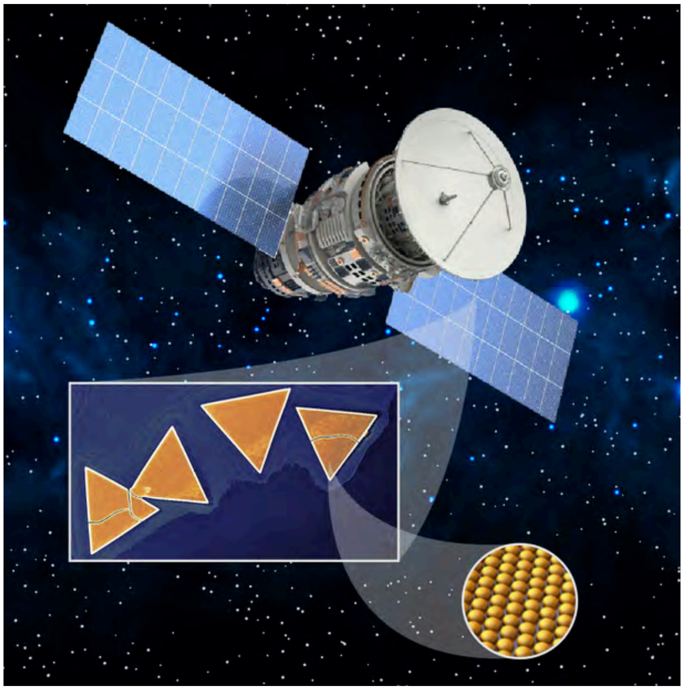
Equipment investments will focus on refurbishing workhorse analytical instrumentation while building one-of-a-kind capabilities to maintain our sharp technical edge. A new high-resolution Nano-Secondary Ion Mass Spectrometer for high-precision isotopic mapping; a medical cyclotron to produce isotopes of interest locally; upgrades to CAMS, including actinide AMS and cosmogenic AMS beamlines for improved sensitivity; and ultra-low background counting capabilities 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**
  Methods are needed to accelerate the creation of bespoke feedstocks and tailored materials with designed functionalities. Advances in computational material development and kinetic control to access metastable states are needed to produce tailored functional materials. 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 >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. 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. Increasingly, new functional materials and interfaces present unique characterization challenges that span atomic to macroscopic length scales and multiple time scales. To understand, develop, and exploit these materials, new capabilities are needed for 3D imaging, spectroscopy, and scattering with unprecedented sensitivity. In-situ and in-operando techniques are also required to probe materials and interface properties and performance under ambient and extreme conditions that arise during fabrication, processing, and/or operation. These emerging techniques can often leverage existing dedicated facilities. Developments in materials characterization are further enhanced by complementary consideration of rapid data analysis and modeling tools. Additionally, in-situ diagnostics will 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.

- **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 network of academic, FFRDC, NNSA laboratories and production facilities, and U.S. industry will benefit LLNL significantly through the generation of new and novel ideas, improved processes for our programmatic applications, and establishment of pipelines for new talent to access the laboratory. This will be further enabled 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 to meet 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 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 areas—AM of optics and free-form optics—could change the way optics are made, opening new applications 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 affect 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 are key to innovation and mitigating mission uncertainty risks. Applications range from optical-surface science for advancing optical damage resistance, novel optical materials, novel fiber laser designs, to improved optical manufacturing.

- **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.

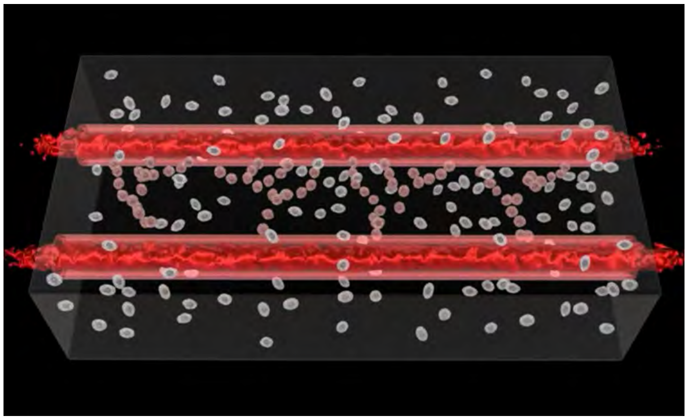
- **Industrial and commercial applications**
  LLNL will develop an S&T portfolio targeting commercial applications of lasers and manage the portfolio so that competencies developed also benefit our core national security missions. The Laboratory's presence in laser-based advanced manufacturing can attract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

LLNL couples a deep understanding of emerging national security needs with the ability to define the underpinning science and develop solutions. Behind this longstanding core competency are world-class capabilities in genomics, bioinformatics, molecular and cellular simulations, bioengineering, biosensors, bioprinting, select agents, toxicology, and bioanalytical science.

A central grand challenge in our mission is to predict, synthesize, and control complex biological systems. LLNL is making strategic investments in the areas of synthetic and mimetic biology, next-generation biosensing and bioanalytic instrumentation, computational biology, human tissue and disease models, and biochemistry and systems biology to build a long-term capability to understand and counter currently unforeseen threats.



LLNL researchers are printing 3D structures with biomaterials and living cells, engineered to enable small blood vessels to develop on their own.

R&D Priorities

LLNL must enhance its efforts in understanding human biochemistry and physiology, host/pathogen interactions and the interdependence of microbial communities through advancements in: human measurement systems; ex-vivo model systems; bioinformatics; forensic analysis and attribution; predictive pharmacology and toxicology; synthetic biology; and the understanding of mechanisms of action for therapeutics and vaccines. Likewise, LLNL must continue to grow its computational biology efforts, building on strengths in scientific simulations and data analysis. To this end, we must bolster our ability to fundamentally understand the biological drivers for specific outcomes and translate that understanding into models that allow adequate predictions to be made with full mechanistic underpinning.

- **Models, algorithms, and software for the simulation and analysis of complex biological systems**
  Simulations and predictive models at multiple scales of very complex biological systems are needed to understand how environmental changes (exposure to toxins, infectious agents, diseases, changing climate) effect the organism and then predict how the organism will respond after exposure. These types of models will also be needed to design and optimize synthetic biology platforms to meet the country's needs in the energy, health, and national security sectors. Key challenges include integrating data-driven and mechanistic approaches for biological systems; devising multiscale approaches linking molecular, cellular, and organismal scales; handling emergent complexity; and understanding the impact of model and parameter uncertainty.

- **Platform tools and techniques to engineer and instrument synthetic biological systems at multiple scales**
  Synthetic engineering approaches to biology have the potential to transform our response to the national security and energy needs of the country. Tools and techniques need to be developed to create, control, and measure the collective behavior of biomimetic ex-vivo systems at a variety of scales (molecular, cellular, tissue/community) that can be used to effectively address emerging problems. Development of novel bio-analytic or biosensor approaches with innovative biotic–abiotic interfaces will provide quantitative data never before obtained from such complex biological systems.

- **Detecting and characterizing emerging threats to enable provision of rapid and effective countermeasures**
  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. Combining strengths in detection technology with high-performance computing (HPC) simulation, advances in data science, and human-relevant microphysiological systems enables a revolutionary, holistic approach to accelerate the development of solutions to newly identified threats and understand the risk of perceived future threats. High-performance computing efforts are focused on developing high- fidelity simulation models that will enable thorough evaluation of new therapeutic candidates for both safety and efficacy against a target.

- **Understanding fundamental mechanisms and pathways of host–pathogen interactions, drug response, and microbial community interactions** Research to understand the critical events, sequences, and routes by which pathogens and toxins affect normal metabolism and physiology is critical to accurately model and understand human-relevant outcomes. Understanding how communities of microorganisms interact is also critical for quantifying how these communities influence human health and how they can be manipulated for better outcomes. We are developing unique capabilities to characterize and understand microbiomes, drug pharmaco(toxico) kinetics and dynamics, and the biochemistry of the genome.

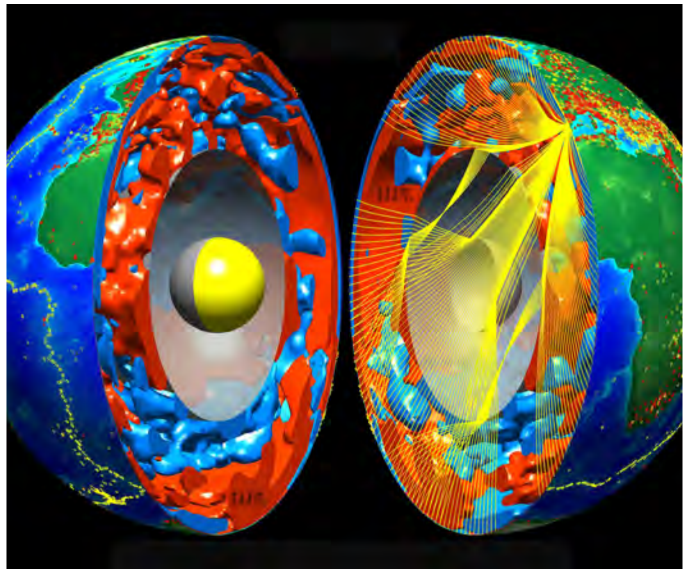
Earth and Atmospheric Science

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, underground coal gasification, 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). The validated simulation models developed by LLNL scientists have provided predictive capabilities that find wide-ranging energy, environmental, and national security applications.

Atmospheric science is a cross-cutting core competency that is central to climate change modeling, as well as renewable energy system modeling, and atmospheric chemistry, transport, and dispersion modeling. The National Atmospheric Release Advisory Center (NARAC) and the Program for Climate Model Diagnosis and Intercomparison (PCMDI) represent major areas of longstanding LLNL leadership. NARAC modeling capabilities, which are continually improved, provide essential data to government decision makers in the event of hazardous emissions, such as the Fukushima radioactivity release in 2011. PCMDI's research includes efforts in uncertainty quantification, 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 contributing factors to climate change and potential consequences.

In Earth science, LLNL has developed world-class capabilities in subsurface modeling, including shock physics, seismic simulation, and fracture mechanics (including 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**
  The current successful, empirically based nuclear-explosion-monitoring capability depends critically upon seismic data analysis. 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 lower monitoring thresholds and confidently monitor new areas.

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

- **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 transportation tunnels to terrorist attack.

- **Climate change and consequence analysis**
  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 among the most difficult for climate models to represent. In addition, many of the important climate change impacts exist at the interface of the atmosphere and land/subsurface systems, and subsurface hydrology is not included in models. Climate simulations also lack a comprehensive characterization of uncertainties, including uncertainties in model formulation, model structure, model parameters, and model output.

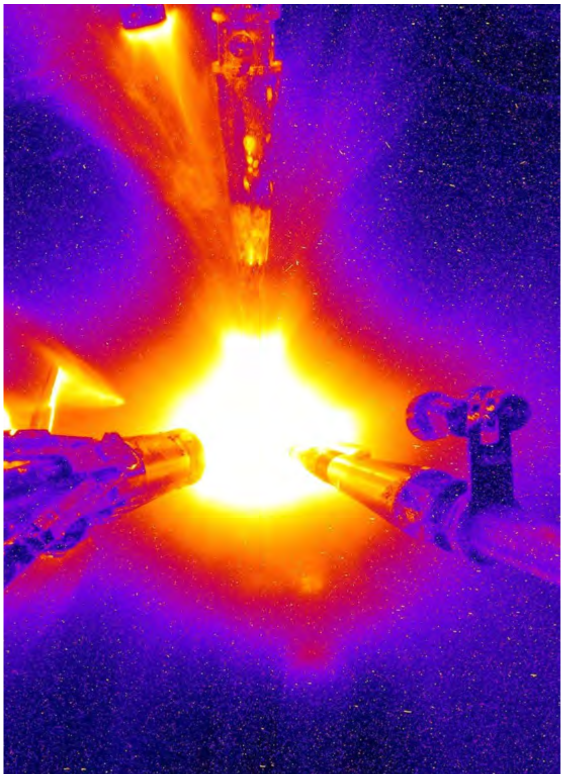
- **Atmospheric modeling for renewable energy**
  Forecasting of wind and solar generation requires modeling skills in atmospheric flow, atmospheric physics/microphysics, and integrated computational fluid dynamics modeling that are currently not available. Atmospheric models cannot handle the complexity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

Nuclear Weapons Science

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

Our Laboratory's national security program is anchored in nuclear weapons science. Innovative science and technology impart creative solutions to maintaining the current stockpile, extending the life of the stockpile, and helps to ensure long-term stockpile sustainment. The smaller size 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 hydro-dynamic 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 is to capture all the crucial physics at all scales. Some key areas of interest to nuclear weapons science are:

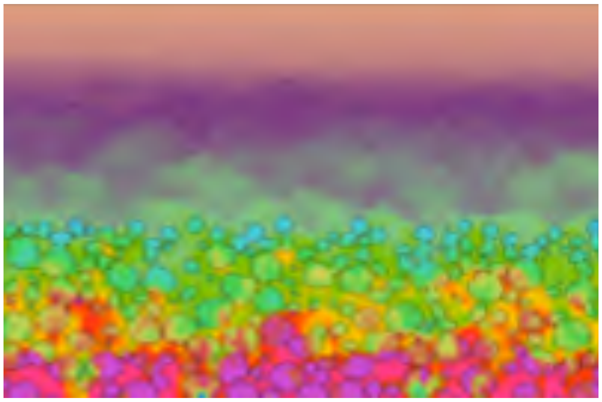
- *First-Principles Understanding of Fundamental Science*—Predictive simulation is the centerpiece of Stockpile Stewardship. To the extent possible, simulation codes are based on physics "first principles" rather than use of parametric models normalized to data. An overarching need is improved scientific understanding and development of reduced model descriptions of microscale physics. Such understanding is achieved through the development of advanced experimental platforms, diagnostic capabilities, theory, and improvements in multiscale modeling. Special focus areas include material properties as a function of age and manufacturing process, high-energy-density science (boost physics, inertial confinement fusion, radiation-hydrodynamics), energetic materials (e.g., high explosives), data science, and uncertainty quantification.

- *Inertial Confinement Fusion*—A primary scientific challenge for our institution is laser-driven fusion using specialized facilities such as the National Ignition Facility. From innovative design concepts to target fabrication, and beyond to novel diagnostics, creativity coupled to disciplined scientific execution is sought to further our understanding of this regime. This area is also important to workforce training in relevant design and engineering skills.

- *Advanced Manufacturing for Weapons Applications*—Research into new manufacturing techniques offers the potential to tailor material properties beyond those available through traditional techniques. 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 is the future workforce that will come to us knowledgeable in the most current manufacturing techniques, the best of whom are unlikely to be attracted to working with 1960s-era manufacturing approaches.

High Explosive Physics, Chemistry, and Material Science

Improving our understanding and prediction of high-explosive behavior to support the nation's nuclear deterrent and keep the U.S. safe from emerging explosives and nuclear proliferation.



ALE3D mesoscale calculations of shock propagation through a bed of aluminum particles infiltrated with the explosive TNT.

LLNL has a mission need to enhance capabilities for understanding and predicting the behavior of high explosives (HE), which are an integral part of every nuclear weapon system. We provide high confidence in the safety, security, and effectiveness of both the U.S. nuclear and conventional deterrent and are enabling a transformation to an all-Insensitive HE (IHE) nuclear stockpile and the increased use of insensitive technologies in conventional munitions. Enhanced expertise in HE also is crucial for informing and providing solutions to detect, mitigate, and interdict explosive proliferation threats.

High-resolution, predictive simulation of HE requires advances in modeling and algorithms that must leverage LLNL's high-performance computing resources. Novel diagnostics and techniques for enhanced characterization of HE materials (including non-destructive radiography and tomography) need to be developed for in-situ and remote applications. New manufacturing methods, such as additive manufacturing (AM), can 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 can now study a reacting material at length and time scales not previously possible. Advances in HPC enable longer runtimes for ab-initio molecular dynamics, mesoscale representations, and methods for bridging the gaps in multiscale modeling from micrometers to miles. Novel diagnostics take never-before captured data for model validation and discovery science.

- *Investigate manufacturing methods to enable options for an all-IHE stockpile, advanced surety, and improved responsiveness of HE component production, and studies of improvised 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.

- *Design and qualify new HE molecules for stockpile use and characterize home-made explosives*—Efficient and timely evaluation of prospective HE molecules and simulants requires scalable manufacturing processes, such as continuous flow reactor technology, that maintain high purity and reproducibility. Computational chemistry enables the discovery of designer molecules and synthesis routes.

- *Evaluate innovative applications of HE*—HE used as energy sources for batteries or pulsed power, and laser–matter interaction, enable LLNL to meet national security needs in unique ways.

Nuclear Threat Reduction

Developing innovative technologies and systems to prevent, detect, counter, and respond to use or threatened use of nuclear weapons or weapons-usable materials.

LLNL provides science-based, intelligence-informed expertise to our national and international partners to: **prevent** and **detect** state and non-state actors' development of nuclear or radiological weapons or acquisition of weapons-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.

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

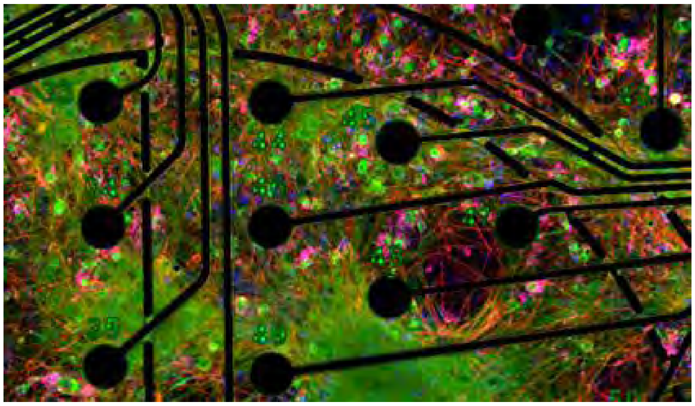
Sponsors of nuclear threat reduction activities seek deployable technologies to use flexibly and quickly. Focus areas include:

- *Data analytics*—We need to develop new data analytics to ingest and search massive amounts of heterogeneous data and extract actionable threat information. The analysis will use model-based templates developed with subject matter expert input, along with experimentally verified simulations.
- *Improving detection of nuclear tests*—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.
- *Understanding potentially unique materials*—We need validated models of how unique materials used by proliferators behave in order to evaluate and disable potential threats.
- *Advancing threat detection*—Accurate detection of potential threat devices requires higher-resolution scintillator materials, as well as more intelligent data fusion and machine learning technologies for sensor networks. Innovative threat-relevant sensors and signatures are also needed.
- *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.
- *Quantifying uncertainties for decision-makers*—Techniques to quantify and communicate uncertainties in our determinations are lacking, yet essential to accurately responding based on limited information.
- *Consequence management*—Improved source models are needed at LLNL's National Atmospheric Release Advisory Center to provide more accurate estimations of where a plume will go to better guide evacuation decisions.

Chemical and Biological Countermeasures

Providing innovative systems and capabilities to rapidly detect and effectively respond to intentional use of pathogens (or chemical agents) or natural outbreaks of pandemic diseases.

LLNL supports the nation in defending our military, homeland, and allies against chemical and biological (CB) threats. The rapid pace of global advances in S&T is resulting in a complex and diverse CB threat space. Mission responsibilities to reduce the likelihood and minimize the impact of 21st-century CB threats are spread across numerous government agencies. The Laboratory works with many of these agencies on their strategic priorities and implements an integrated biosecurity program that addresses a broad spectrum of needs in this area.



Neuronal cultures, including astrocytes and oligodendrocytes, grown on multielectrode arrays are a step towards recapitulating brain complexity and can be used to understand disease mechanisms and conduct toxicity testing.

The mission includes understanding the threat, preventing the malicious use of CB agents, providing CB surveillance and detection capabilities, and building a resilient response capability that includes medical countermeasures, consequence management, and forensics for attribution. Key areas of research and development focus include:

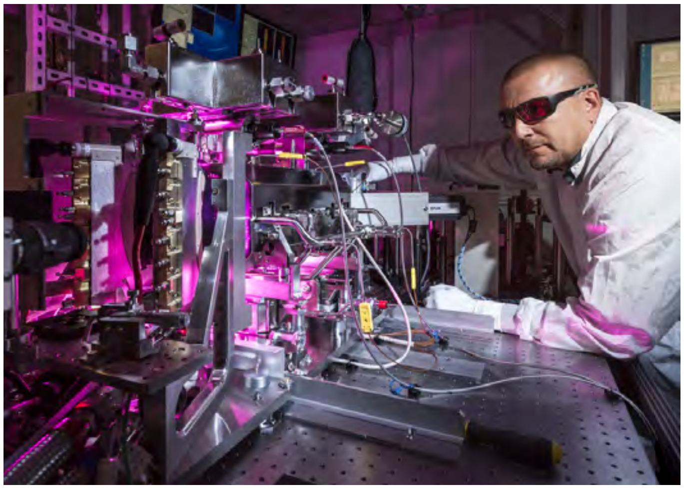
- *Risks and appropriate responses*—Understanding how advances in S&T may impact the evolving threat space and developing a scientific basis for understanding risks and appropriate responses.
- *CB detection*—Developing capabilities including CB detection (environmental and/or clinical) and data analytics to provide CB surveillance of a very large and complex set of chemical and biological agents.
- *Rapid development of medical responses*—Enhancing our ability to rapidly develop medical responses by advancing HPC simulation and modeling capabilities in concert with developing and applying innovative experimental platforms that advance our understanding of biological systems, validate models, and/or enhance testing and validation of medical countermeasures.
- *CB countermeasures*—Developing a diverse set of physical, chemical, and biological countermeasures that can protect personnel, defeat agents, or enhance recovery from a broad range of threats.

Achieving the goals above will require strong partnerships with academia, industry, non-profits and other government institutions. LLNL partnerships may often leverage the S&T overlap between the national security mission and the missions in healthcare, agriculture, and basic life science research.

Directed Energy

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

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.



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

Livermore has long provided S&T leadership in the development of high-energy and high-average-power laser technology. Robust directed energy with high-average-power 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 1–1.1µm band; high pulse energies (e.g., >1 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 1–1.1µm 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. Forensic scientists and the Forensic Science Center at Livermore support a broad set of mission areas. To meet mission needs, researchers develop innovative new techniques, materials, and analytical methodology that can be applied toward 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.

- *Forensic signatures of threat activity*—Identifying, validating, and developing methods for detecting signatures of CBRNE and other threat activities. The goal is to identify and validate signatures resulting from various threat activities, particularly in the material acquisition and weapon development/testing phases of the threat pathways. Signatures ranging from simple indicators of ongoing or historic activity to forensic signatures enabling a deeper understanding of weapon-related activities are desired.

- *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 these key signatures and determine their relevance to specific forensic scenarios. Approaches could include key mass-spectral fragment prediction/recognition, integration of nuclear magnetic resonance methods with chromatography/mass spectrometry, and development of methods to evaluate the potential relationships of various markers within a sample.

- *Exposure signatures*—Understanding the scope and nature of human exposure signatures for various existing and emerging threats, including chemical weapons, narcotics, and pharmaceutical-based threats as well as other biological or radiological materials. Developing a robust pharmacokinetic and metabolic understanding would enable improved determinations of exposure levels (including chronic low-level), timelines, and metabolite signatures.

- *Objective forensic science methodology*—Reducing reliance on subjective methods in forensic analysis. The research focuses are to improve current forensic methods, including converting subjective into objective methods, and to develop new forensic methods not reliant on subjective techniques, a critical priority.

- *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.

The miniCarb nanosatellite, scheduled for launch in 2019, is collaboration between LLNL and NASA Goddard Space Flight Center.

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 small satellite (masses of 100 kg or smaller) and the interest is in innovative technologies at the sensor, payload, and spacecraft level that can enable new space security missions or would provide space situational awareness (SSA) and intelligence, surveillance, and reconnaissance (ISR) 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.

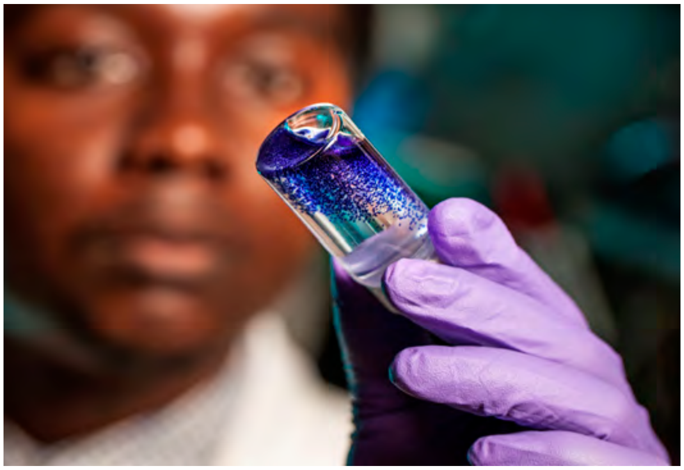
- *Cyber-physical resilience*—Cyber-physical systems play an integral role in many civilian and military systems. Potential areas for investment include: cyber-physical characterization and measurement, modeling and simulation techniques for mixed hardware–software systems, data fusion and analytics 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 S&T 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.

One focus is on developing and demonstrating innovative materials, including wide-bandgap semiconductor materials, to improve technology performance at affordable costs while consuming less energy. A second focus is on the delivery of advanced materials and innovative manufacturing processes to produce 3D structures for batteries yielding higher energy and power densities, greater lifetimes, and enhanced safety.

- *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.

- *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 advanced 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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