Los Alamos 2030: A Vision for Science



To communicate the diversity of the Laboratory's career opportunities in science for potential recruits to LANL and for early career staff.

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Los Alamos 2030: A Vision for Science

Los Alamos National Laboratory (LANL) commissioned this report to communicate the diversity of the Laboratory's mission and career opportunities in science for potential recruits to LANL and for early career staff. It provides a vision for scientific research at Los Alamos as we look forward over the next one to two decades.

1. SCIENCE AT LOS ALAMOS

Los Alamos National Laboratory's mission is to solve national security challenges through scientific excellence. Science at Los Alamos, through 2030 and beyond, will underpin a safe, secure, and effective stockpile; protect against the nuclear threat; and provide solutions to strengthen energy security. A breadth of technical disciplines is pursued at Los Alamos, including physics, engineering, chemistry, biology, computer science, and mathematics. The hallmark of our work is multidisciplinary national security science linking theory, modeling, computation, experiment, and manufacturing, with significant depth in materials and "all-things nuclear."

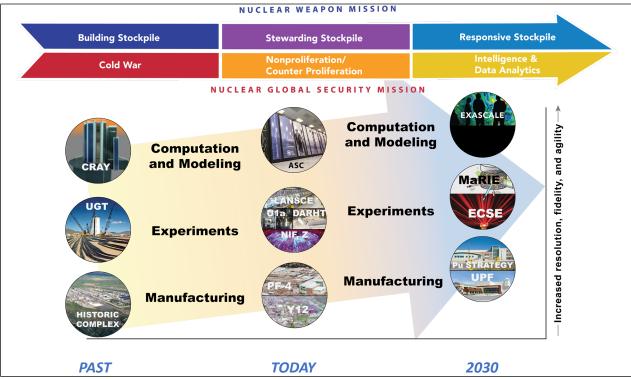


Figure 1. An illustration of how DOE/NNSA scientific facilities are being advanced through 2030, enabling Los Alamos to solve problems for our missions in nuclear deterrence, nonproliferation, and energy. The facilities shown in 2030 are Exascale computing (simulations with >10¹⁸ operations per second); Matter-Radiation Interactions in Extremes (MaRIE) – an anticipated x-ray free-electron laser light source; Enhanced Capabilities for Subcritical Experiments (ECSE) in Nevada; and Los Alamos plutonium facilities, as well as Oak Ridge National Laboratory's Uranium Production Facility (UPF). Other facilities are described in the text.

Scientific excellence has always been central to Los Alamos. The Laboratory was established to design and build the atom bomb, and a few years later the first hydrogen bomb, by bringing together the world's greatest scientific minds. Since then its missions have broadened. It is still very much a nuclear weapons laboratory; about 75% of the US stockpile is designed by Los Alamos. LANL also plays a leading role in the national nuclear counter-terrorism program, developing and leading the world in nuclear material nonproliferation and safeguards with a close International Atomic Energy Agency (IAEA) partnership, and operating the nation's only capability for nuclear criticality experiments. We discovered the neutrino; we have an enduring space science and security mission; and we also provide nuclear batteries and detectors for NASA spacecraft. Our medical isotopes treat more than 30,000 patients a month across the United States. Such accomplishments have been enabled by scientific strength across the Laboratory that must be nurtured into the future. Our scientific reputation, as measured by peer-reviewed publications and citations, awards, and Fellowship in scientific societies, is on a par with that of Department of Energy (DOE)/Office of Science labs, and we are working to ensure that the compelling scientific challenges ahead of us will continue to attract the best talent.

Scientific research at Los Alamos spans the breadth of our principal Department of Energy missions and our strategic partnerships with the Department of Defense and other agencies. Our missions include many aspects of nuclear security and areas in basic and applied science supported by the DOE/Office of Science and in collaborative partnerships of the National Science Foundation, for example. Our research is supported by these programs and by the Laboratory Directed Research and Development program. Throughout the history of Los Alamos, the interplay between basic and applied research has proven beneficial to both.

The long-term success of Los Alamos is based on the scientific talent that we attract. Our ability to publish in open literature has given us visibility and prestige within the scientific community that has enabled us to continue to hire "the best and the brightest." At a more pragmatic level, we have seen the direct transfer of knowledge, tools, and techniques between basic and applied research. For example, the development of proton radiography, which enables us to measure dynamic events related to our stockpile, was a direct outgrowth of the nuclear physics program at the Los Alamos Neutron Science Center (LANSCE).

Similarly, our work in space-based detection of nuclear explosions led to the discovery of gamma-ray bursts — the most powerful explosions in the universe. This synergy continues today with our capabilities in material science and their direct applicability to our national security mission, both in the development of improved sensors and understanding the behavior of materials in harsh service conditions.

As we steward the stockpile, we face some significant challenges. Lifetime Extension Programs (LEPs) are extending the service of our weapons systems as they age, but we need new experimental, theoretical, and computational tools to ensure that we understand, and mitigate, the various aging processes that occur. New weapons components — to replace aged components or to add new safety features — must be developed using advanced manufacturing processes, and the scientific tools of stockpile stewardship need to be advanced to diagnose and qualify these materials. There is a recognition that the National Nuclear Security Administration (NNSA) complex must become more agile, with the ability to quickly address future threats in a responsive manner, a so-called "Responsive Stockpile." Figure 1 shows an overview of anticipated facilities that will simultaneously increase our agility and enable scientific breakthroughs.

Another challenge we face is the need for more efficient production and qualification of strategic materials at Los Alamos and at other facilities across the United States, in the areas of plutonium, uranium tritium, insensitive high explosives, and detonators. While the first two decades of the Stockpile Stewardship Program were successful in creating many tools — high-performance computing and new experimental facilities (Dual-Axis Radiographic Hydrodynamic Test Facility [DARHT], LANSCE, high explosives firing sites, and plutonium facilities), with additional important facilities through DOE/Office of Science (Center for Integrated Nanotechnologies [CINT]) and the National Science Foundation (National High Magnetic Field Laboratory–Pulsed Field Facility [NHFML-PFF]) — the development of modernized efficient production capabilities across the NNSA complex has been less successful. This has led to our focus on "production science," where we will be bringing our scientific skills to develop responsive solutions to help solve this problem.

The United States will also need to address threats to our security in an increasingly complex and challenging environment. Nuclear threats facing the nation from proliferation, and from new technologies used by our adversaries, are likely to increase. Los Alamos has specialized expertise in being able to detect and assess foreign weapon activities, and by 2030, new technical capabilities will be needed to understand and counter such threats. Other challenges involve the development of capabilities needed in space technologies, analytics associated with vast amounts of data collection, and controlling the flow of information across the spectrum of communication.

One of our greatest responsibilities is to ensure we have the skilled workforce needed for the future, researchers who have the expertise, passion, and experience to solve challenges for the nation.

The Laboratory's greatest strength is our multidisciplinary capabilities. Los Alamos has defined four Pillars (*Materials for the Future, Nuclear and Particle Futures, Science of Signatures,* and *Information Science and Technology*) that represent our enduring focus areas. Section 2 of this document describes the scientific 2030 visions for the Pillars. Section 3 then provides an overview of notable crosscutting capabilities at Los Alamos: high-performance computing and simulation; accelerators and dynamical imaging; and plutonium and uranium science.

2. LABORATORY PILLARS: SCIENCE CAPABILITY NEEDS FOR FUTURE MISSIONS

Science breakthroughs will come as we approach difficult problems in revolutionary ways. We draw upon researchers across many science and engineering fields to solve specific national security science problems. The Pillars approach gives these experts a framework for working together and allows them to apply their skills across the traditional boundaries of their disciplines. Visions for the four Pillars in 2030 are given below.

A. Materials for the Future Pillar

The Materials for the Future Pillar provides materials with controlled functionality and predictable performance, with the agility to respond to current and future needs in the three areas of Nuclear Deterrence, Energy Security, and Global Security. Our strategy builds on materials science and engineering, for the following areas of leadership:

- Complex Functional Materials
- Material Resilience in Harsh Service Conditions
- Manufacturing Science
- Actinides and Correlated Electron Systems
- Integrated Nanomaterials
- Energetic Materials
- Materials Dynamics

We must steward our stockpile in the recognition that it is not static due to aging, manufacturing, material replacement, and the possibility for new mission deliverables. Mission success relies on the principle of co-design, the feedback loop between experiment, theory, modeling, and simulation. Computing will be used pervasively to innovatively manufacture materials and products and by 2030 will be an indispensable part of design-for-production, design-for-certification qualification paradigms at the Laboratory.

Energy security can only be achieved with a focus on domestically produced energy including the entire portfolio of oil and gas exploration, renewable sources, and nuclear energy. Material needs arise from the generation of energy such as radiation-resistant cladding for nuclear fuel rods, as well as storage and conversion in fuel cell systems and flow batteries. By 2030, we will have developed the tools to design new cladding and fuel materials — enabling advanced reactor concepts — and demonstrated the ability to accelerate the qualification of these materials. To enable widespread utilization of cyclical renewable energy generation technologies, energy storage and conversion will become increasingly important. Materials-by-design approaches — integrating our modeling and experimental capabilities — will invent new materials for critical energy storage and conversion technologies. Examples include platinum-group metal free catalysts, materials for robust, reliable, and cost-effective fuel cell systems, and scalable storage systems such as flow batteries. For all of these systems, energy efficiency is a driving force to demand constantly improving material solutions.

Strategic deterrence and non-proliferation are key components of our Global Security mission. Material needs arise in agile space applications with a focus on light weight, radiation resistance, and reduced cost, as well as in the dominance of the electromagnetic spectrum to ensure secure communication paths between ground and space-based terminals. Further, there is a need to develop sensor and detector materials to capture and interpret signatures from electromagnetic, chemical, or biological sources. By 2030, we will have developed the ability to predict and design new sensor and detector materials for evolving threat signatures as well as the ability to quickly deploy from design concept to deployable instrument.

The Materials Pillar has identified three science themes, namely *Defects and Interfaces, Emergent Phenomena,* and *Extreme Environments*, described below.

Defects and Interfaces. Imperfections and associated interfaces in otherwise homogeneous materials often dominate the properties of materials and can be exploited to control desired functionality, ideally in a predictive fashion. Novel manufacturing techniques set the stage to manipulate defects and interfaces to our advantage: atomic-scale manipulation and new characterization techniques at multiple length and time scales, including capabilities at the nation's light sources, combined with next-generation computational tools. Our materials-by-design vision involves predicting the ideal defect and interface structure in a material to yield a set of properties, as well as the controlled material synthesis and manufacturing techniques to create those specified structures.

Emergent Phenomena. A similar revolution is taking place in the area of emergent phenomena, which are new collective behaviors that are not merely the result of summing the material behavior of the components. Emergent phenomena manifest themselves whenever we have multiple degrees of freedom in charge, spin, orbital, and lattice that interact in unexpected ways. The challenge is to design, assemble, and optimize materials to ultimately control their functionality and predict their behavior. Emergent behavior is ubiquitous — from the evolution of life, to superconductivity and topologically protected states such as in vortices and skyrmions, as well as quantum entanglement. Advancements in this area will provide the fundamental physics understanding required to predict and control new materials for future technologies such as quantum or neuromorphic computing.

Extreme Environments. The study of a material response to an extreme environment, and the deliberate design to withstand this environment's effects on its performance, is a central theme of our mission needs. There are key factors that need to be considered in this context. In some scenarios, threat radiation levels may exceed those that can be easily probed in laboratory-scale experiments. In others, the duration of exposure may convert an otherwise benign environment into an extreme one, and it may not be possible on a realistic timescale to conduct experiments that allow us to explore the full temporal regime. Computation and modeling are critical. One of the daunting challenges of qualifying new materials for extreme environments, e.g., nuclear reactor applications, is the intensive experimental qualification program sometimes lasting 25 to 30 years. Validated modeling and simulations tools, coupled with in situ experimental characterization, will enable us to predict material response under combined extreme environments and significantly shorten this qualification.

By 2030, we strive to make significant progress in our areas of leadership. For example, we want to achieve sciencebased product certification, including the prediction of the aging behavior of plutonium, develop a predictive capability for explosive reactive burn based on microstructure suitable for integration into continuum explosive burn models, and implement a robust, well understood manufacturing process for every material within a weapon's nuclear explosive package (NEP). These successes will build on our investments in all areas of leadership to develop the underlying fundamental materials science and appropriate diagnostic tools. Spanning multiple decades of length and timescales in a continuous fashion through measurement and modeling, to understand and predict mesoscale phenomena, will be indispensable. The Matter-Radiation Interactions in Extreme (MaRIE) facility will fill a critical gap in our ability to probe materials at the requisite time and length scales so as to predict mesoscale phenomena in bulk samples. It will provide in situ measurements of materials synthesis and manufacturing to understand the kinetic pathways for our predictive modeling tools. Development and validation of microstructure-aware materials models for performance will require MaRIE to probe the dynamic response of materials at the mesoscale.

To prepare for an uncertain future and transform our stockpile, we will mature advanced manufacturing technologies such as additive manufacturing to improve the efficiency, responsiveness, and flexibility of our national security manufacturing enterprise. Since many of the materials we will manufacture via additive manufacturing will not have a commercial source, we will need to develop and qualify these novel feedstocks. Qualification of additive manufacturing will be the largest challenge to overcome in the implementation of this new manufacturing technology. Our vision is to develop a Science-Based Qualification strategy. We will couple advanced modeling and simulation tools (developed with the Information Science and Technology Pillar), with advanced diagnostics measuring critical process and microstructural parameters (developed with the Science of Signatures Pillar) and in situ performance validation testing using proton radiography (pRad), Enhanced Capability for Subcritical Experiments (ECSE), MaRIE, and other National Light Sources (developed with the Nuclear and Particle Futures Pillar).

B. Nuclear and Particle Futures Pillar

As we look to the future, it is essential that Los Alamos continues to lead the world in nuclear science. We must have strong theoretical and experimental programs and robust fundamental and applied programs. At LANSCE, we will build upon the existing partnership between DOE's Office of Science and NNSA. The national user program will continue to attract hundreds of students, postdocs, and university faculty performing research in nuclear physics and material science. Nuclear data obtained at LANSCE and at radiochemistry labs and nuclear criticality facilities in Nevada will be used to develop accurate nuclear cross section databases to simulate neutron transport in a broad range of environments and the performance of the nuclear stockpile. In partnership with the Office of Science, we will continue to probe the fundamental symmetries of nature and deepen our understanding of nuclei. This work will be carried out at LANSCE and at Office of Science facilities, such as the Facility for Rare Isotope Beams (FRIB) at Michigan State University. Such work is essential for understanding nuclear reactions in neutron rich environments that exist in extreme astrophysical processes and in nuclear weapons.

LANL will remain a leader of "all things nuclear." By 2030, exascale-class computing will provide high-fidelity simulations of radiation transport enabled by a comprehensive understanding of nuclear reactions on actinides and light (thermonuclear) processes. We anticipate breakthroughs in our understanding of fission and neutron capture for radiochemical diagnostics, through the development of a new suite of radiation particle detectors and physics models to describe complete and highly correlated fission observables. This will enable comprehensive LANSCE measurements of all fission decay processes with their correlations. Machine learning algorithms coupled with a large database of experimental differential and integral nuclear data will lead to significantly more accurate information to be used in advanced neutron and photon transport simulation codes.

By 2025–2030, the new underground Enhanced Capabilities for Subcritical Experiments (ECSE) facility in Nevada will be online. This Los Alamos-led NNSA facility will transform the way we steward the US stockpile, using multi-pulse x-ray imaging of scaled dynamic plutonium implosions, together with measurements of (subcritical) dynamic nuclear reactivity using a new diagnostic: neutron-diagnosed subcritical experiments (NDSE). The successful exploitation of NDSE will require advances in our understanding of neutron-actinide scattering physics and detection. Breakthroughs will follow large-scale simulation of both the imploding nuclear device and of the underground environment through which the neutron source and emitted gamma-rays traverse. These will be combined with underlying neutron transport code methods and algorithm advances.

Novel accelerator concepts are also being advanced by this Pillar. These include a vision of miniaturized accelerators that dramatically reduce the size of scientific and programmatic facilities and enable portable applications such as nuclear interrogation.

The National Criticality Experiments Research Center (NCERC) facility in Nevada maintains a substantial special nuclear material (SNM) inventory, fully operational critical assembly machines, and global expertise. NCERC can perform both subcritical and critical experiments, including the ability to measure a wide variety of nuclear properties, meeting a wide range of sponsor needs. This one-of-a-kind facility will continue to be used to train criticality safety engineers, test nuclear emergency response equipment and methods, prototype new concepts for compact reactors, and provide essential validation data to advance our simulation codes.

High energy density (HED) physics (the response of systems at pressures of ~1 million atmospheres and above) is an essential part of our program. Advances in plasma physics, radiation transport, and thermonuclear fusion will emerge through continued Los Alamos collaboration with national facilities at Lawrence Livermore National Laboratory (National Ignition Facility [NIF]), the University of Rochester (Omega Laser Facility), and Sandia National Laboratories (Z machine) with concomitant advances in simulation capabilities. Major questions to be addressed include: how hydrodynamical turbulent processes interact with and affect fusion burn; what conditions (and drivers) are required to demonstrate significant fusion yield in the laboratory; what are the opacities of materials under these conditions; and what are the appropriate transport models (kinetic and radiation) in these extreme regimes. This will set the stage for a better understanding of how to achieve laboratory energy producing inertial-confinement fusion to support stockpile stewardship and energy science.

Los Alamos nuclear, particle, astrophysics, and cosmology (NPAC) scientists are exploring the frontiers of nuclear physics, particle physics, and astrophysics. Within nuclear and particle physics, by 2030 we will be answering some of the most fundamental questions about the universe. Why is the universe composed only of matter? What is the dark matter that comprises 23% of the energy density of the universe? What is the nature of the dark energy? Experiments such as the Deep Underground Neutrino Experiment (DUNE), the next generation neutrinoless double beta decay experiment, and the Large Synoptic Survey Telescope (LSST) will be operational and providing answers to these deep questions. The ultra-cold neutron source at LANSCE will continue to probe the nature of the matter-antimatter asymmetry and will develop novel ways to understand fundamental symmetries.

Advances in astrophysics will be dominated by multi-messenger approaches, utilizing data from gravitational wave experiments, x-ray and gamma ray telescopes, and advanced optical telescopes, such as the James Webb Space Telescope and the 30-meter telescope. Success in this area will depend upon our ability to perform complex three-dimensional modeling of complex astrophysical systems, such as supernova explosions, galaxy formation, and black hole physics over an enormous range of length and timescales. Rapid-response, wide-angle telescopes fielded by the Laboratory will play a prominent role in multi-messenger studies of the most violent cosmic explosions and explain discoveries that will follow from gravity-wave and neutrino astronomy.

C. Science of Signatures Pillar

The Laboratory has a long and distinguished history of making measurements to understand complex systems or to detect phenomena or events. Under the Science of Signatures (SoS) Pillar, we apply science and technology to problems of system/threat/impact identification and characterization in areas of global security, nuclear deterrence, space, energy, and health.

The framework for the SoS Pillar centers around three cross-cutting themes: *Detection of new signatures, revolutionizing approaches or technologies for signature measurement,* and *deploying sensing and detection technologies into the field and remote or inhospitable locations.*

We focus on six leadership areas needed for traditional nuclear security missions as well as for emerging concerns in chemical and biological threat surveillance, climate change, signatures of energy production, and a global understanding of infectious disease progression:

- Radiological and Nuclear
- Chemistry and Materials
- Biological
- Climate
- Energy, and
- Space

SoS relies on integration with the other Pillars. Increases in speed and capacity to detect and measure systems result in massive increases in the quantity of data. The ability to manage, manipulate, and evaluate data at scale necessitates advances in data mining and machine learning, data fusion, and pattern recognition from the Information Science and Technology (IS&T) Pillar. Likewise, as we look for new signatures or create advanced measurement systems, new materials with advanced properties will be sought, building upon discoveries from the Materials Pillar. Finally, science supporting the Nuclear and Particle Futures Pillar will provide fundamental knowledge that enhances our ability to detect and qualify materials under the SoS radiological and nuclear area of leadership.

The three cross-cutting theme areas for the SoS Pillar are described below.

Detection of New Signatures. By 2030, we will routinely use data analytics, including data fusion approaches to investigate multiple data streams. Advanced machine learning techniques will enable detection of unexpected signatures. Signatures based on multiple signals (social media, physical and chemical measurements, humint etc.) will be analyzed and fused to diagnose change in systems in ways that are impossible today.

Revolutionizing Measurements. Although remarkable advances have occurred in the 21st century, where we can already detect single molecules and a few femtograms of special nuclear materials, there remain many opportunities for innovation in measurement techniques applied to signature science. By 2030, in addition to progress in scintillators and instrument design, dramatic new techniques such as quantum sensing could offer unprecedented sensitivity and resolution of measurement in a broad range of areas. Quantum sensing is a new technology that utilizes quantum coherence for ultrasensitive detection. This capability is an exemplar of the new technologies that may be available in the 2030 timeframe. Similar to quantum computation, quantum sensing relies on initialization, control, and readout of quantum bits (i.e., qubits). While practical quantum computation needs control of many physical qubits, quantum sensing requires control and measurement of only one or a few qubits. Construction, control, and measurement of few-qubit systems have been proven feasible in many physical systems, thanks to the foundational research for quantum computation.

Deploying New Technologies. By 2030, we will see many technology and system engineering advances that support the deployment of technologies and sensors. Low power utilization on measurement platforms, signal processing on platforms communicating processed information without huge data streams, highly miniaturized sensors for multiple modalities, sensor reconfiguration and relocation in response to what is sensed, protection in harsh environments, and remote deployment in denied or difficult to access sites are all potential requirements for a successful technology deployment. The vision in this area is the ability to deploy tools that allow the routine detection of materials important to national security, including nuclear, biological, and chemical materials from remote locations, including space. Over the course of the next 10 to 15 years, tools will come online that are steps on the way to ubiquitous situational awareness of domains critical to nuclear security using intelligent, self-configuring swarms of sensors based on drones, small robots, and miniature fixed emplacements — the currently oversold "Internet of Things" finding its true maturity. Applications will come first in permitted scenarios, such as nuclear safeguards, and move towards more difficult environments.

As we think about programmatic needs in 2030, there are many areas in which SoS advances are required. In support of Weapons Program production goals and the plutonium strategy, we want to create a suite of analytical capabilities that provide agile and possibly remote process characterization and monitoring of nuclear materials in advanced manufacturing. Adaptation of these capabilities will position us to more quickly and accurately characterize and attribute materials for our nuclear forensics mission and achieve standoff detection of nuclear materials in areas we cannot access. Similarly, we are working to create the next generation of signatures, models, and detection platforms for non-nuclear threats such as explosives, chemical, and biological agents, and universal approaches to pathogen detection. Pioneering approaches to extract or attribute signatures from underground nuclear detonations, assess behavior of Earth systems across multiple timescales and energy production are also under development. The ability to perform many of these measurements from space may be possible by 2030. Our vision is that by coupling advanced sensing and measurement with sophisticated IS&T capabilities, we will provide unique knowledge and a predictive understanding of both natural and engineered systems important for our missions.

D. Information Science and Technology Pillar

Modern computational science (e.g., Monte Carlo methods) has its roots in the Manhattan Project at Los Alamos. Today, a Los Alamos strength continues to be computational physics research, methods development, and applications that run on the world's most powerful computers to help solve the nation's most urgent needs. Advances in theory, algorithms, and the exponential growth of high-performance computing are accelerating the integrative and predictive capability of the scientific method. By 2030, the scope of simulation science will be even broader, to include data science and machine learning.

However, it is not entirely clear *how* we will do that computation by 2030, given the variety of hardware approaches being explored. It seems likely that we will continue to physically host large-scale capability computing at scales beyond exascale, including the associated power and cooling infrastructure. Further, non-traditional "Beyond Moore's Law" computing approaches will likely be an area of active research, with some technologies deployed to solve all or part (e.g., in hybrid configurations) of mission problems.

Finally, the impact and scale of distributed and "cloud" computing will surely continue to increase. It will be essential for Los Alamos to be a consumer of each of these computing technologies and be a thought leader in defining their future development and utilization roadmaps.

At the application level, the computational physics methods and workflows will have experienced a data science and — in particular — machine learning revolution. Computational methods and frameworks will exist that seamlessly incorporate data-based learning and first-principle physics models. Many of these methods will be developed at LANL. We will have a sizable workforce of theoretical physicists, computer scientists, foundational machine learning experts, and discrete and other applied mathematicians that co-design these methods. Integrated machine learning and computational physics will have led to the deployment of new data management technologies, partially developed under Los Alamos' leadership in scientific visualization.

The HPC software stack will have developed a novel computing branch that has started to complement (and in some cases, replace) the traditional stack. Quantum computing will be leading among a set of novel computing technologies that includes neuromorphic computing and application-specific CMOS-based chip design. Leveraging early investments in building a quantum capable workforce and a strategy of consistently acquiring leading quantum computing platforms and technologies, LANL will have emerged as a global leader in quantum software design with applications in optimization, and quantum simulation, particularly in connection with the Materials Pillar. We will also maintain a significant presence in other novel computing technologies, particularly in application-specific chip design.

Cyber security is another important area of research. Security threats to complex cyber-physical systems take place on many levels including sensors, information processing components, cyber-coupled operational technology control systems, and physical actuators. Countering these threats requires understanding, models, and data that span the entire system. LANL will take an approach that is aligned with the Laboratory's scientific foundation by encouraging the creation of interdisciplinary teams that pair cyber sciences domain experts with theoretical and experimental scientists, to develop innovative research results and solutions.

In all of our efforts, co-design will continue to be central to our strategy, both in terms of computational co-design as described above, and the broader integration of experiment/observation, theory/simulation, and computation/analysis. We will also continue to steward capability in data science at scale and complex networks. Los Alamos can help shape the future by integrating high-performance computing, computer science, and statistics expertise to fill the substantial gaps between data and understanding/prediction/uncertainty quantification (UQ). The new era of data/communication democracy means that Los Alamos must excel by decreasing the time from discovery science to impact on technologies programs. Further details on high-performance computing are given in the Section 3A below.

3. ENABLING SIGNATURE FACILITIES

A. Computing

By 2030, scientific computing will be increasingly pervasive in all aspects of the LANL mission. Modeling and simulation will be used more and more often in the analysis of experimental data and the predictive extrapolation to inaccessible regions of experimental phase-space for "matter in extremes." In addition, simulations will continue to be used to optimize the design and interpretation of experiments, guide uncertainty quantification through large ensemble calculations, and provide scientific foundations for the safety of facility operations.

Today, LANL's Trinity computer provides large-scale high-performance computation for the complex. Our next highperformance computer, Crossroads, is being designed and procured, and by 2030, exascale computing will be routine. As discussed in Section 2D, comprehension of the resulting profusion of data will require revolutionary advances in HPC technologies (memory, storage, networks), programming methodologies, data science, and computer-aided analysis. Guided simulation, enabled by machine learning, may emerge to play a significant role.

In our nuclear deterrence mission, computational advances — validated with measured data — have enabled us to steward the stockpile for more than 25 years without nuclear testing. The improvement in predictive capability has been staggering. Nevertheless, gaps remain that drive the need for yet more computing power together with underlying algorithm and model improvements in hydrodynamic, radiation flow, and burn physics. These fall into three

main areas: 1) the need for high-fidelity 3D simulations to accurately model dynamic material motion in the presence of certain features; 2) survivability simulations for devices as they face extreme environments; and 3) the Grand Challenge of predicting material properties from the underlying microscopic structure properties (defects, interfaces, grain sizes, etc.). The latter multi-scale modeling effort would seem to be a solvable problem using traditional reductionist scientific methods, although to date it has proven to be very difficult. Our computational science thrust in this field is paired with LANL's vision for a future experimental MaRIE light source facility (described below) to provide new capabilities that will revolutionize our scientific understanding for our national security and energy missions. Also, our ocean and sea ice modeling (COSIM) project is used by the DOE in its development of the E3SM (Energy Exascale Earth System Model) for climate change assessments.

B. Accelerators

Los Alamos has always been an accelerator laboratory. Such technologies are used to create x-ray, proton, and neutron beams to interrogate matter. Our 2030 plans for accelerators — the x-ray dynamic-material imaging DARHT and ECSE facilities, our LANSCE neutron science center, and the future MaRIE brilliant light-source — are described below.

DARHT and ECSE. The Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) uses two electron accelerators to create intense bremsstrahlung x-ray sources to image dynamic weapons implosions using surrogate (non-plutonium) materials. This facility is used by Los Alamos and Lawrence Livermore National Laboratories to understand and assure the operation of a nuclear weapon primary. DARHT is one of the successful tools developed for stockpile stewardship in the post-nuclear testing era. DARHT's capabilities will be advanced to provide further-improved image fidelity to validate our weapons implosion computational models and stockpile solutions. But the most significant new advance underway is the Enhanced Capabilities for Subcritical Experiments (ECSE) project that is using our DARHT expertise to design and build a new underground capability at the Nevada National Security Site (NNSS) for imaging scaled plutonium weapon implosions.

The new ECSE radiographic machine, Scorpius, is being designed by a Los Alamos, Livermore, Sandia, and NNSS (Nevada) collaboration, with the goal of reaching its initial operating capability underground at the Nevada U1a facility in the 2025–2030 timeframe. Los Alamos and Livermore have concluded that this capability is needed to more completely understand dynamic compressed plutonium behavior; it will be an important tool for stockpile stewardship in the future. We anticipate that in 2030 this new tool will be tremendously valuable for enabling weapon designers to assess and certify the performance of stockpile devices, including changes that may be made for enhanced safety purposes. It will also provide invaluable integral data to challenge the predictions of designers, providing essential experience to help assure that we do not exhibit overconfidence or hubris in the accuracy of our simulation capabilities.

Even though we already have much experience in designing and operating the DARHT facility, building Scorpius underground in tunnels at U1a presents its own challenges for our accelerator engineers. In addition to Scorpius, LANL has made breakthroughs in developing a new neutron-diagnosed subcritical experiment (NDSE) diagnostic that will also be fielded at U1a, as described in Section 2B.

LANSCE. The Los Alamos Neutron Science Center is one of the most versatile accelerator facilities in the world. It is composed of an 800-MeV proton linac with five target stations and 16 flight paths — all of which can operate simultaneously. The 800-MeV protons are directly used at the proton radiography facility to radiograph dynamic events in order to understand material behavior in extreme conditions, the role of instabilities in material response, and to further our understanding of high explosive performance. Three independent neutron spallation targets provide neutrons with energies from 10 nano-eV to 800 MeV to study nuclear and material properties and probe the fundamental symmetries of nature using ultra-cold neutrons. In addition, 100 MeV protons are used to generate radionuclides for medical use.

Over the past decade we have made, and continue to make, significant investments in the accelerator and its experimental capabilities to ensure that LANSCE will provide vital data into the future. By 2030, LANSCE is planning to restore high-powered (MWatt class) operations, which would enable the production of large quantities of actinium-225, an alpha-emitting isotope used to treat cancer and study radiation damage effects on materials and electronics. The proton radiography facility will be a dual-axis system capable of obtaining nearly 100 image frames. These experiments

will provide a window into three-dimensional behavior needed to resolve important stockpile stewardship issues. These facilities will be coupled to MaRIE to provide a predictive capability of material performance based on micro and mesoscopic material properties.

Nuclear weapons operate on the principle of neutron multiplication in fission and fusion, and new neutron detector upgrades will allow, by 2030, an unprecedented understanding of the underlying physics of neutron scattering and fission reactions. The Lujan Center at LANSCE was one of the first accelerator-driven neutron spallation sources in the world. While more modern facilities operate at higher power, we have the unique ability to perform classified experiments on high explosives and special nuclear material. As we look to the future, we will focus on the characterization and qualification of materials made through advanced manufacturing processes, including high explosives and special nuclear material. This will support the 2017 American Nuclear Society Grand Challenge to "accelerate development and qualification of advanced materials and to ensure the continuous availability of radioisotopes." LANSCE currently produces roughly 60% of the strontium-82 used for cardiac imaging in the United States. As we look to the future, we will perform R&D needed (and potentially develop a production and separation capability) to produce radionuclides for novel cancer therapies, such as actinium-225.

MaRIE. The Matter-Radiation Interactions in Extremes (MaRIE) light-source facility is envisaged to be coming online sometime in the early 2030s, providing a unique DOE/NNSA capability to understand and test how material structures, defects, and interfaces perform in extreme environments, such as nuclear weapons. To do this, MaRIE will be an x-ray free-electron laser, brilliant and energetic enough to study critical materials such as actinides. MaRIE will provide us with more rigorous science-based approaches to manufacturing and certification and enable a responsive and agile nuclear enterprise. It will also provide experimental data needed for exascale dynamic material simulations for increased fidelity and high resolution.

Dynamical Imaging. Dynamical imaging of materials has proved to be an essential component of stockpile stewardship. This is a field that Los Alamos leads for the nation. The high-intensity x-ray multi-pulse radiography at the DARHT facility images dynamic weapons implosions using surrogate (non-SNM) material, while proton radiography (pRad) at LANSCE images detonator initiation/high explosives (HE) burn and dynamic material shock response to qualify weapons components. Our future in 2030 and beyond will focus on plutonium, providing higher spatial resolution to resolve features and more penetration to experiment on denser systems. ECSE in Nevada will extend our DARHT capabilities to image macroscopic quantities of plutonium in late-time configurations in weapons primaries. Plutonium at pRad (Pu@pRad) will study other features of dynamic plutonium science, and MaRIE will provide light source imaging of the microscopic properties of plutonium to advance our understanding.

C. Plutonium and Uranium Science

Knowledge of actinide science continues to be essential to the United States and central to the mission of the DOE and NNSA, including national defense, energy security, environmental restoration, and radioactive waste management. Expertise in the production, processing, purification, characterization, analysis, and safe disposal of actinide elements is essential to US national security. The actinide elements plutonium and uranium are central to the national security mission of the Laboratory.

Los Alamos plays a special role for the nation as the center of excellence for plutonium research and pit production for weapon primaries. Our responsibilities include the nuclear security aspects of plutonium and helping the nation address questions associated with the safe handling and disposition of DOE high-level legacy wastes from weapons' plutonium production and civilian reactor spent fuel. Spent fuel also includes other actinides (uranium, neptunium, americium, and curium) and fission products. This presents serious technical challenges in the chemistry, physics, and material science of plutonium. Our 2030 vision for plutonium research has the following objectives:

- 1. An improved fundamental understanding of the electronic structure, which like our recent Los Alamos discoveries will come from experimental work using resonant ultrasound, ultra high-magnetic fields, LANSCE neutron scattering, and many other experiments, with related computational material science advances;
- 2. Quantification of the aging, phase stability, and corrosion of plutonium and its alloys;
- 3. Breakthroughs in our understanding of the dynamic behavior of compressed plutonium. Previous insights from our Nevada subcritical experiments, our measurements with Sandia at its Z facility, and at our plutonium facility will be much advanced in 2030 through small-scale plutonium experiments at pRad and in weapons-like regimes at ECSE;
- 4. Enhanced chemical and radiochemical separation capabilities for plutonium and other actinides;
- 5. An understanding of the fate of plutonium and other actinides in the natural environment to address legacy contamination and in the context of nuclear forensics; and
- 6. Expansion of our capabilities in the detection, measurement, and analysis of actinides.

The nation lost much of its expertise in pit manufacturing following the closure of Rocky Flats in the 1990s. The plutonium facility at Los Alamos has rebuilt this capability with modern techniques at a smaller scale. A major focus area for us now must be to demonstrate pit production at increasing capacity levels through 2030, enabled by breakthroughs in plutonium production science of metallurgy, analytical chemistry and material qualification, and related successful operations involving integrated criticality safety and waste disposition.

Most important is maintaining and developing an expert workforce of sufficient size and quality to meet the challenging and changing needs of new processes, prototype demonstrations, capacity production, and the building of special items for our growing subcritical plutonium experiment program.

Our Sigma Complex is playing an expanded role in providing underlying uranium materials research for the nation, including scientific expertise supporting the Y12 National Security Complex's mission in uranium component production. This role includes expert knowledge across many processing techniques and spans weapons components and reactor fuel development support for national nonproliferation programs. At the same time, Sigma develops the next-generation advanced manufacturing processes ranging from electron beam additive manufacturing to direct casting methods for uranium components.

4. CONCLUSIONS

Los Alamos National Laboratory's mission is to solve national security challenges through scientific excellence. This report has laid out some of the main thrust areas being advanced by the Laboratory to support our vision of delivering science and technology to protect our nation and promote world stability.

To meet this challenge, we will continue to work closely with our partners, including federal sponsors, collaborators at other US national laboratories and universities, and those who advise us through service on external review committees. Our goals will be accomplished through the talents of our staff, students, and postdocs, improvements in our facilities, evolution of our instruments, and application of secure modern tools supporting data sharing and computing.

Los Alamos is on the path to dramatic improvements in predicting and controlling complex systems, global ubiquitous sensing of nuclear threats, and leading the acceleration of the theory-simulation-experimental cycle that is the engine of science.







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