U.S. DEPARTMENT OF ENERGY

The U.S. Department of Energy's Ten-Year-Plans for the Office of Science National Laboratories FY 2021

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INTRODUCTION

The Department of Energy (DOE) is responsible for the effective stewardship of 17 national laboratories, of those ten are stewarded by the Office of Science and focus on discovery science. The DOE national laboratories were created as a means to an end: victory in World War II and national security in the face of the new atomic age. Since then, they have consistently responded to national priorities: first for national defense, but also in the space race and more recently in the search for new sources of energy, new energy-efficient materials, new methods for countering terrorism domestically and abroad, and addressing important critical national needs.

Today, the national laboratories comprise the most comprehensive research system of their kind in the world. In supporting DOE's mission and strategic goals, the SC national laboratories perform a pivotal function in the nation's research and development (R&D) efforts: increasingly the most interesting and important scientific questions fall at the intersections of scientific disciplines—chemistry, biology, physics, astronomy, mathematics—rather than within individual disciplines. The SC national laboratories are specifically designed and structured to pursue research at these intersections. Their history is replete with examples of multi-and inter-disciplinary research with far-reaching consequences. This kind of synergy, and the ability to transfer technology from one scientific field to another on a grand scale, is a unique feature of SC national laboratories that is not well-suited to university or private sector research facilities because of its scope, infrastructure needs or multidisciplinary nature.

As they have pursued solutions to our nation's technological challenges, the national laboratories have also shaped, and in many cases led, whole fields of science—high energy physics, solid state physics and materials science, nanotechnology, plasma science, nuclear medicine and radiobiology, and large-scale scientific computing, to name a few. This wide-ranging impact on the nation's scientific and technological achievement is due in large part to the fact that since their inception the DOE national laboratories have been home to many of the world's largest, most sophisticated research facilities. From the "atom smashers" which allow us to see back to the earliest moments of the Universe, to fusion containers that enable experiments on how to harness the power of the sun for commercial purposes, to nanoscience research facilities and scientific computing networks that support thousands of researchers, the national laboratories are the stewards of our country's "big science." As such, the national laboratories remain the best means the Laboratory knows of to foster multi-disciplinary, large-facility science to national ends.

In addition to serving as lynchpins for major laboratory research initiatives that support DOE missions, the scientific facilities at the SC national laboratories are also operated as a resource for the broader national research community. Collectively, the laboratories served over 34,000 facility users and more than 8,000 visiting scientists in Fiscal Year (FY) 2020, significant portions of which are from universities, other Federal agencies, and private companies.

DOE's challenge is to ensure that these institutions are oriented to focus, individually and collectively, on achieving the DOE mission, that Government resources and support are allocated to ensure their long-term scientific and technical excellence, and that a proper balance exists among them between competition and collaboration.

This year, DOE engaged its laboratories in a strategic planning activity that asked the laboratory leadership teams to define an exciting, yet realistic, long-range vision for their respective institutions based on agreed-upon core capabilities assigned to each.[1] This information provided the starting point for discussions between the DOE leadership and the laboratories about the laboratories' current strengths and weaknesses, future directions, immediate and long-range challenges, and resource needs, and for the development of a DOE plan for each laboratory. This document presents strategic plans for ten national laboratories for the period FY 2021-2031.

[1] A table depicting the distribution of core capabilities across the science and energy laboratories is provided in Appendix 1, along with the definitions for each core capability category.

AMES LABORATORY

Lab-at-a-Glance

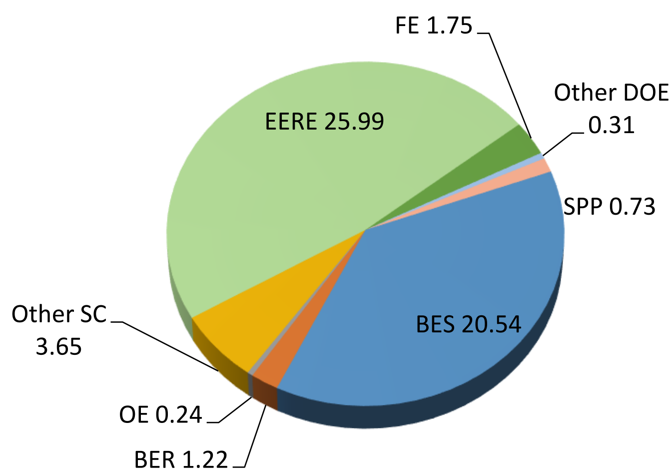
Location: Ames, IA
Type: Single-program Laboratory
Contractor: Iowa State University of Science and Technology
Site Office: Ames Site Office
Website: www.ameslab.gov

- **FY 2020 Lab Operating Costs:** $51.43 million
- **FY 2020 DOE/NNSA Costs:** $53.70 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $0.73 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 1.3%
- **FY 2020 DHS Costs:** $0 million

Physical Assets:
- 10 acres and 13 buildings
- 340,968 GSF in buildings
- Replacement Plant Value: $107 M
- 0 GSF in 0 Excess Facilities
- 0 GSF in 0 Leased Facilities

Human Capital:
- 305 Full Time Equivalent Employees
- 46 Joint Faculty
- 38 Postdoctoral Researchers
- 115 Graduate Student
- 66 Undergraduate Students
- 0 Facility Users
- 96 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

Ames Laboratory delivers critical materials solutions to the nation. For more than 74 years, Ames Laboratory has successfully partnered with Iowa State University of Science and Technology to lead in the discovery, synthesis, analysis, and use of new materials, novel chemistries, and transformational analytical tools. Ames Laboratory is doing today's fundamental science for tomorrow's critical chemistry and materials challenges with a focus on three long-term strategic directions: critical materials and upcycling science, atomistic and molecular design and control for energy and chemical conversion, and novel synthesis to manufacturing. Each strategic direction has a particular focus on rare earth elements, alloys, and compounds. Building upon our chemistry, physics, and materials sciences core strengths in the science of interfaces, science of synthesis, science of quantum materials, and science with rare earths, and a proven track record of transitioning basic energy science through early-stage research to licensed technologies and commercialization, Ames Laboratory will lead the nation in translating foundational science for energy and chemical conversion into critical technology innovation. To address these challenges and future unforeseen challenges, the Laboratory will focus its fundamental research to: accelerate the discovery, design, and implementation of new chemistry, materials, and associated processes enabling critical technologies; create novel approaches for precision synthesis and chemical transformations across length scales to enable scientific discoveries and their implementation into technology; devise better ways to apply chemistry and materials for re-use, recovery, and efficient and clean conversion of end-of-life products; and integrate communication, computation, and Artificial Intelligence/Machine Learning across the basic and applied spectrum to optimize complex chemical and synthetic processes to enable rapid device integration and optimization.

Our goals are to continue to transform the way we do science and to create next-generation materials and chemistry to enable a more sustainable future. Our scientific success depends on a high-quality diverse workforce, modern business systems, safety-focused research and operations, renewed infrastructure and facilities, and a cultural ecosystem unique to Ames Laboratory and Iowa State University.

Core Capabilities

The strengths of Ames Laboratory's core capabilities are key to achieving our mission to deliver critical materials solutions to the nation. Ames Laboratory research is focused on transformational breakthroughs in the fundamental understanding of the chemistry and physics of matter using innovative approaches that arise from the core capabilities and our foundational strengths of science of interfaces, science of synthesis, science of quantum materials, and science with rare earths. New fundamental discoveries in the core areas of *Chemical and Molecular Science* and *Condensed Matter Physics and Materials Science* enable successes in *Applied Materials Science and Engineering*. Each of the three core capabilities identified by DOE's Office of Science involves interdisciplinary teams of world-leading researchers that utilize unique expertise and capabilities to address areas of national need and deliver on DOE's mission.

Ames Laboratory's core capabilities support DOE's strategic objectives, and those of DOE's Office of Science, in particular, to:

- Deliver scientific discoveries, capabilities, and major scientific tools that transform the understanding of nature;
- Strengthen the connection between advances in fundamental science and technology innovation;
- Support a more economically competitive, secure, and resilient U.S. energy infrastructure; and
- Accelerate scientific breakthroughs and develop new innovations for more sustainable U.S. energy production, conversion, and usage.

Applied Materials Science and Engineering

A well-known strength of Ames Laboratory is the application of knowledge derived from fundamental experimental, computational, and theoretical chemistry and physics research to design, discover, and synthesize advanced materials with specific energy-, information-, and environment-relevant functionalities. Ames Laboratory develops, demonstrates, qualifies, and deploys materials that accelerate technological advancements in a wide range of fields—from materials that keep things cool in the European Space Agency's Planck satellite, to a lead-free solder used in virtually all electronics, to analytical techniques that can detect harmful chemicals at parts-per-trillion concentrations, to new materials for efficient electrical transmission.

Based on more than 70 years of rare-earth element research, this core capability is further strengthened by the highly successful Critical Materials Institute (CMI), a DOE Energy Innovation Hub, led by Ames Laboratory. The mission of the CMI is to accelerate the development of technological options that assure supply chains of materials essential to clean energy technologies, enabling innovation in US manufacturing and enhancing energy security. Rare-earth elements are the most prominent of the critical materials today. CMI's efforts aim to assure economically viable processing techniques for improved availability of these materials for clean-energy technologies, to develop new techniques to recover materials from waste and scrap, and to find acceptable alternatives to critical materials for use in devices such as generators, motors, and magnets. CMI-funded researchers have published 335+ journal articles, filed 140+ invention disclosures, filed 58 patent applications, had 16 patents issued, and have six active licensed technologies.

Advances in fundamental science through BES-funded research in chemical and molecular sciences and condensed matter physics and materials has motivated expansion into applied areas, such as new catalysts for biofuel production, magnets, alloys for extreme environments, and sensors or cooling technologies with caloric materials, which are thermodynamically responsive but need better response and control. Caloric materials research is accelerating innovation by designing, discovering, and deploying materials in which reversible, thermal (caloric) response is triggered by magnetic, stress, and electric fields, or any combination of these fields. In less than three years of operations this research has produced 12 disclosures, five patent applications and one patent issued. We have deployed a one-of-a-kind device, CaloriSMART®, to benchmark caloric compounds. This demonstrates our ability to exploit phenomena discovered during their basic research phase of development.

Ames Laboratory’s world-leading advanced powder processing capabilities are advancing rapid and low-loss additive manufacturing of metal and metal oxides. This is being achieved through improved process yield, powder surface quality and passivation, and particle size/shape uniformity and yield to tailor feedstock for advanced manufacturing processing by gas atomization. Ames Laboratory also developed an additive powder feed testbed to enable rapid process development and informed qualification of the additive manufacturing components and processes.

With our applied research in decision sciences, we work to integrate models, information, and other artifacts related to a product or process. We challenge the notion that one cannot integrate analysis into decision making on-the-fly. In partnership with the National Energy Technology Laboratory, Ames Laboratory is working to build the middleware tools needed to integrate the concepts of cyber-physical systems and digital twins into the energy system and materials development process of research and development, design, and deployment. This will create a “discovery-application feedback loop” in which newly conceived ideas can be rapidly tested and sorted, and challenges can be overcome more effectively, thus reducing the development process from decades to years.

Major Sources of Funding: Office of Energy Efficiency and Renewable Energy, Office of Fossil Energy, Office of Advanced Research Projects Agency-Energy, and Strategic Partnership Projects.

Chemical and Molecular Science

This core capability recognizes Ames Laboratory's world-leading competence in developing and applying theoretical, computational, and experimental methods to study structure and reactivity of chemical and biological materials, with emphasis on interfacial interactions relevant to catalysis and separations. These efforts support the DOE mission of addressing energy-related materials and processes, as well as environmental challenges.

Ames Laboratory improves the fundamental understanding of molecular design and chemical processes for energy needs by developing and utilizing both electronic structure theory and non-equilibrium statistical mechanical and multiscale modeling. The primary focus is on methods that enable the study of condensed-phase chemistry and surface reaction phenomena, including at liquid-solid interfaces in heterogeneous catalysis. Theory developments include fragment molecular orbital, effective fragment molecular orbital, effective fragment potential approaches, and orbital reduced space methods that can be applied to systems comprising large numbers of atoms. An integral component of these efforts is the advancement of computational chemistry codes, especially GAMESS and NWChemEx, and the development of interoperability between these two computational chemistry codes. Our unique competencies in theory include the development of highly scalable computational chemistry codes to take advantage of exascale computers.

We are also globally acknowledged for our research focused on bringing together homogeneous and heterogeneous catalysis by developing 3D interfacial, selective catalysts that combine the best characteristics of both to mediate efficient reductive transformations under less forcing reaction conditions. Our core capabilities include synthetic techniques, rigorous spectroscopic characterization, and mechanistic studies. The focus is upon reduction of functional groups that are abundant in biorenewable compounds and energy-relevant molecules, whose conversion suffers from a lack of selective and energy efficient catalytic processes.

An entirely new approach that further advances our core capabilities in interfacial chemistry aims to create a new generation of cooperative catalysts that enable chemical upcycling of energy-rich macromolecules and thereby help to effectively utilize hydrocarbon polymer waste. This Ames Laboratory-led Energy Frontier Research Center, the *Institute for Cooperative Upcycling of Plastics* (iCOUP), is developing new catalytic methods for upcycling hydrocarbon-based polymers and establishing principles of cooperativity in catalytic materials that are specifically designed to interact with macromolecules on multiple length scales.

Central to the success of our chemical sciences programs are advances in the development, implementation, and applications of world-leading characterization tools. Atomic-scale characterization of catalysts, energy storage materials and other solids is available through state-of-the-art solid-state nuclear magnetic resonance (NMR) technologies, including ultrafast magic-angle spinning and dynamic nuclear polarization (DNP) NMR. These methods are being advanced in our Laboratory to reach groundbreaking sensitivity and resolution levels. We have recently added operando MAS-NMR that enables us to deconvolute complex reaction pathways and achieve kinetic control of selective production of specific chemicals. We have also developed and applied in situ Raman imaging to measure the distribution of biomolecules important for energy capture within plant tissue. We continue to develop other chemical analysis tools that enable us to measure biological function in live plants and study spatial and chemical inhomogeneities in separation media with unprecedented spatial resolution.

Separation science has been a key component of Ames Laboratory since its inception. Continuing in this vein, we are developing an in-depth understanding of the use of ionic liquids and deep eutectic solvents as separation media. Taking advantage of our spectacular characterization technologies and our rich chemical knowledge, we are able to probe the key interactions that make selectivity possible in these systems, unlocking pathways to better separation media and processes. We are also using our theoretical and computational expertise to develop and implement methods to aid in the design of ligands for selective separation of metals as part of the CMI. These methods hold the potential to reduce the number of experimental trials that are required and, therefore, the overall costs of finding new, selective ligands.

Looking forward, we will further expand our synthesis methods, analytical tools, and theory. By combining advances in exascale computing, quantum chemistry, data driven science, catalysis, separation science, and world-class characterization tools, we will ensure that Ames Laboratory continually strengthens its research programs and guides the scientific discourse in chemical and molecular science.

Primary Source of Funding: Office of Science.

Condensed Matter Physics and Materials Science

Ames Laboratory is a leader of condensed matter physics and materials science within the national scientific enterprise. Specifically, Ames Laboratory has been at the forefront of research in rare-earth science and novel electronic and magnetic materials since the Laboratory was started, seven decades ago. Ames Laboratory provides the Nation with the highest quality materials for conducting fundamental research, invents new materials, and provides key insights into the fundamental physics and chemistry of these materials. We do this by working collaboratively both within the Laboratory and with external collaborators. Ames Laboratory's deep understanding in precision and demanding synthesis of the highest quality materials allows the science community to disentangle the truly novel physics and chemistry from inherent impurity-caused materials issues that so frequently impact the scientific enterprise's understanding of the nature of materials.

Ames Laboratory continues to enhance and bolster its core capability in *Condensed Matter Physics and Materials Science* by carrying out world-leading experimental and theoretical research in the science of synthesis, science of quantum materials, science with rare earths, and the science of interfaces.

Synthesis: We are continuing to develop our *in-situ* and *in-operando* capabilities, guided by theory, to enable direct observations of nucleation, growth of many metals, intermetallics and self-assembly of nanoparticles using advanced TEM techniques at our Sensitive Instrument Facility. We have established a new rare-earth, transition metal and pnictide system and innovation synthesis routes for tunable quantum materials with strong spin orbital coupling and non-centrosymmetric symmetry, key structural features in materials exhibiting topologically protected states. We continue to reveal mechanisms of 2D growth of nanomaterials, most recently for graphene-protected nanosystems. We have developed several theoretical approaches for predicting new materials, from ground state crystal structures of complex compounds, to high-throughput prediction of alloys for harsh conditions.

Quantum materials: Ames Laboratory's Energy Frontier Research Center for the Advancement of Topological Semimetals (CATS) underpins our effort to understand and discover new quantum phenomena and functionality in topological materials. A recently awarded FWP in 'Light-Matter Quantum Control: Coherence and Dynamics' is using ultra-short mid-infrared and terahertz pulses to isolate and control the surface properties of photovoltaic materials. The ability to coherently excite materials have led to new understanding of topological insulators and new insights into photovoltaics. These methods are also proving invaluable in understanding quantum coherence in 3D topological insulators and superconductors. Our experimental efforts are underpinned by new theory tools to understand and control emerging 2D phenomena with special emphasis on magnetic spin states. A new FWP, 'Quantum Computing Enhanced Gutzwiller Variational Embedding Method for Correlated Multi-Orbital Materials,' is implementing a hybrid quantum-classical computational framework for predicting correlated material behavior onto state-of-the-art quantum hardware. This framework will be used to investigate a series of rare-earth (RE) based multi-orbital materials for their complex phase diagrams and coherent quantum dynamics.

Ames Laboratory's leadership and expertise in quantum materials is being utilized as part of two of the new Office of Science *Quantum Information Centers.* The *Superconducting Quantum Materials and Systems (SQMS) Center*, led by Fermi Lab, seeks to build and deploy a beyond-state-of-the-art quantum computer based on superconducting technologies. Ames Laboratory is providing expertise to understand coherence in qubit materials. For Brookhaven's *Co-design Center for Quantum Advantage (C2QA)*, Ames Laboratory is applying its expertise in quantum computing to advance predictions of correlated materials behavior.

Rare earths: Rare earth research remains a strong focus in the area of materials design and prediction, from unique magnetic and quantum phenomena to developing the understanding on how to manipulate their phase transitions for energy harvesting. We are leading areas of utilizing magnetic caloric materials, and discovering new earth-abundant caloric materials. Our theoretical efforts in first principles methods development are advancing our understanding of strongly correlated systems and guiding materials discovery and synthesis in this area. We continue to develop the fundamental understanding that underpins extraordinary magnetocaloric, magnetoresistive, and magnetorestrictive materials that owe their functionality to rare earth compounds.

Interfaces: Understanding and controlling interfaces spans a wide range of phenomena that includes control over the propagation of light with matter, guiding self-assembly and engineering interfaces that control phase transformations, both in growth of solids from liquid- and solid-state transformations. We continue to develop unique methods coupled to advanced theory to expand dynamic nuclear polarization NMR, providing unprecedented atomic-level characterization of surfaces and disordered materials. We are advancing theory for predicting self-assembly and solid-state phase transitions, in close collaboration with experiment.

Accelerating materials discovery is a key motivation in developing computational methods for the scientific community. This is accomplished by developing methods to better understand functional materials using quantum Monte Carlo simulations, self-consistent electronic structure calculations incorporating total energies, spin excitations spectra, and classical and quantum molecular-dynamics simulations. Understanding synthesis far-from- equilibrium requires new algorithms to predict the structure and properties of complex materials, extending to novel compositions where little experimental data exists. Pioneering theoretical methods with innovative numerical algorithms are being created to enable computational discovery of new materials and to fashion materials by design using DOE's significant leadership computing resources. We seek to create predictive tools that may be utilized by the research community, and to implement these in computationally effective ways. These methods serve to guide experiments and reduce the time needed to develop advanced materials to serve the Nation's energy needs. These capabilities in theory and discovery bolster Ames Laboratory's capabilities in Material Science and enable the DOE to maintain world leadership.

While Ames Laboratory has developed science and capabilities to utilize the full palette of the periodic table to achieve its mission, it continues to develop the fundamental science and synthesis methods of rare-earth materials. From its unique facilities to produce, process, manipulate, and characterize rare-earth materials to the highly visible BES projects and applied programs such as the Critical Materials Institute (CMI) and caloric materials research and systems, all have benefited from and contributed to sustaining this key core capability. Basic research on rare earths at Ames Laboratory is distinguished by its strong tradition of inspiring and enabling novel energy technologies such as magnetostrictive actuators and magnetic refrigeration. The applications of rare earths have evolved rapidly in recent years. While intuition, serendipity, and trial-and-error have been successful strategies in the past, modern demands for precise tuning and control require a clear theoretical basis and the mining of huge physico-chemical datasets.

Primary Source of Funding: Office of Science

Science and Technology Strategy for the Future/Major Initiatives

Ames Laboratory's mission is to deliver critical materials solutions to the nation. Critical materials are those materials and chemicals that are both currently in short supply and subject to supply chain disruptions, and new materials and chemicals that are critical to advancing our nation's energy, economic, environmental, and national security. Ames Laboratory is enabling a sustainable future and addressing national challenges facing the country through the discovery, application, and recovery of materials and chemicals that enable critical technologies.

Our vision is to lead the nation in foundational science for energy and chemical conversion, and to translate this into innovative critical technologies. This is reflected in our strategy: *Today's fundamental science for tomorrow's critical chemistry and materials solutions*. Ultimately, our goals are to transform the way we do science, to create next-generation materials and chemistry, and to enable these developments into manufacturing, to achieve a more sustainable future.

Ames Laboratory focuses its priority research on the following strategic directions:

1. *Discovery for a Sustainable Future – Critical Materials and Recycling Science.* Ames Laboratory conducts basic and applied science to achieve a sustainable future through efficient separations, chemical transformations, and materials design and synthesis. We are developing novel approaches to better reuse and recover materials, in order to efficiently convert end-of-life products into useful resources. We are developing alternate materials for use in energy conversion, reducing our dependence on critical minerals. We are developing materials for extreme environments, for more efficient energy conversion and for new materials for clean energy.
2. *Making Every Atom Count – Atomistic and molecular design and control for energy and chemical conversion.* Ames Laboratory utilizes atomistic and molecular control to master interfacial, atomic, and electronic phenomena to create transformative capabilities in directing chemical and material behavior. We are understanding and directing novel material behaviors that underpin new quantum technologies, new optical properties. We develop and use highly sensitive probes that enable atomistic understanding of catalytic processes, separations, magnetic behaviors, and quantum devices. We study and develop materials that enable energy savings: from caloric materials for reduced energy solid-state cooling technologies, to novel superconductors and topological materials that minimize energy dissipation, to stronger, more conductive wires for a more efficient energy grid. Ultimately, our fundamental understanding, expertise, development, and implementation of new chemistry and materials capabilities provide the basis to enable new technology.
3. *Innovating for Science and Industry – Novel Synthesis to Manufacturing.* Ames Laboratory develops the fundamental knowledge to control synthetic pathways and chemical transformations to precisely fabricate materials across length scales. We make new materials out of compositions never before explored, efficiently predict materials properties to accelerate their development, and enable additive manufacturing and materials synthesis of components with revolutionary properties. We discover, design, and make magnetic materials that reduce our dependence on critical materials, and that enable efficient energy conversion. Our ability to predict, direct, and control atomic and molecular transformations results in new materials with transformative properties, new approaches to make these materials across length scales, and to transform materials into new resources.

These key strategic directions build upon our foundational pillars—science of interfaces, science of synthesis, science of quantum materials, and science with rare earths—to enable impactful advances in chemical and molecular sciences, condensed matter physics and materials, and applied materials science that transform science and lead to technological breakthroughs.

We accomplish this through three high-priority scientific initiatives, and by utilizing a diverse workforce, modern business systems, safety-focused research and operations, renewed infrastructure and facilities, and a cultural ecosystem unique to Ames Laboratory and Iowa State University.

Infrastructure

Overview of Site Facilities and Infrastructure

Ames Laboratory, with a mission to provide critical materials solutions to the nation, is located in Ames, Iowa, on the campus of Iowa State University (ISU). The Laboratory occupies 10 acres of land leased from ISU where 13 DOE-owned buildings reside (see the Ames Laboratory *Land Use Plan*). There are four research buildings, an administrative building, and eight support buildings on the campus. The four research buildings are for general use and support research for all three of our core capabilities: applied materials science and engineering, chemical and molecular science, and condensed matter physics and materials science. The Ames Laboratory campus consists of 340,968 gross square feet (GSF) with a replacement plant value (RPV) of $107M.

In the 2014 DOE Laboratory Operations Board (LOB) infrastructure survey, 10 out of 13 of the DOE-owned buildings were rated as *Adequate* (31.4% of the GSF). The three older research buildings (Harley Wilhelm Hall, Spedding Hall, and Metals Development) were rated *Substandard* (68.6% of the GSF). In 2020, a Facilities Condition Assessment (FCA) was conducted of these three facilities. The FCA rated each of these facilities in below average (Spedding Hall) and poor condition (Harley Wilhelm Hall, Metals Development), highlighting the need for significant renovation investment in major infrastructure systems (electrical, HVAC, plumbing, building envelopes, and elevators). These buildings were constructed 60 to 72 years ago. The buildings have good structural integrity, but they were designed for research needs of the mid-1900s. In FY 2020, Ames Laboratory and the Ames Site Office also deemed two maintenance and general storage facilities substandard since this 8,246 GSF is also in poor condition.

Ames Laboratory has no utility-generating plants. Electricity is purchased through the local municipality (City of Ames). Water, steam, chilled water, and natural gas are purchased through Iowa State University. Natural gas for the support buildings is purchased from Alliant Energy. ISU has updated utility systems that support Laboratory operations. Since 2015, ISU has upgraded its distribution systems for electricity and chilled water, and also upgraded some of its boilers from coal to natural gas. Future plans include updates to the storm and sanitary sewers, power, and the conversion to natural gas for more boilers. ISU has invested $74M in infrastructure improvements that have had a positive impact on Ames Laboratory operations.

Harley Wilhelm Hall
(1949)

Spedding Hall
(1953)

Metals Development Building
(1961)

Technical & Administrative Services Facility (1995)

Sensitive Instrument Facility (SIF)
(2015)

Shop Buildings and Warehouse
(1964-1991)

Campus Strategy

To meet its mission, Ames Laboratory relies on an outstanding scientific and operations staff, a strong partnership with ISU, unique laboratory and mid-scale scientific infrastructure, as well as national user facilities. Judicious investment in Ames Laboratory facilities and infrastructure has expanded the potential of our highly skilled staff and motivated new opportunities to impact the scientific community. As we continually advance such facilities and capabilities, we also continuously improve upon the collaborative Ames Laboratory scientific competencies.

Ames Laboratory has increased its investment in the main research buildings, replacing 50+ year-old electrical and HVAC components, and renovating individual laboratories. The progress is slow, but steady. As Ames Laboratory focuses on our three key strategic scientific directions and strives to meet our mission to provide critical materials solutions to the nation, we must also optimize our infrastructure and facilities to accelerate progress. We will continue to maintain our legacy research buildings through infrastructure modernization to provide a safer and more operationally efficient campus while reducing deferred maintenance costs. As we embark on these efforts, the design and planning must include consideration for a Net Zero environment that focuses on the deliberate reduction of carbon emissions and utilization of environmentally friendly energy sources across the laboratory campus. We are planning for future capabilities with the evolution of our research; for modern and flexible research space to advance DOE's and the Nation's desire to reduce dependence on the supply of critical materials from foreign entities. Ames Laboratory, in partnership with ISU, has earmarked a site adjacent to

Rendering of Critical Materials and Supply Chain Research Facility (CMRF)

Ames Laboratory for a Critical Materials Supply Chain Research Facility (CMSCF). ISU is nearing completion of the demolition of the existing facility on this site in preparation for the CMSCF. This state-of-the-art facility will advance the DOE strategy to reduce dependence on the supply of critical materials from foreign entities by providing an integrated platform that allows early stage research from fundamental science through applied technology and development that spans the supply chain. The CMSCF will support DOE's efforts to unlock new sources of critical materials, and will serve as a regional resource recovery facility for materials recovered from the central and northern plains. The facility will also support DOE's critical materials mission by developing environmentally benign processing to address end-of-life recovery of critical materials from wind generation and other renewable energy sources, as well as from end-of-use plastics and other materials important to clean energy technologies. The research enabled by this facility will:

- Provide for innovative technological solutions to unlock primary and non-conventional sources of critical materials and rare earths.
- Develop fundamental understanding of separations and processes required for process intensification and reduction of energy intensity for mineral processing.
- Reduce the environmental and energy intensity of processes for the conversion of mineral sources to refined materials used for manufacture.
- Accelerate materials discovery and design of both chemical and functional materials using integrated computational/high throughput/rapid assessment methods using Artificial Intelligence and Machine Learning.
- Discover and develop environmentally friendly methods for the recovery of materials during manufacturing and from end-of-life products.
- Leverage and improve on advanced manufacturing methods for decreasing embodied energy, decreased use of critical materials and reducing waste.
- Create a bridge for manufacturing from creation to commercialization.
- Serve as a teaching and research facility for workforce development.

The Sensitive Instrument Facility (SIF) provides Ames Laboratory with an advanced platform to pursue science-driven development and operation of state-of-the-art analytical tools within specialized laboratory environments that enable rapid onsite analysis of materials to expedite discovery. It is the instrumentation and computational resources (atomic- to macro-scale capability) of our mid-scale scientific infrastructure within Ames Laboratory that provide a competitive advantage to deliver high impact science and achieve scientific breakthroughs.

Ames Laboratory Strategic Plan prioritizes facilities investments for success of the Laboratory's strategy. Given the general purpose of our facilities, each project supports our core competencies of 1) Applied Science and Engineering, 2) Chemical and Molecular Science, and 3) Condensed Matter Physics and Materials Science. See *Infrastructure Investment Table*.

Ames Laboratory utilizes the Mission Readiness process to identify new and review existing facility improvement requests. Projects are prioritized through use of the Capital Asset Management Process (CAMP) and management review. During the FY 2021 Mission Readiness interviews, several common themes were discussed. First, the COVI-19 pandemic has forced a majority of the operations staff and some research staff to primarily telework. Even when the pandemic conditions improve and staff are able to come back to onsite work, not all will come back full-time. Some team members will be 100% work from home, and some will have hybrid schedules with a blend of onsite work and telework time.

This may free up some office spaces overall. However, to accommodate hybrid schedules, Ames Laboratory is considering converting some office space to hoteling configurations. These will be generic desk spaces that can be used by multiple hybrid staff members for short visits to the Laboratory when they need to be onsite. Second, the COVID-19 pandemic has forced the Laboratory to conduct a majority of its business via virtual meetings. Even when the pandemic conditions improve, a significant amount of business activities will stay in online formats. Leaders across the Laboratory are assessing their small conference rooms' capabilities and looking to improve technology in those spaces through their overhead budgets. Technology updates for the larger Lab-managed conference rooms are also being considered. Priority will go to updating the Spedding Hall 301 conference center.

Current Gaps

Through continued investment, we plan to fulfill our Strategic Plan objectives and goals to provide facilities to support scientific objectives, provide infrastructure that supports mission readiness, and pursue opportunities for future scientific capabilities.

In the Laboratory Plan Investment Table, the Laboratory identifies several facility improvement projects, some of which are broken into phases, to modernize the oldest buildings at the Laboratory. These improvements total $90 million in facilities gaps, with more than 95% of the facility investments for the three older research buildings (approximately $85 million).

To address the needs of its aging facilities, the Laboratory recommends advancing the $30 million SLI Line-Item project, Ames Infrastructure Modernization (AIM) to the design phase (CD-1). The Laboratory also recommends that DOE invest $3-4 million of General Plan Project (GPP) capital funding each year for the next 12 years. This sustained level of capital funding represents a volume of work that the Laboratory can effectively manage, and helps with staff capacity planning. The Laboratory does not have alternate space available to temporarily move activities. Therefore, the buildings must remain operational during major renovations and infrastructure upgrades, and utilities interruptions must be limited in order to avoid negative impacts to the Laboratory's research mission. This additional coordination time extends the duration for a majority of the improvement projects.

Several recurring gaps are identified for all three of our older research buildings and the Laboratory, with DOE's support in closing the gaps:

Fire Alarm and Emergency Notification Systems: These Laboratory-wide systems are at the end of their useful life, and the Laboratory is currently in the construction phase for the complete replacement of the fire alarm system, funded with BES-GPP ($1.5M). Construction will be completed in early FY 2022, and the scope includes the replacement of control panels, detection devices, fire alarm devices, mass notification LED signage, and new wiring. The complex-wide upgrades for the fire alarm and emergency notification systems will provide assurance the systems are working accurately, while also improving the Laboratory's capabilities to effectively communicate fire, severe weather situations, and other safety notifications.

Building Envelopes: Building envelopes include roofs, exterior walls, windows, and other exterior building systems. The three general use research buildings require upgrades or repairs to their building envelopes. Future projects will need to add insulation to the roofs of the three primary research buildings to improve energy efficiency and improve each building's ability to protect people and equipment. A new white roof system will increase energy efficiency, eliminate the need for damaging ballast, and add at least 25 years to the life of the buildings.

Backup-Emergency Power & Uninterruptible Power Supply (UPS) Systems: The two existing diesel generators used for backup/emergency power on the main campus are past their useful life and do not have the capacity to add additional backup/emergency loads for new equipment. They can only handle 25% of the total electrical demand of the Laboratory, which is enough for life/safety systems only. Critical research equipment, information technology equipment, and operational equipment are protected by several smaller, decentralized UPS systems (most at point of use). These decentralized systems require various forms of maintenance, upkeep, and upgrades, which demands a great deal of effort and coordination. A centralized UPS system for each mission critical building would benefit the Laboratory by improving uptime and providing facility-wide protection for sensitive electronics. These larger UPS systems are also capable to ensure critical systems will keep running during power disturbances such as blackouts, brownouts, sags, surges, or noise interference.

Plumbing Systems: Most of the water supply piping and sewer drain piping are original to their respective buildings, and these systems were evaluated as deficient during the 2014 LOB Infrastructure Assessment. Water leaks, complaints of sewer smells, and clogged drains have increased dramatically in recent years. The Laboratory inspected the sewer lines below the concrete floors utilizing cameras in FY 2016, and conducted surveys of pipe chases in FY 2018. The original sewer lines under the concrete floors and in the vertical pipe chases are deteriorating. Major cracks were found and repaired in several sewer drains behind vertical chase enclosures in FY 2017 and FY 2018.

Condition of Research Laboratories: The 2014 LOB infrastructure survey identified 101,000 square feet in poor or fair condition. Many of these Laboratory spaces have original fixtures, rusted cabinets that are difficult to operate, pocked work surfaces from chemical exposure, asbestos-containing materials, and inadequate lighting. Since FY 2014, the Laboratory has renovated 20,000 square feet of this poor or fair condition space. Our capacity to renovate space is approximately 4,000 to 5,000 square feet per year. At the current pace, it will take the Laboratory approximately 15 to 20 years to renovate the substandard spaces.

Helium Recovery System: The Low-Temperature Laboratory (LTL) requires several important upgrades to support the Ames Laboratory mission. Laboratory helium liquefaction and recovery services allows research efforts to obtain liquid helium on demand, at a lower price, and helps in the recycling of this precious natural resource. In-house production makes delivery independent of weather conditions, helium mining, and helps address the challenge of the limited world supply. Supply of liquid helium in quantities necessary for complete laboratory operation (5,000 liters per month) is not a reliable or consistent source through local providers. The Laboratory received BES-GPP funding in early FY 2020, which will be used to upgrade the helium storage tanks ($500K) and SLI-GPP funding, which will be utilized to upgrade the compressor on the helium recovery system in the LTL ($1M). Ames Laboratory is working closely with ISU to ensure the infrastructure in Zaffarano Hall (ISU building) is sufficient to support the new Helium recovery storage tanks and compressor.

Telecommunications Infrastructure: The majority of emerging technologies require the fast and efficient transmission of data from sensors and devices and greater bandwidth than is currently available. The Laboratory completed a feasibility study and is now proceeding with the planning and design to upgrade the physical telecommunications infrastructure needed for current and future computing needs with BES-GPP funds. The plan includes creating a new IT room in Spedding Hall, with new telecommunications equipment, cabling, racking, and ventilation.

Electronic Access Control: The Laboratory began converting its door access from physical keys to electronic proximity card readers with American Recovery and Reinvestment Act (ARRA) funding. When the ARRA funds were exhausted, the Laboratory allocated GPP funds to continue progress. The exterior doors for all buildings, the property protection areas for the site, and the interior doors for two buildings were completed. This electronic system provides the operations staff a greater amount of control for different access situations and helps to provide better safety, security, and accountability for room use. We have used this capability to secure exterior doors during the pandemic to control access. With the electronic access control system, it would only take one command to lock down all Laboratory exterior and interior doors in the case of an active shooter. However, most of the interior doors in Spedding Hall and Metals Development are still physical key access only and require conversion to electronic card access. The Laboratory received $3M in FY 2021 SLI-GPP funding for this gap, and is currently developing the project plan with design and construction to follow.

Heating, Ventilation, and Air Conditioning (HVAC) Systems: The FY 2020 Facilities Condition Assessments (FCAs) completed for Harley Wilhelm Hall, Spedding Hall, and Metals Development identified some significant deficiencies in their HVAC systems. Though some HVAC updates have been completed by the Laboratory over the last 12 years utilizing GPP funds, the aging systems still require more resources to better support current and future research. The building automation systems need updated as the current Metatsys hardware and software systems are close to obsolete and will not be supported by Johnson Controls International (JCI) in the future (ROM $3M). Multiple air handlers in each of the three older research buildings are nearing the end of their life expectancy and need replaced (ROM $10M). The FCAs also identified a significant amount of HVAC distribution ductwork that is nearing the end of its life expectancy and needs replaced. Legacy contamination concerns will also have to be addressed as a part of the efforts to replace the ductwork (ROM $20M).

Building Maintenance & Repair: The maintenance program, funded from overhead dollars, consists of activities necessary to keep the existing inventory of facilities in good working order and extend their service lives. It includes regularly-scheduled maintenance, corrective repairs, and periodic replacement of components over the service life of the facility. It also includes facility management, engineering, documentation, and oversight required to carry out these functions. The condition of the research buildings has been maintained even as they age beyond normal service life. The Laboratory anticipates it will need to continue to operate in the older buildings over the 10-year window of this plan. Historically, the Laboratory has invested approximately 2.0% of Replacement Plant Value (RPV) per year into maintenance and repair activities. This level of resources has been able to control deferred maintenance in the buildings. However, the combination of limited capital improvements and aging facilities has placed a greater demand on maintenance resources. Maintaining the condition of the facilities does not ensure they will continue to meet the needs of research activities. In recent years, maintenance and repair expenditures have ranged from 2.0% to 2.8% of RPV.

Spedding Hall
Existing Built-Up Roof
(circa 1985)

Harley Wilhelm Hall
Backup/Emergency Generator
(circa 1970)

Harley Wilhelm Hall
Poor Condition Lab Space
(circa 1950)

Spedding Hall
Deteriorating Sewer Piping
(circa 1953)

Spedding Hall
Deteriorating Brick/Limestone Exterior
(circa 1953)

Investment Summary

The Laboratory made significant progress in FY 2020, completing the renovation of 5,000 square feet of space on the third floor of Spedding Hall. This created an enlarged and consolidated solid-state Nuclear Magnetic Resonance Laboratory, and completed the project to replace one of the main air handlers in Metals Development. The Laboratory has awarded two construction contracts so far in FY 2021 for the helium recovery system storage tanks, and the fire alarm system upgrades. Contractors will mobilize and start construction in Third Quarter for these two projects. Design and procurement activities continue for the new telecommunications room in Spedding Hall, and for the replacement of helium recovery system compressor in the Low-Temperature Laboratory. Construct contracts should be awarded this summer, with construction occurring in Fourth Quarter FY 2021 and First Quarter FY 2022.

Ames Laboratory developed a project plan, *Ames Infrastructure Modernization (*AIM), to address facilities gaps primarily in Harley Wilhelm Hall, Spedding Hall, and Metals Development. Gaps that will be addressed with this project include plumbing systems, building envelopes, UPS and emergency power systems, telecommunication systems, and deteriorating research laboratory spaces. This project is focused on major infrastructure systems whereas SLI GPP investments are targeted at ancillary projects, renovations and other minor facility modifications that work to improve the physical work environment along with the safety and security of personnel, equipment, and facilities. The Mission Need was approved by the Office of Science on September 9, 2019 followed by the approval of CD-0 on September 16. The Total Project Cost (TPC) range for the preliminary alternatives identified during Mission Need is $10M to $90M (target $30M). Ames Laboratory is currently working toward achieving CD-1 and starting the design effort for this project in FY 2022. Pre CD-1 activities completed so far by the Laboratory include: Facilities Condition Assessments (FY 2020), IT Feasibility Study (FY 2020), and conceptual designs for the plumbing, electrical and building envelope gaps (FY 2021). The Laboratory is currently developing an Analysis of Alternatives (AoA), Conceptual Design Report (CDR), and Preliminary Project Execution Project Plan (PPEP) in preparation for CD-1 reviews. The planned construction window for this project is FY 2023 to FY 2026.

These recent and projected investments by DOE will allow the Laboratory to accelerate its capital planning and positively impact our mission. Ames Laboratory plans to fund maintenance and repair activities through overhead at 2.0%-2.4% of RPV for the duration of this plan. Support of this investment strategy will result in the three older research buildings moving from “Sub-Standard” to “Adequate” for their Overall Asset Condition, and contribute to the success of the Laboratory’s mission. Deferred Maintenance (DM) was re-baselined in FY 2020 as result of the updated guidance from the Office of Science DM Working Group. DM at Ames Laboratory is $4.4M.

We have aligned planned infrastructure activities with our Strategic Plan objectives, as follows:

Objective 1: Provide facilities that support our scientific objectives. Through SLI-GPP funds, the Laboratory has updated and modernized approximately 5,000 square feet in Spedding Hall for Dynamic Nuclear Polarization (DNP) research expansion, and Nuclear Magnetic Resonance (NMR) research consolidation in FY 2020 ($3M).

Objective 2: Provide infrastructure that supports mission readiness. The Laboratory replaced one of the main HVAC air handlers in Metals Development in FY 2020 ($1M). Design was completed in FY 2020, and the construction contract awarded in early FY 2021 for the replacement of the fire alarm system across the complex ($1.5M). The Laboratory received $3M of SLI-GPP funding in FY 2021 for upgrading the access control systems in Spedding Hall and Metals Development. The Laboratory recommends advancing the $30 million SLI Line-Item project, AIM, to the design phase in FY 2022. The Laboratory requests sustained funding of $1M per year (BES-GPP), and $2-3M per year (SLI-GPP) from FY 2022 to FY 2032 to focus on mission readiness renovations and additional infrastructure updates.

Objective 3: Pursue opportunities for future scientific capabilities. Discussions during Strategic Planning and Mission Readiness have guided the Laboratory to consider repurposing several areas across the campus to support future research activities. New research initiatives will be defined with supporting facilities and infrastructure projects. The Paint & Air Conditioning Shop, the Records Storage Building, and some spaces in Metals Development are being considered for supporting new activities.

ARGONNE NATIONAL LABORATORY

Lab-at-a-Glance

Location: Lemont, Illinois
Type: Multi-program Laboratory
Contractor: UChicago Argonne, LLC
Site Office: Argonne Site Office
Website: www.anl.gov

- **FY 2020 Lab Operating Costs:** $784 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $80 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 12%
- **FY 2020 DHS Costs:** $23 million

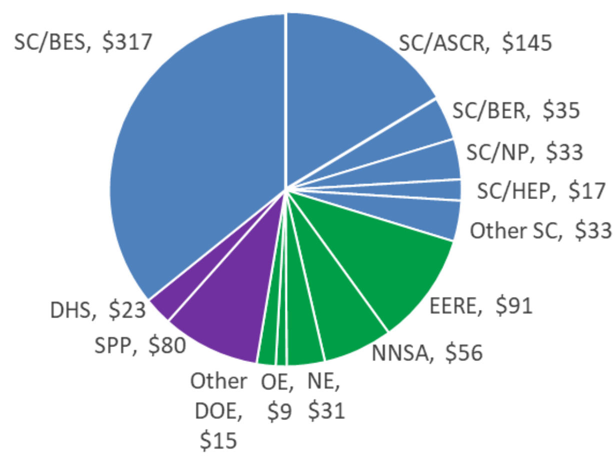
Physical Assets:

- 1,517 acres and 155 buildings
- 3.9 million GSF in buildings
- 5.1 million GSF in buildings
- Replacement Plant Value: $3.9B
- 0.4 million GSF in 13 Leased Facilities
- 0.02 million GSF in 16 Excess Facilities

Human Capital:

- 3,442 Full Time Equivalent Employees (FTEs)
- 424 Joint Faculty
- 324 Postdoctoral Researchers
- 200 Graduate Students
- 276 Undergraduate Students
- 6,715 Facility Users
- 825 Visiting Scientists

FY 2020 Costs by Funding Source ($887 million total)



Mission and Overview

For 75 years, Argonne National Laboratory has accelerated science and technology to drive American prosperity and security. We are recognized internationally for pioneering discoveries in multiple fields of research and for technology innovations that are embraced by industry. We support the U.S. Department of Energy (DOE) mission through four signature contributions:

- Our ***discovery science*** unravels Nature's deepest mysteries in materials, chemistry, physics, and biology, laying the foundation for new technologies that improve the quality of life
- Our ***energy and climate research and development*** provides critical new insights into climate processes, builds on discoveries in the physical sciences to deliver advanced technologies to overcome challenges in clean energy, and translates these technologies to the marketplace
- We strengthen ***global security*** through our work in nuclear nonproliferation, infrastructure resilience, critical materials, physical and cyber security, and disease response
- We design and operate ***large-scale research facilities*** that provide unmatched capabilities in computing, climate science, nuclear physics research, and the use of x-rays and nanoscience to

explore physical and biological systems: these facilities support the second largest user community in the DOE complex.

Argonne's impact on science and technology is amplified by extensive interdisciplinary collaborations, both internally and with universities, industry, and other national laboratories. We are proud to lead five multi-institution research centers for DOE, focused on development and recycling of batteries, materials for energy conversion and water treatment, and quantum information science.

Since Argonne's founding, we have operated under the auspices of the University of Chicago, currently through UChicago Argonne, LLC. We have long conducted joint research with the University; current collaboration areas include climate change, sustainability, quantum information science, computing, and cosmology.

Our main campus is in the Chicago suburbs, with satellite research and collaboration centers in Washington, D.C., and Chicago. Our Chicago location supports our growing role as a regional convener, as we expand partnerships with Midwestern industries and universities and broaden our STEM outreach to disadvantaged communities to build the science and technology workforce of the future.

Core Capabilities

Argonne's broad base of expertise in science and engineering, which comprises 18 of the 24 core capabilities defined by DOE for its laboratories, is a powerful asset to meet national needs for scientific and technological leadership. We use these capabilities to advance the missions of our sponsors as we accelerate science and technology to drive U.S. prosperity and security. Our collaborations with other research institutions and industry enrich our contributions to society.

UChicago Argonne, LLC, enables Argonne to effectively use our capabilities by providing guidance, advocacy, and oversight. Led by UChicago, the Joint Task Force Initiative (JTFI) identifies and pursues opportunities for Argonne, UChicago, and Fermilab to drive breakthroughs in research, engage with sponsors, and boost the efficiency of operations. In addition, the JTFI partnership has been critical to Argonne throughout the COVID-19 pandemic, in bringing medical advice to the Laboratory and providing support in testing and vaccinating Argonne employees.

Our core capabilities are listed below and summarized on the following pages. The expertise of our scientists and engineers both supports, and is supported by, our suite of large-scale experimental facilities that serve thousands of researchers from outside Argonne:

- Advanced Photon Source (APS)
- Argonne Leadership Computing Facility (ALCF)
- Argonne Tandem-Linac Accelerator System (ATLAS)
- Atmospheric Radiation Measurement Southern Great Plains (ARM-SGP) site
- Center for Nanoscale Materials (CNM)

Argonne National Laboratory core capabilities

Accelerator science and technology	Condensed matter physics and materials science
Advanced computer science, visualization, and data	Cyber and information sciences
Applied materials science and engineering	Decision science and analysis

Applied mathematics	Large-scale user facilities and advanced instrumentation
Biological and bioprocess engineering	Nuclear and radio chemistry
Chemical and molecular science	Nuclear engineering
Chemical engineering	Nuclear physics
Climate change sciences and atmospheric science	Particle physics
Computational science	Systems engineering and integration

Accelerator science and technology

Capability

Argonne's accelerator science and technology capabilities center around the APS, ATLAS, and the Argonne Wakefield Accelerator (AWA) and range from electron storage rings and linear accelerators operated as x-ray sources to hadron linear accelerators and advanced accelerator technology. This portfolio of expertise is the foundation for our successful operation of a suite of facilities that support a broad range of scientific research; it also forms the basis for developing enabling technologies for future research and facilities at Argonne and across the DOE complex. Activities among facilities are coordinated and communicated via the Argonne Accelerator Institute. We also have broadened our expertise and outreach with several joint faculty appointments with accelerator groups at Chicago-area universities.

The nearly 200 Argonne scientists and engineers who work in this field are recognized internationally for their expertise in six areas:

- *Modeling, design, and operation of photon sources, electron accelerators and storage rings, x-ray free electron laser seeding and oscillators, and insertion devices, particularly superconducting undulators.* We have complementary expertise in beam diagnostics and feedback systems and in vacuum system engineering. These capabilities underlie the APS Upgrade (APS-U) project as well as future x-ray sources at Argonne and elsewhere in the DOE complex.
- *Generation, acceleration, and reliable delivery of stable- and rare-isotope ion beams serving nuclear physics research at ATLAS.* We support several DOE and worldwide accelerator initiatives using expertise gained at ATLAS over the past 40 years in linear accelerator design and modeling and in the design and development of state-of-the-art superconducting radio-frequency cavity systems, especially for ion accelerators. We are drawing on our unique expertise and infrastructure for superconducting cavity production, testing, cleaning, and processing to support five major efforts. Those efforts are the Facility for Rare Isotope Beams at Michigan State University, R&D for the future electron ion collider at Brookhaven National Laboratory, the APS-U bunch lengthening system, cavity development and related hardware for the SLAC National Accelerator Laboratory's Linac Coherent Light Source II, and the Proton Improvement Plan II project at Fermilab.
- *Advancements in high-gradient, two-beam acceleration using dielectrically loaded structures,* in support of high-energy physics research. This work is centered at the AWA, a unique facility combining the world's highest electron bunch charge produced by a photocathode gun with a state-of-the-art linear accelerator and beam instrumentation. Using the AWA, we are working to evaluate emittance manipulation techniques in support of future capabilities in photon science. The AWA also is open to the user community for general accelerator R&D in structure and plasma wakefield acceleration, radiation generation, and electron source development.

- *Areas vital to future accelerators and colliders,* including high-power radio frequency sources, generation and preservation of high-brightness beams, photo-injectors, collective beam instabilities, and two-beam acceleration with high transformer ratios. This research is synergistic with our work to improve the performance of light sources and colliders and address national security applications.
- *State-of-the-art accelerator modeling and controls:* our advanced accelerator modeling codes *elegant* and TRACK are used worldwide, and we develop EPICS software tools and applications for distributed control systems for accelerators.
- *Support for accelerator outreach, training, and education* via the U.S. Particle Accelerator School based at Fermilab, the summer undergraduate Lee Teng Fellowship in collaboration with Fermilab, and the DOE-funded graduate accelerator education program led by Michigan State University.

This capability supports the broad DOE/SC mission to enhance the capabilities of its current accelerator-based scientific user facilities while driving development of next-generation user facilities. Current sponsors include DOE/SC-BES, -HEP, and -NP and DOE/NNSA.

Advanced computer science, visualization, and data

Argonne is a leader in computer science, visualization, and data science. We are recognized for our innovation in extreme-scale systems software, scientific software productivity, and high-performance computing tools for data-intensive science and visualization. This leadership is critical to achieving DOE's exascale computing objectives. We continue to enhance and promote this capability and to build capacity in the following areas:

- Foundational computing software and algorithms for quantum and neuromorphic computing, with a focus on software and methods for science
- Automation of scientific discovery through machine learning (ML), cloud computing, and high-performance computing; this includes platforms to support the basic and applied sciences
- Concepts and strategies that capitalize on our work in data visualization, analysis, and management for the capture, transport, reduction, transformation, storage, and understanding of data in DOE applications
- Systems architectures for end-to-end computing to enable progress from today's sensing-analysis-simulation-reasoning-control approach to tomorrow's fully automated science, applying our expertise in system software, distributed computing, and high-performance computing
- Fundamental concepts and techniques to support and enhance scientific simulations and data analytics reliability and correctness through advanced resilience, data reduction, and error analysis

Our computer science benefits multiple disciplines. For example, our SciDAC-4 RAPIDS Institute for Computer Science and Data is enhancing computer science and data analysis capabilities in these strategic research areas:

- In hard x-ray science: data transfer from APS to ALCF, real-time analysis, and parallel algorithms
- In earth system science: coupled data analysis across multiple models
- In cosmology: emulations of cosmic microwave background power spectra using deep probabilistic generative models

- In fusion energy: use of ML to develop low-cost surrogate models for magnetohydrodynamic models
- In applied materials: novel active learning for additive manufacturing
- Other examples of how Argonne's computer science supports multiple disciplines includes our development of:
- Edge computing: The Waggle project is enabling a new breed of edge computing for smart-city applications and sensor-driven environmental science, and the Array of Things and Sage projects are deploying them in Chicago and around the U.S.
- A quantum simulation capability for understanding quantum architectures, quantum compilation, quantum networks, and quantum sensors
- DLHub for materials and chemistry research: this self-service platform for publishing, applying, and creating new ML and deep learning models makes it easier for researchers to benefit from advances in those technologies
- Applied artificial intelligence (AI) in response to COVID-19: we continue to build infrastructure to integrate AI/ML tools with physics-based tools to form a workflow to screen orders-of-magnitude more compounds than is possible with traditional drug-screening workflows (Argonne was part of the team that won the First ACM Gordon Bell Special Prize for High-Performance Computing-based COVID-19 Research, awarded at the SC20 supercomputing conference)

Argonne-developed software is tested and deployed at the ALCF, Oak Ridge Leadership Computing Facility, and National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory. Argonne and Fermilab are exploring the future of data storage and networking using a unique Illinois networking infrastructure. Production supercomputer systems worldwide use Argonne's research software tools and, in exascale computer science, we are highly regarded for our development of operating system and runtime software. We are deeply involved in managing and executing DOE's research plan for exascale computing, and we maintain partnerships with researchers in Japan and Europe. In 2020, an Argonne computer scientist won an Ernest Orlando Lawrence Award from DOE.

This capability supports the DOE/SC-ASCR mission to develop and deploy high-performance and leadership computing resources for scientific discovery. Additional current sponsors include DOE/ECP; DOE/SC-BER and -BES; NIH; NIST; DOD; NSF; and VA. Much of this additional funding supports co-design activities, basic and applied research, and interdisciplinary research partnerships with scientists in various application areas.

Applied materials science and engineering

Argonne applies internationally recognized expertise in materials design, development, synthesis, processing, and scale-up to drive advances in materials science and technology. Applied and basic science teams from across the Laboratory execute research using a broad suite of resources. These resources include the APS and CNM, used for materials characterization; the ALCF, used for computational materials science; the joint Argonne-UChicago Center for Molecular Engineering; and our Materials Engineering Research Facility (MERF).

The MERF enables scientists and engineers to bridge the gap between bench-scale science and industrial implementation through synthesis, process R&D, scale up of materials, and fabrication/testing of components and devices. Researchers develop scalable processes and advanced manufacturing techniques to produce quantities of innovative materials sufficient to enable industrial testing and accurate cost modeling. For example, capabilities at the MERF allow integration of new nanostructured and soft matter materials developed at Argonne into state-of-the-art flexible electronic devices for use as sensors and detectors.

Argonne is a leader in creating innovative materials and applying them to real-world needs. For example, we develop one-, two-, and three-dimensional nanomaterials such as fibers, coatings, thin films, particles, and powders, using state-of-the-art synthesis and processing capabilities that include electrospinning and microfluidic reactors. We extend those technologies to a variety of demanding applications, including solid-state batteries, catalysts for fuel cells and polymer upcycling, radio-frequency energy harvesting, water treatment, advanced communication devices, and antiviral filter media in support of COVID-19 response.

We also develop membrane materials and systems for gas- and liquid-phase separation for uses such as hydrogen production, biofuels processing, lithium metal manufacture, and water treatment. An expanding focus is upstream and midstream processing for critical energy storage materials and the recovery, reconstruction, and upcycling of specialized materials, an example of which is the DOE/EERE-funded ReCell battery recycling center.

The integration of basic and applied materials science at Argonne has produced more-efficient batteries, new solar panel designs, high-performance sponges for oil adsorption and chemical separations, nanofiber magnets, and improved nuclear energy fuels and materials. Ongoing work has shown promise for more-efficient nuclear fuel reprocessing, lighter-weight transportation alloys, advanced building materials, and higher-performance superconducting materials for use in detectors, accelerators, and energy transmission. Argonne's extensive experience in energy storage materials R&D positions us to make significant contributions to future storage solutions for stationary and mobile applications.

We recently expanded the MERF to enable additional materials manufacturing, synthesis, and processing capabilities for varied applications. The expansion enables us to focus on decarbonization across the energy system and to enhance partnership opportunities, including workforce development with a special emphasis on underserved communities. Over time, we plan to extend our manufacturing research and development capabilities to DOE priorities such as quantum information systems and pandemic response/biosecurity.

Argonne's applied materials science and engineering capability supports diverse collaborative research efforts. These efforts include the Joint Center for Energy Storage Research, a DOE/SC Energy Innovation Hub that creates transformative battery materials, and Argonne's Collaborative Center for Energy Storage Science, which facilitates maturation of novel battery materials and their deployment to industry. We develop materials technologies to solve global water challenges through the Advanced Materials for Energy-Water Systems, a DOE/SC Energy Frontier Research Center, and the Collaborative Water-Energy Research Center, an international consortium supported by DOE and Israel. We also partner with industry through DOE/EERE Manufacturing USA institutes such as PowerAmerica, NextFlex, and REMADE (Reducing EMbodied-Energy and Decreasing Emissions).

This capability supports the missions of DOE and other sponsors in the areas of nuclear energy, energy efficiency, renewable energy, energy storage, and environmental stewardship. It builds on discoveries in our core capabilities in condensed matter physics, materials science, and chemical engineering, with the goal of enhanced impact from moving those discoveries to market. It also supports many of the DOE/EERE consortia, including Chemical Catalysis for Bioenergy (ChemCatBio) and Lightweight Materials (LightMat).

Applied mathematics

Argonne is recognized for broad-ranging foundational research in mathematical modeling, analysis, and algorithm development, implemented in scalable software for the world's largest computing systems. We excel in the scalable solution of partial differential equations (PDEs) and provide best-in-class expertise in automatic differentiation (AD). We also are a recognized leader in mathematical optimization algorithms, modeling, software, and theory. Our strategy for the future emphasizes:

- Creating time- and energy-efficient PDE and optimization solvers for the exascale era and beyond
- Extending and combining AD, data assimilation, optimization, and PDE capabilities to support efficient solution of design, decision, and control problems while accounting for error estimates and uncertainty
- Applying expertise in optimization, statistics, and AD as building blocks for ML for scientific applications
- Expanding our capabilities in ML, statistics, quantum algorithms, and other strategic areas
- Combining approaches – ML, statistics, and optimization – to solve inverse and analysis problems associated with simulation, observation, and experimental data

Important recent advances in Argonne's applied mathematics capabilities include the following:

- Scalable computational frameworks for modeling and solving large-scale-optimization-under-uncertainty problems by using high-performance computing for the planning, design, and control of networked systems such as electrical, gas, transportation, and water networks
- Multimodal ML, statistical modeling, and algorithmic approaches to analyzing experimental, observational, and simulation data, including APS data and environmental observations
- Automated ML, multi-objective optimization, and differentiation algorithms applied to post-Moore architectural concepts and deployed for applications such as transportation modeling, supercomputing performance, and oceanographic modeling

Argonne's advances in applied mathematics are captured in state-of-the-art software, including:

- The Nek5000 and NekCEM software packages, which employ the spectral element method to efficiently solve large problems in computational fluid dynamics and computational electromagnetics
- PETSc, used by hundreds of scientific applications, which provides scalable linear solvers, nonlinear solvers, and time integration methods for solving discretized PDEs
- The ADIC, OpenAD/F, Rapsodia, and SWIG-PyADOLC AD tools for C, Fortran, Python, and R
- DSP and MINOTAUR, which solve optimization problems with both discrete and continuous variables
- Scalable solvers, such as TAO and PIPS, for optimization problems with billions of variables and constraints

This software ecosystem, designed to run on the most powerful supercomputers in the world, makes it possible to answer a broad range of science and engineering questions, including how to operate and upgrade the power grid, how mantle convection affects the earth's geological evolution, and how to cool nuclear reactors efficiently. These capabilities have been recognized repeatedly through R&D 100 awards, DOE Early Career Research Program awards, and the naming of staff members as Fellows of the Society for Industrial and Applied Mathematics.

This capability supports the DOE/SC-ASCR mission to develop and deploy high-performance and leadership computing tools for scientific discovery. Other current sponsors include DOE/ECP; DOE/EERE; DOE/NE; DOE/OE; DOE/SC-BER, -BES, -FES, -HEP, and -NP; DARPA; DHS; IARPA; NSF; and the private sector. Much of this funding entails interdisciplinary research partnerships that draw on our applied mathematics expertise.

Biological and bioprocess engineering

Argonne's approach to biological and bioprocess engineering incorporates methods from synthetic biology and synthetic chemistry to create biological systems and biomaterials with tuned functionalities. We apply understanding of complex biological systems to design, test, and validate process components, technologies, and systems relevant to bioenergy production, environmental contaminants processing, and global carbon cycling and biosequestration. We also apply biochemical engineering principles to develop scalable new processes for biofuels and bioproducts. Primary supporting disciplines include biology, chemistry, chemical engineering, materials science and engineering, environmental and agricultural science, computational sciences, and systems science.

This capability draws on the experimental systems at the CNM and APS. CNM's tools for imaging and manipulating biomolecules, cells, and processes over multiple scales are used extensively for bioprocessing. We use APS beamlines to determine the structure of biological macromolecules and characterize catalysts in thermochemical conversion processes; associated capabilities include bionanoprobe and micro-diffraction tools. Our Advanced Protein Characterization Facility at the APS produces and characterizes tens of thousands of unique proteins each year. We have leveraged our computational expertise and resources to become leaders in developing bioinformatic tools for the larger research community. The proposed Sensing and Imaging at Argonne (SIA) building would enable nondestructive methods to study biologically driven processes using advanced sensors and computer vision. It also would further development of new quantum methods for advanced sensing.

Through recent advances in biological and bioprocess engineering, we have demonstrated the ability to predictively engineer microbes from the environment for biotechnology, energy, and food proteins with radically altered function and enzymes to transform biomass. This synthetic biology ability enables us to design microbes and communities for fundamental understanding of biological functions, biomanufacturing, novel polymer production-transformation, the energy-water nexus, and biohybrids.

Our work also includes directed molecular evolution for photosynthetic systems, catalyst separation and reuse, bioreactor design and operation, and selective extraction and separation of products and inhibitors from bioreactors. To support a circular economy, Argonne also designs and synthesizes sustainable plastics and develops bioprocesses to convert waste to energy and products.

Current research directions and investments focus on:

- *Synthetic biology for biosystems design.* We analyze and model microbial and microbiome systems to enable predictive design of strains and communities and develop an ecological understanding of them. We are a major contributor to the development of the DOE/SC-BER Systems Biology Knowledgebase, which integrates metabolic modeling with cheminformatics, omics, and meta-omics in support of bioengineering of microbes, plants, and microbial communities. We also develop methods to rapidly design and engineer novel microorganisms and collaborate with Northwestern University and UChicago on automated laboratories to support this effort.
- *Global carbon cycle and environmental chemical cycling.* Argonne research seeks to understand elemental cycling in the biosphere in a variety of environmental contexts. One focus area is the biogeochemical processes that affect iron, carbon, and contaminant speciation within the wetland sediment, rhizosphere, and stream environments. We also work to discover the plant genes important for adaptation and sustainability in the face of environmental change.

- *Bioprocesses and biomanufacturing.* As the lead laboratory for the DOE/EERE Bioprocessing Separations Consortium, Argonne has developed technologies to separate and recover organic acids and terpenes produced during fermentation. We also have developed a pilot-scale fermenter system to scale up bioprocesses. We contribute to the development of biomanufacturing technologies as part of two DOE/EERE efforts, the Agile Biofoundry Project and the Feedstock Conversion Interface Consortium. In addition, we have core competencies in lifecycle, techno-economic, and environmental risk analyses of bioenergy-related processes and assessments of the impacts of bioenergy system deployment on soil carbon, water footprint, water quality, and landscape design.

This capability supports the missions of DOE and other entities that seek to better understand microbes, plants, and biohybrids to engineer them for energy applications. Current sponsors include DOE/EERE, DOE/SC-BER and -BES, national security agencies, industry, and local government entities.

Chemical and molecular science

Chemical and molecular science is central to many of Argonne's research programs. World-leading strengths include computational and theoretical chemistry; electrochemistry; functional, interfacial, and mechanistic chemistry; molecular control of chemical transport and chemical reactivity; molecular design and synthesis; and interactions of light and matter.

Studies explore trends in chemistries across the periodic table, applying our expertise in gas-phase, liquid-phase, and solid-state chemistries. In support of the DOE/SC mission, these strengths deliver scientific discoveries relevant to catalysis, electricity production from chemical energy, energy storage, geochemistry, heavy-element separations, and solar and photosynthetic processes. These core efforts are supported by our expertise in theoretical and computational chemistry. Our atomic and molecular physics and solar photochemistry programs use unique competencies in ultrafast characterization of reactions. Our catalysis research draws on unique expertise in organometallic chemistry combined with heterogeneous catalysis and, most recently, electrochemistry. Efforts in geoscience and heavy element chemistry build on extensive expertise and capabilities in the characterization of interfaces.

Computational resources and characterization tools available through the ALCF, APS, and CNM are integral to this capability. The upgraded APS will enable us to study chemical processes in real time, under realistic conditions. The APS upgrade also will lead to an expected 30-fold increase in the time resolution of observations of catalytic processes; will enable geoscientists to image complex structures and morphologies directly, rather than probe average properties of samples; and will improve our ability to study interfacial chemical dynamics important to chemical separations.

Other relevant facilities include Argonne's unique High-Throughput Research Laboratory, atomic layer deposition laboratories, and Advanced Electron Paramagnetic Resonance Facility. In addition, our DOE/SC-BES programs in heavy-element chemistry and separations science are now based in new radiological facilities in the Materials Design Laboratory. That location will further a systems approach by fostering new interdisciplinary science within a state-of-the-art research complex.

In addition, our core capability in condensed matter physics and materials science complements these strengths through materials design and synthesis and functional material development. We advance our DOE/SC-BES discoveries in chemical and molecular science through collaborations with industry and in conjunction with our core capabilities in chemical engineering and applied materials science. We lead the Energy Frontier Research Center on Advanced Materials for Energy-Water Systems (AMEWS), which is focused on the science of water/solid interfaces, in collaboration with UChicago and Northwestern University.

Argonne takes an integrated, systems approach to the chemical and molecular sciences. We seek to unify the understanding of the periodic table, taking advantage of our expertise in the chemistry of the light elements, transition metals, and heavy elements. We seek to understand transient processes within molecules through our ultrafast chemistry and ion and electron transport expertise. Expertise in photosynthetic systems offers an opportunity to study spin quantum effects important for quantum information science.

Additionally, competing reactions are at the core of our strategy. Complex environments with competing reactions are studied through detailed explorations of the underlying dynamics and kinetics, including the role of rare events and energy transfer processes. Efforts in understanding dynamics, structure, and transport within complex environments and at interfaces will impact areas such as separations, catalysis, geochemistry, and photochemical processes.

Recent investments will expand capabilities in polymer design and upcycling; sustainable manufacturing science; carbon dioxide capture and conversion; electron transfer in molecules, including light-driven electron transfer in natural and artificial photosynthetic systems; and prediction and control of the flow of electrons, ions, and molecules at interfaces relevant to geochemistry, separations, catalysis, and electrochemical processes. To address the challenges and opportunities of predictive chemistries, we will further integrate our expertise in computational, theoretical, and data science into experimental chemistry research, building on expertise in artificial intelligence for science.

Precision synthesis for controlled chemical conversions will continue to be at the fore in addition to the necessary characterization of atoms and molecules spanning length scales from atomic to microns and time scales from ultrafast to seconds under *in situ/operando* conditions. This core capability will benefit from the proposed Sensing and Imaging at Argonne building (Sec. 6.2), particularly through proposed capabilities in attosecond spectroscopy.

This capability supports the missions of DOE/SC-BES and other DOE/SC offices. Current sponsors also include DOD.

Chemical engineering

Argonne's chemical engineering research addresses the nation's energy and security challenges by building on and informing basic energy research while developing transformational technologies for electrochemical energy storage, water cleanup, chemical and light energy conversion, and conversion of biomass (including post-use carbon resources). This capability integrates chemical engineering expertise with our core capabilities in chemical and molecular science, condensed matter physics and materials science, and biological and bioprocess engineering.

We are globally recognized for our research in lithium-ion (Li-ion) batteries, solar conversion, combustion chemistry, and fuel cells, based on our success in applying our foundational knowledge of electro-, photo- and thermo- chemistry and catalysis (from our core capability in chemical and molecular science) and of interfacial sciences (from additional core capabilities). We are advancing the next generation of Li-ion batteries, looking beyond Li-ion batteries, developing solid-state batteries and solutions for stationary storage, and advancing methods to recycle Li-ion batteries through the DOE/EERE-funded ReCell center.

Our multidisciplinary efforts also develop advanced membranes, electrodes, and electrocatalysts to reduce the cost and improve the durability of fuel cells based on solid-oxide and polymer-electrolyte membrane technologies. Recent work is advancing rail, marine, and aviation applications of fuel cells.

Our expertise in gas-phase chemistry and chemical and material scale-up is leading to new engine designs and pathways for translating DOE/SC discoveries and DOE/EERE foundational research to meet industry and consumer needs.

In addition, we accelerate the development of catalysts that do not use platinum-group metals for fuel cells, by using high-throughput materials synthesis, characterization, and performance evaluation of equipment and methodologies. This activity is a cornerstone of the DOE/EERE ElectroCat research consortium, which we co-lead with Los Alamos National Laboratory. We also lead a thrust of the DOE/EERE Fuel Cell Consortium for Performance and Durability (FC-PAD), applying our sophisticated characterization capabilities, including those at the APS, to study electrocatalysis. Other efforts are intended to reduce the costs of producing renewable liquid transportation fuels through advances in catalysis. Additional research is aimed at moving basic science discoveries in polymer upcycling catalysis to market.

Argonne operates a unique suite of facilities for energy storage and conversion R&D, a suite that is integrated with our process and systems modeling capabilities. Our modeling capabilities include process unit modeling, performance vs cost modeling, supply chain analysis, and techno-economic and life cycle analysis. Our facilities, funded mainly by DOE/EERE, include:

- *Cell Analysis, Modeling and Prototyping Facility*. Cells manufactured in this facility enable realistic, consistent, and timely evaluation of candidate battery-cell chemistries in a close-to-realistic industrial format.
- *Electrochemical Analysis and Diagnostics Laboratory.* This laboratory provides battery developers with performance evaluation of cells, modules, and battery packs, allowing diagnostic analysis of battery components after use to identify mechanisms that limit battery life.
- *Post-Test Facility.* This facility is designed to understand failure modes in batteries with air-sensitive materials, such as those from lithium-based or sodium-based battery technologies.
- *High-Throughput Research Laboratory.* This laboratory provides robotic tools and reactor systems for fast, automated, and parallel approaches to chemical synthesis and materials development, thereby accelerating optimization of new materials for catalysis, energy storage, fuel cells, solar energy, and nanoscale chemistry.
- *Materials Engineering Research Facility.* This facility allows researchers to explore the scale up of materials and chemical processes as we work with industry to move national laboratory and industry innovations to the marketplace. It is described in more detail under our applied materials science and engineering capability.

This capability supports the missions of DOE and other agencies to advance energy storage and fuel cell science and engineering. Current sponsors include DOE/EERE, DOE/IP, DOE/NNSA, DOD, and industry.

Climate change sciences and atmospheric science

Argonne's research improves understanding of atmospheric and environmental systems and advances efforts to address climate-related energy, water, and security challenges. We make leading contributions in atmospheric measurement and analysis, earth science simulations, and soil and biogeochemical science; we integrate these areas to develop a predictive understanding of the role of heterogeneity in water, energy, and carbon exchange in earth systems.

Argonne's strengths in atmospheric science are grounded in our ability to make sophisticated atmospheric measurements at an unprecedented scale and under challenging circumstances. We are actively involved in the science teams for mobile facility deployments under the DOE/SC-BER Atmospheric Radiation Measurement (ARM) program. We oversee operational activities across all ARM sites and operate the ARM Southern Great Plains (SGP) site, the world's largest and most extensive research facility for *in situ* and remote sensing of cloud, aerosol, and atmospheric processes. We also design and deploy open-source best-practices software that researchers use to read, process, and visualize atmospheric data.

Argonne is pioneering edge computing that makes use of artificial intelligence (AI) and advanced wireless technology (5G and beyond) for agile sensing to measure at spatial and temporal scales optimized for the science question being asked. We have deployed edge computing to the ARM-SGP site and will soon have nodes at ARM sites in Alaska and Texas. Our computational and domain scientists collaborate to develop AI applications to improve the predictability, speed, and efficiency of earth system models.

Argonne provides the global scientific community with unique expertise and software for retrieving geophysical variables from atmospheric remote sensing instruments. Our Py-ART software for radar data is internationally recognized, as are our tools to understand tropical/ equatorial convection and to work with time series.

We apply our aerosol/cloud science and instrument expertise, along with ARM data, to understand terrestrial-atmospheric coupling and the role of cloud processes in the hydrologic cycle and to define the impact of surface- and boundary-layer coupling on low-level clouds. Argonne made fundamental contributions to the science of absorbing aerosols by identifying brown carbon as a potential atmospheric warming component, and we continue to focus on the life cycle of aerosols from burning biomass. We have made fundamental contributions to the physics of low-level clouds using ARM data and developed novel methods for retrieving atmospheric thermodynamic and cloud properties from remote sensing data.

To advance earth science simulation, Argonne applies high-performance computing to develop robust predictive capabilities. We support the computational objectives of DOE's flagship Energy Exascale Earth System Model (E3SM) and the data and analytical needs of other DOE climate and atmospheric science programs. We develop models and use them with field observations to understand the influence of aerosols and aerosol life cycle on low-level clouds and the earth's radiation budget. Using the APS, we pioneered the application of synchrotron technology to analyze the chemical and physical characteristics of atmospheric dust, aerosols, and soils. The APS Upgrade will vastly expand the capabilities of this technology for environmental science.

Argonne is an international leader in downscaling earth system models to project possible local climate conditions. Our 12-km-resolution climate projections for North America support quantitative analysis of risks from extreme weather. We have collaborated with DOE/EERE-WETO and NOAA to improve the accuracy of numerical weather prediction models over complex terrain, in support of wind-energy production. We are now making North American continental-scale simulations at a 4-km resolution that fully accounts for convection physics.

Our soil and biogeochemical scientists develop a deep predictive understanding of soil response to environmental change, from the molecular to the regional scale. We collaborate with the broader scientific community to develop novel syntheses of regional carbon dioxide flows from arctic and boreal soils, producing the first high-resolution, spatially explicit estimate of organic carbon stocks in permafrost soils. We apply microbial ecology to advance knowledge of soil processes, develop novel technologies to characterize soil properties, and use geospatial analytics to extend field measurements. Our rapid mid-infrared spectroscopy technique enables researchers to quickly assess the degradation of organic matter in those soils. This information is vital to predicting future carbon emissions from soils in high-latitude regions.

This core capability supports the missions of DOE/SC-BER and other federal entities with climate and atmospheric science initiatives. Additional sponsors include DOE/EERE-WETO, NSF, DOD, NASA, NSF, and industry.

Computational science

Computational science, a cornerstone of Argonne's R&D enterprise, advances the solution of critical problems in many scientific disciplines. Our Laboratory-wide computational activities involve more than 350 scientists and engineers working in interdisciplinary project teams that include applied mathematicians, computer scientists, and computational scientists with expertise in various domains. Argonne's computational science effort is strongly supported by the capabilities of the ALCF, Joint Laboratory for System Evaluation, and Laboratory Computing Resource Center.

We will continue to enhance and promote our computational science capabilities, in the following ways:

- Leverage our computational science division and data science and learning division to build strong collaborative projects with scientists and engineers across Argonne in modeling, simulation, data-intensive applications, and machine learning (ML). We are facilitating crosscutting Laboratory-wide engagement in computing and fostering multidisciplinary teams for conducting leading-edge computational science.
- Through our computing divisions, provide computational scientists and engineers with ready access to broad and deep expertise in traditional and emerging scientific computing methods and tools. These methods include modeling and simulation, data science, machine and deep learning, software development and optimization, and next-generation technologies such as quantum and neuromorphic computing.
- Use a matrix model to integrate domain expertise with methodological expertise in computational science, data science, and ML.
- Take advantage of the co-location of hardware and staff expertise to strengthen proposals of both internal and external computational science groups as they apply for DOE's *Innovative and Novel Computational Impact on Theory and Experiment* and *ASCR Leadership Computing Challenge* awards.

Some examples of the impact and leadership of Argonne's computational science capability follow:

- We have performed some of the world's largest high-resolution cosmological simulations with Argonne's HACC code, modeling the universe over billions of years. HACC plays an important role in benchmarks for future DOE computing systems and is a significant part of two major efforts within DOE's Exascale Computing Project (ECP).
- We have developed and implemented algorithms and toolkits for analysis of large datasets from Argonne's APS, the Large Hadron Collider in Switzerland, and the Legacy Survey of Space and Time carried out at the Vera C. Rubin Observatory in Chile.
- Our peers have recognized the computational science enabled by our PETSc library with multiple Gordon Bell prizes and the joint prize in Computational Science and Engineering awarded by the Society for Industrial and Applied Mathematics and the Association for Computing Machinery.
- Our NekCEM/NEK5000 code has been used in applications spanning fluid flow, thermal convection, combustion, magnetohydrodynamics, and electromagnetics. It won an R&D 100 award in 2016 and is used in two ECP application projects.
- Argonne staff engage in development of community codes such as NAMD, QMCPACK, and LAMMPS.

- We participate in 10 SciDAC application partnerships spanning environmental science, fusion, high-energy physics, nuclear physics, and nuclear engineering.
- We have developed and contributed to a spectrum of applications: these include *elegant* (accelerator simulation), TomoPy (x-ray tomographic analysis), Green's Function Monte Carlo (properties of nuclei), and QMCPACK studies of the electronic and structural properties of semiconductors.
- Argonne is a member of a multi-laboratory partnership under the auspices of the High Energy Physics Center for Computational Excellence, which works to employ exascale computing resources for simulation and data analysis for high energy physics experiments.

This capability supports missions across all of DOE and other entities that fund R&D. Current sponsors include ARPA-E; DOE/EERE; DOE/OE; DOE/SC-ASCR, -BER, -BES, -FES, -HEP, and -NP; NIH; NASA; NSF; and industry.

Condensed matter physics and materials science

Argonne's research in condensed matter physics and materials science predicts, designs, and creates new materials and advances understanding of their behavior. Our program is internationally recognized in multiple areas, including magnetic, superconducting, ferroelectric, and topological materials; quantum metamaterials; correlated oxides; polymers and active soft matter; and electrochemical systems. Our leadership in these fields relies on the breadth and depth of our expertise in materials chemistry and physics, scattering and imaging, theoretical and computational science, and the integration of capabilities at the APS, CNM, and ALCF.

Our programmatic strategy rests on understanding and exploiting the science of defects and interfaces across three core themes: quantum materials and materials for quantum information science (QIS), materials to enable interface- and defect-directed energy and information transduction, and static and dynamic order in soft matter. Our expertise and capabilities together make Argonne's portfolio unique, positioning us to deliver scientific breakthroughs in materials discovery related to defects and interfaces.

For example, our experimental and computational research is advancing discovery of defect-based materials platforms for QIS. We recently launched a program focused on targeted repair of interfacial defects, offering a route to new physical phenomena in diverse materials systems. We support our core themes with crosscutting and enabling strategies in precision synthesis and *in situ* and *in operando* coherent x-ray and electron studies coupled to modeling and theory. Artificial intelligence (AI) and data-driven science underpin all areas of our research. Our programs are making full use of Argonne's new Materials Design Laboratory, including a laboratory outfitted to support ultrafast laser research. Our expertise in soft matter and in semiconductor- and superconductor-based QIS materials platforms is enhanced through joint staff appointments between UChicago and Argonne's Center for Molecular Engineering.

Collaboration within and outside Argonne is a key element of our strategy. Our materials science strengths are complemented by Argonne's core capability in chemical and molecular science, particularly in the areas of molecular design and synthesis, the role of interfaces, and electrochemistry. Our activities are synergistic with Argonne's efforts in circular economy research, AI applications in science, and hard x-ray sciences. We lead the Midwest Integrated Center for Computational Materials, a collaboration with UChicago and four other universities. Our core materials science complements the work of the Argonne-led Joint Center for Energy Storage Research and Q-NEXT center, and we play a principal role in several other materials-focused multi-institution projects funded by DOE/SC-BES. Across our portfolio, we seek to transfer fundamental materials discoveries to applied Argonne research that can leverage them.

Argonne's research has had recent impact at frontier areas of science, including discovery of higher-temperature emergent interfacial superconductivity in oxides; use of AI to design polymers with specific properties; discovery of new materials that exhibit topological behavior; and use of machine learning on diffuse scattering data to understand fluctuations of structural order.

Looking ahead, we will build on our materials discovery expertise to extend our basic research on novel quantum materials to explore emergent behavior that arises because of defects and interfaces, and to gain a fundamental understanding of quantum materials relevant to both QIS and microelectronics, in part with a view toward materials circularity. We will follow opportunities to understand non-equilibrium behavior in soft matter. We will develop a synthesis framework to create electrochemical environments that repair materials, and we plan new fundamental research at the materials frontier that capitalizes on our expertise in AI, for example to explore autonomous polymer discovery.

We will develop approaches to materials design that will make use of Argonne's AI- and data-centric Aurora exascale computer. We will focus on simulation of heterogeneity in hard and soft matter, including the role of topological defects, and develop methods to treat strong electron-phonon interactions that today are very challenging. To help shape the scientific mission of the upgraded APS, we will develop and deploy measurement and analysis frameworks for coherent x-ray diffractive imaging, focused on applications in soft matter, defects for QIS, and time-resolved behavior in response to environments. We will also expand our synchrotron- and laboratory-based efforts in ultrafast science. In addition, we will propose scientific programs that incorporate electron probes into our coherent imaging frameworks and make use of the planned Sensing and Imaging at Argonne building across our portfolio.

This core capability supports the missions of DOE/SC-BES and other DOE/SC programs. Additional sponsors include DOE/EERE, DOE/NNSA, DOD, and industry.

Cyber and information sciences

Through our cyber and information sciences programs, we protect, analyze, and disseminate information from computer systems and other electronic sources to defend the U.S. from cyber attacks. Our research supports critical national missions: it strengthens the overall cybersecurity of national infrastructure, including the electric grid, water systems, transportation assets, and supply chains. Additionally, our work underpins national efforts in nonproliferation and counterproliferation of weapons of mass destruction, military decision support, and radiological response and recovery.

We take a collaborative cross-disciplinary approach to address emerging problems in this arena and deliver results of global impact. Our cyber and information sciences activities leverage Argonne's fundamental sciences, advanced computing and engineering capabilities, and the APS, ALCF, and Laboratory Computing Resource Center. Our external partners include researchers from Iowa State University, UChicago, Mississippi State University, Hitachi ABB, Commonwealth Edison, additional universities and businesses, and other national laboratories.

We help protect the nation as a trusted partner to government agencies, through our research into the resiliency of critical cyber assets, the security of cyber-physical systems, and the collection and dissemination of intelligence needed to defend against cyber threats. Through our cyber and information sciences strategy, we:

- Conduct proactive cybersecurity research in critical infrastructure risk and resilience, moving target defense, autonomous vehicle security, the trustworthiness of algorithms driven by

artificial intelligence (AI) and machine learning (ML), and other proactive technologies to improve national security
- Share cyber threat information using real-time, machine-to-machine methods for the defense of the energy sector using the Cyber Fed Model, while also working to define the next generation of information sharing to enable coordinated cyber threat discovery
- Design tools and testbeds, such as the SECURE testbed, to evaluate the resiliency, dependencies, and defenses of computer systems that operate critical infrastructure and industrial control systems, as well as the consequences of attacks on those systems
- Explore the risk/benefit trade-off for applications of quantum communication and quantum sensor technologies in cybersecurity of critical infrastructure.
- Apply cutting-edge research and development to design systems supporting power grid operations that will be resilient to the cybersecurity threats of the future, in support of the DOE/CESER Cybersecurity for Energy Delivery Systems program
- Partner with DOE/CESER and DOE/SC to develop the cybersecurity workforce, including hosting the annual CyberForce Competition™ to increase college students' understanding of cyber-physical risk to systems like high-performance computers
- License Argonne's patented MORE Moving Target Defense technology, recipient of an R&D 100 Award, which enhances cybersecurity through a rotation of multiple operating systems
- Deploy advanced algorithms and tools that monitor the physics of the power grid to detect and mitigate attacks on cyber-physical systems
- Extract structured data from unstructured sources, including the darknet, using information retrieval methods that employ natural language processing and ML to better understand proliferation patterns in support of U.S. enforcement efforts
- Develop and operate searchable databases and document repositories for a variety of missions, including nuclear forensics and nonproliferation
- Develop edge-computing platforms for detection of moving objects such as unmanned aerial vehicles and birds
- Integrate cutting-edge research into complex models for analysis of military transportation, disaster response and recovery, storage and transportation of spent nuclear fuel, and supply chains

Facilities that support this capability include enterprise data centers that host a multi-agency secure private cloud and a state-of-the-art testbed to model physical and cyber dependencies.

This capability supports the missions of DOE, DHS, DOD, and industry. Current DOE sponsors include DOE/CESER, DOE/EERE, DOE/IN, DOE/NE, DOE/NNSA, DOE/AU and DOE/OCIO. Current DHS sponsors include the Federal Emergency Management Agency, Office of Intelligence and Analysis, Countering Weapons of Mass Destruction Office, Office of the Chief Security Officer, and Cybersecurity and Infrastructure Security Agency.

Decision science and analysis

Argonne is recognized for developing and applying novel decision science and analysis approaches to inform decision makers as they address pressing national, cross-border, and global challenges in rapidly changing environments with incomplete/imperfect data. These approaches include agent-based modeling, complex adaptive system modeling, system dynamics, life-cycle analysis, and complex network analyses that model parameters of dynamic, complex systems. We are an international leader in the development of high-performance computing software tools (such as Repast and EMEWS), including their use in extreme-scale agent-based modeling applications. This core capability, linked with Argonne's core capabilities in cyber and information sciences and in systems engineering, positions us to deliver impactful solutions to complex problems that require multidisciplinary solutions.

Argonne drew on many aspects of this core capability during the U.S. response to COVID-19. Our researchers updated our Resilience Analysis and Planning Tool to inform emergency managers about vulnerable populations. We also supported the City of Chicago and the State of Illinois with the CityCOVID agent-based model, which we used to forecast the spread of COVID-19 and test the effects of mitigation measures before they were implemented.

More generally, Argonne has applied leadership computing capabilities to the analysis of social and behavioral systems to address problems such as the spread of infectious disease and misinformation in urban settings and the effectiveness of interventions to mitigate both. Facilities that enable this work include an immersive data visualization STudio for Augmented Collaboration (STAC) and the ALCF. Looking to the future, we will make increasing use of advanced computing approaches and architectures, including artificial intelligence, machine learning (ML), and exascale systems.

Staff members across the Laboratory are dedicated to a decision science and analysis strategy in which we:

- Use system dynamics capabilities to build models that enable federal leaders to make data-driven decisions about disaster staffing, taking into consideration key missions, future disaster impacts, and anticipated agency workloads and staffing requirements
- Apply decision science principles and techniques to create assessment frameworks for use across critical infrastructure systems that enable subject matter experts to make cost-benefit tradeoffs for different security and resilience features
- Assess the complex interactions of infrastructure interdependencies in local, regional, national, and international systems to identify potential cascading and escalating failures and inform resilience-enhancement decisions
- Develop optimization models that enable decision-makers to prioritize transport routes that support disaster relief supply chains and identify pre-disaster planning and mitigation measures to protect them
- Model and analyze global supply chains to inform decisions affecting the U.S. stockpile of critical materials that support national security and energy technologies
- Deploy a threat assessment process for federal security personnel that leverages ML to analyze threats and vulnerabilities at federal facilities and optimize recommendations for targeted countermeasures in accordance with relevant security standards (winner of an R&D 100 award)
- Apply our expanded Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET) life-cycle-analysis model to inform decisions about new technologies and concepts within DOE/EERE initiatives in transportation electrification, supply chain sustainability analysis, H2@Scale, and building-embodied-carbon analysis

In addition, we are addressing how best to meet future DOE needs for earth system prediction. A scientific challenge is to capture the reverse feedback from human behavior on the environment. Supporting research focuses on model coupling, ensemble modeling, and uncertainty propagation, with the goal of providing model-generated information to decision makers, and on understanding the social dynamics of how information and misinformation spread through social networks. We are collaborating with UChicago researchers in several of these areas.

This capability supports the missions of DOE, DHS, DOD, and industry. Current DOE sponsors include DOE/CESER, DOE/EERE, DOE/IN, DOE/NE, DOE/NNSA, and DOE/OE. Current DHS sponsors include the

Federal Emergency Management Agency, Cybersecurity and Infrastructure Security Agency, and the Federal Protective Service. Industry sponsors include AT&T and Exelon.

Large-scale user facilities/advanced instrumentation

Argonne is at the forefront in the design, construction, and operation of world-leading scientific user facilities and innovative instrumentation. The capabilities and productivity of these facilities and instruments derive from their strong integration with our research programs and from our commitment to nurture a diverse and vibrant user community. The five facilities described here are part of the DOE/SC portfolio of user facilities.

Three of these facilities – the ALCF, APS, and CNM –supported critical research as part of DOE's response to the COVID-19 crisis. Modeling work continues at the ALCF to identify potential treatments for disease and forecast the spread of viruses. The APS continues to support the effort of structural biologists to characterize viral proteins.

More generally, this capability supports the DOE/SC mission to operate user facilities that provide the highly advanced research tools needed to address the world's greatest challenges in science and technology. In addition to DOE/SC support for the overall operation of these facilities, specific capabilities at individual facilities are also supported by DOE/NNSA, DOE/OE, NIH, NSF, and industry.

Advanced Photon Source (APS)

Funded primarily by DOE/SC-BES, the APS is an internationally leading source of high-energy x-rays for scattering, spectroscopy, and imaging studies over a wide range of length and time scales. Capabilities include *in situ, in operando*, and extreme sample environments (static and dynamic high-pressure, pulsed high magnetic fields, low/high temperatures); x-ray interrogation of electron and lattice excitations; macromolecular crystallography; and real-time studies of evolving systems. The APS Upgrade project is underway to create the world's brightest hard x-ray storage-ring light source. To complement x-ray macromolecular crystallography, we also propose cryo-electron microscopy in the planned Sensing and Imaging at Argonne building.

Argonne Leadership Computing Facility (ALCF)

Funded by DOE/SC-ASCR, the ALCF operates an open-science supercomputer named Theta (an Intel/Cray XC40 system, ALCF-Lithium) that ranks among the 40 fastest machines in the world. The ALCF provides petascale computing capabilities and support services that enable the computational science and engineering community to run the largest and most complex calculations. In 2021, we enhanced Theta by adding 24 NVIDIA DGX-3 GPU nodes. ALCF also hosts the Joint Laboratory for System Evaluation, which gives our staff and collaborators access to the latest production and prototype computing resources. In 2021, the ALCF will deploy Polaris (HPE/NVIDIA, ALCF-Polaris) in preparation for a 2022 deployment of the Aurora exascale system (an Intel/HPE machine, ALCF-3).

Argonne Tandem Linear Accelerator System (ATLAS)

Funded by DOE/SC-NP, ATLAS is a superconducting linear accelerator and the only DOE user facility for low-energy nuclear research. It provides high-intensity heavy-ion beams in the energy domain best suited to study the properties of the nucleus. At ATLAS, the Californium Rare Ion Breeder Upgrade (CARIBU) has the unique capability to provide both stopped and reaccelerated beams of radioactive neutron-rich nuclei. ATLAS offers its users an array of unique experimental systems to take full advantage of the accelerator capabilities.

Atmospheric Radiation Measurement Southern Great Plains (ARM-SGP) site

Funded by DOE/SC-BER, the ARM-SGP site is the world's largest and most extensive field site for climate research. Its instruments are arrayed across 9,000 square miles, with a heavily instrumented central facility on 160 acres near Lamont, Oklahoma. In addition to operating the ARM-SGP site, Argonne oversees operations and instrumentation and provides instrument and measurement expertise to all ARM sites. Scientists from Argonne and other institutions use ARM data to advance scientific understanding of cloud, aerosol, and atmospheric processes, which supports improvements in models of the earth's climate.

Center for Nanoscale Materials (CNM)

The CNM, funded by DOE/SC-BES, supports interdisciplinary nanoscience research, with emphasis on quantum materials and sensing, manipulation of nanoscale interactions, and nanoscale dynamics. Its capabilities include ultrafast electron microscopy, broadband ultrafast optical spectroscopy, nanofabrication, and first-generation user tools for quantum information science. Capabilities achieved through collaborations with the APS include a hard x-ray nanoprobe and a synchrotron x-ray scanning tunneling microscope. In collaboration with DOE, the CNM invests in ongoing instrumentation upgrades. A multi-laboratory Major Items of Equipment DOE/SC-BES project for Nanoscale Science Research Centers Recapitalization has identified opportunities to greatly strengthen this capability. New, dedicated space to house equipment is needed to expand CNM's electron microscopy capabilities; the proposed Sensing and Imaging at Argonne building would provide such space.

Nuclear and radio chemistry

Argonne executes pioneering work in nuclear chemical engineering, chemical separations, and the materials and chemical science of actinides, radioisotopes, and the nuclear fuel cycle. Our strategy to enhance this capability includes gaining new understanding of the:

- Chemical and thermophysical properties of actinides in extreme environments, such as the high-temperature and molten salts encountered in advanced nuclear energy systems
- Production and chemical separation of radioisotopes essential to groundbreaking medical and national security technologies
- Structure-property relationships foundational to actinide and radioisotope chemical separations across a broad spectrum of energy-related areas, from nuclear fuel and materials separations to radioisotope production
- Correlations between ion and neutron radiation damage to nuclear fuels and structural materials to enhance their performance and accelerate their regulatory qualification; these correlations are developed using AI/ML tools
- Technical bases and performance of next-generation separations and safeguards technologies for future nuclear energy systems

A distinctive portfolio of research capabilities and facilities enables this work, including:

- APS, ATLAS, and ALCF
- Electron microscopy tools including the Intermediate Voltage Electron Microscope
- Two co-located, purpose-built radiological facilities: the Low-Energy Accelerator Facility (LEAF) and a chemical separations system for radioisotope production and isolation

- Radiological laboratories that enable development and testing of advanced electrochemical and aqueous separation processes and nuclear fuels, to support development of innovative nuclear fuel cycle and safeguards technologies

We apply these capabilities, including the use of AI/ML, to actinide science that produces novel approaches to the synthesis, characterization, and modeling of actinide-bearing materials and their properties. Our work uses these purpose-built radiological facilities to extend understanding of the pure and applied chemistry of these elements. We target predictive bonding and energetics models, within the context of nuclear fuel development and chemical separations relevant to nuclear energy, by using Argonne computational facilities to interpret x-ray analytical characterization at the APS. We are applying insights from these studies to develop efficient separations processes and associated safeguards technologies that promise to reduce nuclear waste generation in a secure and cost-effective manner.

Within the context of minimizing the world's reliance on weapons-usable nuclear material in reactor applications, we are a leader in R&D in the production of molybdenum-99/technetium-99m, which is currently the most important and in-demand medical isotope for diagnostic nuclear medicine. In collaboration with industrial sponsors, we developed and demonstrated new accelerator-based production channels, as well as chemical separation and purification methods, to facilitate domestic molybdenum-99 production without the use of weapons-usable materials.

We use our radioisotope production expertise at the LEAF and our radioisotope separations capability to perform R&D on, and produce, theranostic (therapeutic and diagnostic) medical radioisotopes. LEAF includes Argonne's electron linear accelerator, one of the most powerful electron accelerators in the DOE complex, and a Van de Graaff accelerator. We supply copper-67 to the DOE Isotope Program for subsequent use by medical researchers and are conducting research to develop production methods for additional medical radioisotopes, including scandium-47 and high-priority actinium-225. Radioisotopes such as these offer great promise in both the diagnosis and treatment of diseases such as prostate and bone cancer.

We also conduct sensor and detector research for national programs in border, cargo, and transportation security, as well as chemical, biological, radiological, and nuclear incident mitigation; our focus includes millimeter wave technologies for remote detection and sensors, as well as forensics to identify sources of nuclear and biological materials.

This capability supports the missions of DOE and other organizations that seek to advance understanding of actinide chemistry, radioisotopes, and technologies for future nuclear energy systems. Current sponsors include DOE/NE, DOE/NNSA, DOE/SC-BES and -IDPRA, and overseas research organizations.

Nuclear engineering

Argonne pioneered nuclear energy systems and continues to be a world leader in advancing nuclear energy science and technology. We are recognized for ground-breaking research in advanced nuclear energy technology and nuclear materials security. Our nuclear engineering capability supports significant national goals in nuclear energy safety and development, nuclear nonproliferation, isotope research and production, and protection of critical infrastructure. Our nuclear engineering staff draws on unique Argonne capabilities in nuclear and neutron physics, thermal-hydraulics, materials science, nuclear and radio chemistry, x-ray imaging, and computational science.

Key facilities that support this work include APS, ALCF, ATLAS, and our Intermediate Voltage Electron Microscopy-Tandem Facility, which has unique capabilities to image changes in materials during irradiation. Using ALCF, Argonne has made groundbreaking advances in exploiting high-performance computing for multiphysics analysis of nuclear-reactor behavior. We use our specialized engineering laboratories to execute detailed studies of nuclear reactor materials and components under extreme conditions representative of nuclear reactor systems. Throughout our history, we have enhanced the efficiency and benefits of our research through national and international collaboration with research and industrial partners. Recent efforts include teaming with Oak Ridge National Laboratory (ORNL) in development of materials for the Transformational Challenge Reactor.

Argonne has long invested significant effort in maintaining and expanding core capabilities in neutron physics and advanced reactor design and safety analysis. We are viewed as the world leader in designing and analyzing fast-neutron-spectrum systems and understanding the performance and safety of fuels and materials in nuclear reactors. Our contributions to the design of passively safe reactor systems and our understanding of nuclear accident phenomena and mitigations are widely recognized by the international community. Building on our work with fast-spectrum reactors, we now lead the core design and safety analysis efforts for the Versatile Test Reactor, one of the priority projects of DOE's Office of Nuclear Energy.

In addition, we use our nuclear fuel cycle expertise, along with our nuclear and radio chemistry capability, to develop methods for separating radioisotopes and recycling actinides to reduce nuclear waste generation. We also have applied our understanding of reactor physics, thermal hydraulics, and materials behavior to the conversion of fuel in research and test reactors around the world from highly enriched to low-enriched uranium.

Our goals in nuclear engineering are to:

- Lead the emerging Advanced Nuclear Security, Waste and Energy Research (ANSWER) initiative, working with ORNL and Idaho National Laboratory (INL), to position the US as the enduring leader in global deployment of advanced civilian nuclear energy systems through a simultaneous focus on science, technology, and policy to advance non-proliferation, security and waste minimization goals.
- Advance technologies for next-generation reactor and fuel cycle systems, including micro-reactors, in partnership with industry, ORNL, INL, and the National Reactor Innovation Center. This includes evaluating new systems for industrial applications and use with grid storage, complementing DOE's energy storage grand challenge efforts.
- Lead the core design and safety analysis efforts for the Versatile Test Reactor, one of the priority projects of DOE's Office of Nuclear Energy.
- Increase fundamental understanding of nuclear energy materials, processes, and systems to enable their optimal application and development. Argonne is exploring the use of artificial intelligence and machine learning (AI/ML) techniques to correlate neutron damage in reactors to ion damage measurements in accelerator facilities such as ATLAS.
- Develop and validate advanced, mechanistic modeling and simulation capabilities to better predict the performance characteristics and safety behavior of nuclear energy systems, leveraging our broader capabilities in AI/ML and high-performance computing.
- Lead the development of the science and technology basis for limiting proliferation risk from nuclear energy systems, including minimizing the use and availability of highly enriched uranium

This capability supports the missions of DOE and other organizations to sustain the benefits of nuclear energy generation; develop new and innovative nuclear energy systems, including advanced testing facilities that support development of future nuclear systems; and enhance the security of nuclear technology applications worldwide. Current sponsors include DOE/ARPA-E, DOE/NE, DOE/NNSA, DOE/SC-NP, DOD, DHS, NRC, the nuclear power industry, and international organizations.

Nuclear physics

Argonne is a global leader of research in nuclear structure, nuclear astrophysics, fundamental interactions, and hadron physics as well as in the enabling areas of nuclear instrumentation and accelerator development. Our ATLAS user facility is at the cutting edge of discovery science with recent upgrades to deliver a unique capability set. Capabilities include beams of stable isotopes at energies up to 20 MeV/nucleon, radioactive ion beams from the californium rare isotope breeder upgrade (CARIBU), and state-of-the-art instruments such as the helical orbital spectrometer (HELIOS). The recent addition of a radioactive ion separator further increases the availability of intense and clean light radioactive ion beams. These capabilities enable ATLAS users to study nuclear structures that depend strongly on the neutron excess and are not readily apparent in stable nuclei, investigate reactions and nuclear properties far from stability, probe astrophysical processes generating the chemical elements, and test nature’s fundamental symmetries and interactions.

Our physicists are leaders in theoretical and experimental quantum chromodynamics, the foundational force that binds quarks and gluons into protons, neutrons, and nuclei. They design, construct, and operate detectors at Thomas Jefferson National Accelerator Facility (TJNAF) and Fermilab to carry out these investigations. Argonne scientists are principal investigators for a significant number of approved TJNAF 12-GeV experiments. At Argonne, we test the limits of the Standard Model by searching for violation of time reversal symmetry in the electric dipole moment measurement of radium-225.

Argonne’s experimental nuclear physics research is supported by our work in accelerator science and by theory efforts that make use of the ALCF and Argonne’s computational capabilities. We are world leaders in quantum Monte Carlo calculations of nuclear structure and reactions and predictions of hadron and nuclear properties using nonperturbative methods in quantum chromodynamics.

Our nuclear physicists also apply their expertise to address national needs, such as characterization of spent nuclear fuel for reactor design; techniques for producing medical radioisotopes in collaboration with Argonne’s radiochemists; and atom trap trace analysis for geophysics, oceanography, and national security applications. Argonne’s accelerator research and development group supports ATLAS and keeps it at the forefront of accelerator technology. Our expertise and facilities for cavity processing and fabrication are also in high demand to support other accelerators funded by DOE/SC-NP, -HEP, and -BES: our capabilities in superconducting radiofrequency technology, especially for ion accelerators, are unique and complement those of other national laboratories. This support includes the design, fabrication and testing of the bunch-lengthening system for the APS Upgrade.

Ongoing upgrades to ATLAS will provide unmatched critical capabilities to complement the strengths of the Facility for Rare Isotope Beams (FRIB). ATLAS will remain the premier stable beam user facility, providing unique opportunities for rare isotopes research. A proposed multi-user upgrade would simultaneously deliver two beams of different species to separate experiments to address user demand; it also would enable an expanded isotope research and development program at ATLAS.

We continue to work with ATLAS users to identify important new capabilities, such as the neutron-generator upgrade to CARIBU and production of neutron-rich nuclei in the N=126 region, essential for astrophysics and nuclear structure studies. We will continue our leadership role in the science and instrumentation at FRIB, leading the construction of the solenoidal spectrometer apparatus for reaction studies (SOLARIS) and making key contributions to instruments such as the Gamma-Ray Energy Tracking Array and the FRIB Decay Station.

We are also developing leadership roles in new areas by leveraging our strengths in materials science, particle physics, accelerator and hard x-ray science, and advanced computing. For the Electron Ion Collider (EIC) at Brookhaven National Laboratory, our goal is to make major contributions to the science program and the design and simulation of the detectors and accelerator. In quantum science, our physicists are building on our strengths in atom trapping, quantum sensors, and quantum algorithms for nuclear physics to build a program in quantum information science in partnership with materials and computing scientists and leveraging the new capabilities developed by Argonne's Q-NEXT center.

This capability supports the DOE/SC-NP and -IDPRA missions. Other sponsors include DOE/SC-BES and -HEP; IAEA; DTRA; NSF; and universities in the United States and abroad.

Particle physics

Argonne's particle physics program is based on the vision to carry out cutting-edge research while becoming a hub of innovation in new computing, detector, and accelerator technologies. This work distinguishes itself through strong collaborative efforts across Argonne and the DOE complex and with local and other universities.

Since the discovery of the Higgs boson in 2012, the Large Hadron Collider (LHC) at CERN in Switzerland has delivered a large data set and will be upgraded for high luminosity (HL-LHC) operations. Argonne has a balanced research program as a part of the ATLAS experiment at the LHC. Our physics studies focus on beyond-standard-model (BSM) searches and precision standard model measurements. Argonne provides significant support for ATLAS detector operation, software, and computing, with emphasis on using Argonne's high-performance computing resources and machine learning techniques. Finally, Argonne carries out critical HL-LHC upgrade activities, including construction of the new silicon pixel detector and development of the state-of-the-art trigger and the new detector readout systems.

The theoretical high-energy physics program at Argonne focuses on high-precision calculations of standard model processes, interprets experimental data in terms of physics within and beyond the standard model, and makes predictions for experimental searches for BSM physics.

Through the high-energy physics community's Center for Computational Excellence, co-led by Argonne, high-performance computing tools are being developed to ultimately use the power of exascale computing for high-energy physics. First-of-a-kind simulations of LHC particle collisions that were carried out using the ALCF have enabled publication of results from the LHC's ATLAS experiment that would otherwise not have been possible. Our particle theory research, using the ALCF, has provided the most precise theoretical quantum chromodynamics predictions ever for standard model processes, essential to the search for new physics.

Our research in theoretical and computational cosmology provides some of the largest simulations currently available world-wide that capture the evolution of the universe. Argonne researchers play leadership roles in extracting science from current and future cosmological surveys. By developing the Hybrid/Hardware Accelerated Cosmology Code framework and the data analysis library CosmoTools, Argonne has become a leader in extreme-scale, high-resolution cosmological simulations. These computational tools are run at the ALCF and other DOE leadership computing facilities. The tools generate synthetic sky maps that enable construction projects, such as the Cosmic Microwave Background (CMB) Stage 4 experiment and the Legacy Survey of Space and Time, to exercise their data analysis pipelines and provide comparisons with actual observations. Such comparisons give, for example, new insights into the dark sector of the universe. We develop advanced statistical tools to extract science from next-generation cosmological surveys. Our cosmology group also leads an exascale computing project sponsored by DOE/SC-ASCR.

Through a multidisciplinary effort, we deployed, at the South Pole Telescope, the largest focal plane to date of transition edge sensors (TES) for the third-generation experiment to detect anisotropies in the CMB radiation and have taken a leading role in proposing the CMB Stage 4 experiment. Our unique capabilities in engineering superconducting TES arrays are being used to develop ultra-sensitive sensors that could be deployed in next-generation dark matter detectors. We also will draw on existing strengths in superconducting devices for quantum science as part of the Argonne-led Q-NEXT center and collaborations made possible via the Chicago Quantum Exchange.

We also play key roles in the construction of Fermilab’s muon-to-electron-conversion experiment, in parallel with our work on providing the most precise magnetic field map for the muon g-2 experiment. We provided critical engineering support for the protoDUNE long-baseline neutrino detector prototype, now deployed at CERN. Argonne was responsible for delivery of the high-voltage field cage and readout for the photodetectors. Based on this work, we are focusing our scientific and engineering activities on Fermilab’s Long-Baseline Neutrino Facility/Deep Underground Neutrino Experiment (LBNF/DUNE). We have delivered a half-wave cryomodule for Fermilab's Proton Improvement Plan-II project, which aims to produce the most intense high-energy neutrino beam for LBNF/DUNE.

Finally, we use the Argonne Wakefield Accelerator for advanced acceleration research, in synergy with Argonne’s other accelerator science capabilities, to advance the science that will be needed for the next generation collider for particle physics research.

This core capability supports the DOE/SC-HEP mission and is fully aligned with the national high-energy physics roadmap. Additional current sponsors include DOE/SC-ASCR and -BES as well as NASA and NSF.

Systems engineering

We bring together multiple engineering disciplines to integrate science discoveries into technological solutions that strengthen the U.S. energy, environmental, and security portfolio and enhance economic competitiveness. We develop experimental facilities, systems engineering methods, and analytical tools to advance understanding of complex systems such as urban environments, communications, transportation, critical infrastructure, and other large-scale systems. Our work also draws on Argonne’s core capability in decision science and analysis.

Our systems engineering research allows us to make major contributions to the nation’s development of future transportation systems. For example, we:

- Assess dynamic transportation system changes at scale to understand new mobility technologies, connectivity and automation, user decisions, and business model evolutions using POLARIS, our high-fidelity agent-based transportation system model.
- Develop and deploy energy-efficient connected and automated vehicle and powertrain control algorithms enabled by knowledge of the environment, using our RoadRunner framework and Argonne methodologies such as Vehicle-in-the-Loop.
- Evaluate the emerging technology of electric aviation for performance requirements, using our Aeronomie simulation tool.
- Compare millions of propulsion and vehicle technologies to quantify energy consumption, performance, and cost impacts with our Autonomie simulation tool, supplemented with

experimental validation at our Advanced Mobility Technology Laboratory, supported by internal investments in our mobility facilities.

- Study and promote decarbonization strategies for engine combustion and fuels to gain larger efficiency and emissions benefits with experimentation and predictive combustion phenomena modeling.
- Apply expertise, hardware, and tools to advance electrification and grid integration at the Argonne EV-Smart Grid Interoperability Center and facilitate integrated communication and control of the electric vehicle charging infrastructure, distributed energy resources, and storage to enable smart charge management and grid resilience.

Argonne also develops analytical and modeling tools, including advanced computational algorithms, to drive engineering improvements in our nation's electrical infrastructure in partnership with industry, academia, and government agencies. Advanced computing at the ALCF, coupled with machine learning and artificial intelligence, is a core component of our systems engineering and integration work, including high-fidelity modeling of electric power grid systems, critical infrastructures, the mobility ecosystem, and engine combustion kinetics. We also develop next-generation computational fluid dynamics code called Nek5000 for predictive engine simulations.

We apply the imaging capabilities of the APS to understand structure and processes in materials and chemistries, such as complex flows in engineered systems. For example, we use the APS to study fuel-injector spray dynamics and combustion chemistry in engines and use the results to improve computational models for multiphase flows.

We have created a spectrum of system engineering methodologies and tools focused on analysis, design, experimentation, and computation that enable us to model security, risk, and resilience for critical infrastructure systems. These resources help analysts study infrastructure interdependencies, evaluate connections within and across networks, and simulate complex scenarios of infrastructure service disruptions. We apply our geospatial, engineering and computer science expertise to build models that predict operational degradations of infrastructure, understand when and how these failures could cascade, and estimate how disruptions could affect the communities and institutions that depend on them.

We use our system engineering competence to boost U.S. manufacturing job creation through our ongoing collaborations with industrial partners. Argonne also manages the DOE/EERE Advanced Vehicle Technology Competition, which is an engineering workforce pipeline for university students.

This capability supports the missions of DOE, DHS, other federal agencies, and industry. Current DOE sponsors include DOE/EERE, DOE/NE, and DOE/OE. Current DHS sponsors include the Federal Emergency Management Agency and the Cybersecurity and Infrastructure Security Agency. Current strategic partners include DOD, DOS, DOT, NERC, NGA, state and local departments of transportation, municipal planning agencies, and businesses such as Cummins, Exelon, Ford, and General Motors.

Science Strategy for the Future / Major Initiatives

Argonne's strategy for the future will establish new research strengths and extend our impact in the world. We will execute this strategy through our major initiatives, core research programs, user facilities, and multi-institution centers. UChicago Argonne, LLC, will support our strategy through seed funding of new research directions under the Joint Task Force Initiative.

Our five DOE Office of Science user facilities are integral to our overall strategy:

- Advanced Photon Source (APS), now being upgraded to transform researchers' ability to explore diverse forms of matter using hard x-rays

- Argonne Leadership Computing Facility (ALCF), soon to be home to the Aurora exascale supercomputer
- Argonne Tandem Linac Accelerator System (ATLAS)
- Atmospheric Radiation Measurement Southern Great Plains (ARM-SGP) climate observatory
- Center for Nanoscale Materials (CNM)

Also key to our strategy are the five major multi-institution collaborations that we lead for DOE: the Advanced Materials for Energy-Water Systems center, Joint Center for Energy Storage Research, Midwest Integrated Center for Computational Materials, and Q-NEXT quantum information science center, all supported by DOE/SC, and the ReCell advanced battery recycling center, supported by DOE/EERE.

Infrastructure

Argonne Facilities and Infrastructure

Argonne's main campus in Lemont, Illinois, a suburb of Chicago, is stewarded by DOE/SC. The average age of Argonne-operated facilities and infrastructure is 51 years, with 64% of the assets being more than 50 years old. Our facilities are roughly 85% occupied. Tables 6.1, 6.2, and 6.3 summarize the type and condition of Argonne's facilities and utilities.

In addition to buildings operated by Argonne, the campus includes the Howard T. Ricketts Regional Biocontainment Laboratory, operated by UChicago, and the Theory and Computing Sciences Building, a privately operated building in which we currently lease 330,468 sq ft. In FY20, Argonne entered into a new lease for 100,719 sq ft of multi-use space in nearby Woodridge, Illinois, in support of the Advanced Photon Source Upgrade (APS-U). To enable Argonne's second location in Chicago, we licensed 20,000 sq ft of space from UChicago in FY20. In FY21, we leased about 18,000 sq ft of space in nearby Bolingbrook, Illinois, to support the Radiological Assistance Program's move into different off-campus space.

We reduce operational risks by focusing investments on substandard support infrastructure and utilities, which account for most of our deferred maintenance (DM). Despite steady investments in infrastructure, we carried $101 million in DM costs in FY19 and $109 million in FY20. In FY20 we completed our five-year cycle of Condition Assessment Surveys (CAS) for all our facilities. We expect to begin seeing a reduction in DM for FY21 compared to FY20, due to targeted investments aligned with our campus strategy. In FY19, we extensively evaluated DM and created a comprehensive ten-year strategy to significantly reduce it. Meaningful, large-scale investments such as the Argonne Utilities Upgrade project are crucial to our strategy for greatly reducing DM. Executing Argonne's Excess Facilities Plan and reinvesting the savings associated with nuclear facility and waste reductions would enable us to eliminate current and future DM. We identify these risk-reduction measures in our ten-year campus modernization plan – entitled *Facility and Infrastructure Strategic Investment Plan*, which aligns with the Annual Laboratory Plan and details our intended facility operations funding portfolio.

Campus Strategy

Overview of 10-year modernization plan

Our vision for the future is driven by a foundational goal of resilient, sustainable facilities and infrastructure to enable mission readiness both during regular operations and under off-normal circumstances. The 10-year modernization plan establishes a roadmap for achieving this vision, with investments aligned to support key research program drivers and position Argonne to prepare for, adapt to, withstand, and rapidly recover from events that affect our facilities and infrastructure.

We saw the positive impact of our infrastructure planning during the COVID-19 pandemic, as we smoothly transitioned from minimum safe operations in March 2020 to limited operations in June 2020 and continued construction projects without interruption. The unprecedented levels of telecommuting in our workforce since March 2020 have led us to begin to investigate the interest in and potential campus impacts of long-term telework by a significant portion of the Laboratory population. Our 30-year planning efforts are considering expanded technology platforms to accommodate remote work and the impacts on facilities. Any potential reduction in on-site work creates a need to identify modern space planning opportunities within buildings and further evaluate vacant and inadequate facilities for shutdown, removal, or reuse. Our 10-year campus modernization plan further explores these emerging workforce trends in visioning the laboratory of the future.

Four main principles guide our campus infrastructure strategy to assure current and future mission readiness: (1) support Argonne's science strategy, (2) construct replacement facilities and complete targeted renovations, (3) repair and modernize support infrastructure, and (4) eliminate legacy waste and excess facilities. Two cross-cutting goals apply to all our infrastructure improvements: strengthen resiliency and increase sustainability.

Our resilience planning establishes campus-specific performance goals for our infrastructure portfolio and mitigating gaps in performance and event recovery time with planned investments. We are investing in artificial intelligence (AI) and machine learning (ML) to drive resilience by optimizing and automating utility, facility, and maintenance operations where feasible. This investment will help us reduce deferred maintenance by making the most effective use of limited resources for maintenance. Execution of the 10-year modernization plan will lead to Argonne's first phase of AI-enabled operations for infrastructure. That plan provides a strategy to reduce deferred maintenance while improving facilities and infrastructure resilience. Section 6.3 provides more information on Argonne's AI for Operations initiative.

Our sustainability strategy is described in Sec. 6.4. We intend to build on our sustainability accomplishments to date to move Argonne toward net-zero carbon by 2035 and serve as a model for place-based decarbonization.

We take an integrated planning approach to establish a comprehensive portfolio of facility needs, align necessary investments, and complete projects within specific timeframes to meet Argonne's science strategy and support foundational investments. Our 10-year infrastructure investment plan includes estimated total capital investments in buildings and utility systems across the Argonne campus of $985 million between FY21 and FY32, consisting of:

- $294 million in Argonne indirect funds
- $400 million in DOE funds (line items, program funds, scientific laboratories infrastructure [SLI], and general plant projects [GPP])
- $176 million in DOE/EM clean-up funds
- $115 million in State of Illinois funding

We will also maintain our robust operations maintenance and repair program with planned spending of $642 million during that period.

Site Sustainability Plan Summary

Argonne's sustainability program is an integral part of our campus strategy, leading efforts to meet DOE's sustainability and resilience goals. Our investments focus on optimizing and upgrading infrastructure, engaging the Laboratory community, and institutionalizing sustainability at Argonne. We leverage synergies that benefit multiple sustainable goals and support overall repair needs and deferred maintenance.

We are developing a strategy for achieving net-zero carbon emissions by 2035, starting with a detailed computer model of our energy use in buildings, utilities, and transportation activities. To date, we have identified a high-level, viable pathway to reduce energy demand and decarbonize our energy sources, in a collaboration between our scientific and operations staffs. Over the next year, we will develop an implementation plan that outlines the sequence of activities and funding needed to achieve our net-zero goal. Argonne's diverse building stock, energy-intensive research facilities, and central utility systems, all within a three-square-mile secure campus, provide an ideal setting to pilot local decarbonization and serve as a model for place-based solutions.

To support our emission-reduction strategy, we propose three new SLI-GPP projects that would reduce emissions from heating and cooling. Two of these projects would install waste heat recovery systems based on conceptual designs completed in FY20, for the 200 and 400 Areas, at a cost of $3.8 million in FY22 and $6.9 million in FY24. The third would optimize heating and cooling in Buildings 202, 203, and 362 in support of the Smart Labs Program, at a cost of $12 million in FY23.

Our sustainability efforts reach every corner of the laboratory. FY20 accomplishments included the following:

- *Increased efficiency and promoted safety with Smart Labs Program*. We initiated development of a Laboratory Ventilation Management Plan and identified $101,600 per year in heating, cooling, and ventilation savings with a ventilation and chilled-water assessment of Building 202.
- *Increased the number of accredited sustainable buildings with completion of the Materials Design Laboratory (MDL).* The MDL is our 17th building that meets *Guiding Principles for Sustainable Federal Buildings* (Council of Environmental Quality, 2016) and the sixth that is Leadership in Energy and Environmental Design (LEED) certified. We have now documented 23% of our buildings as meeting the *Guiding Principles*, exceeding the DOE goal of 15%.
- *Reduced cost of operating and maintaining facilities.* We completed 14 energy- and water-savings projects, adding $121,901 in annual savings to Argonne's portfolio of implemented efficiency projects. We continue to use energy-savings performance contracts to improve infrastructure efficiency and resilience. Efficiency measures are also incorporated into modernization, maintenance, and repair projects funded by Argonne.
- *Identified carbon savings projects and improved resilience through comprehensive planning.* We completed conceptual designs of two waste heat recovery systems: a system in Building 450 that would save about $240,000 per year and provide nearly 55% of the annual APS heating load and a system in the 200 Area that would provide heat for Buildings 241 and 242, resulting in $250,000 in annual energy savings and a 36% reduction in carbon emissions. We also developed an infrastructure resilience strategy that seeks to improve performance before a hazard event and reduce the time needed to recover from disruption.
- *Were recognized for sustainability excellence.* DOE recognized Argonne with an Accelerating Smart Labs Award for our participation in the Better Buildings Smart Labs Accelerator Program

and our quick adoption of best practices to enhance safety, efficiency, and operation of Laboratory buildings. The U.S. EPA also recognized Argonne with a Federal Green Challenge Award for electronics power management, waste diversion through composting, and water management through five acres of natural habitat restoration at the old coal yard site.

Argonne’s sustainability program plays an integral role in our AI-Ops initiative. In FY20, we fully implemented operational efficiency software in Buildings 200 and 401. We are using the software’s analytic tools to identify facility system improvements and predict maintenance needs and savings achieved from completed efficiency projects. Next steps include developing machine-learning algorithms and leveraging other data to automate system optimization and maintenance efforts. Our AI-Ops initiative for infrastructure will improve system resilience and support long-term sustainment of our efficiency investments.

BROOKHAVEN NATIONAL LABORATORY

Lab-at-a-Glance

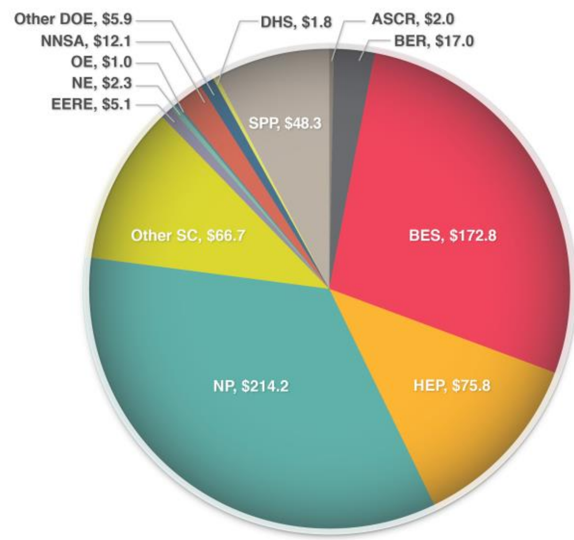
Location: Upton, New York
Type: Multi-program Laboratory
Contractor: Brookhaven Science Associates
Site Office: Brookhaven Site Office
Website: www.bnl.gov

- **FY 2029 Lab Operating Costs:** $625.1 million
- **FY 2019 DOE/NNSA Costs:** $575 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $48.3 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 8%
- **FY 2019 DHS Costs:** $1.8 million

Physical Assets:
- 5,322 acres and 314 buildings
- 4.8 million GSF in buildings
- Replacement Plant Value: $5.95 B
- 161,002 GSF in 28 Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:
- 2,502 Full Time Equivalent Employees (FTEs)
- 137 Joint Faculty
- 159 Postdoctoral Researchers
- 203 Graduate Student
- 183 Undergraduate Students
- 3,473 Facility Users
- 1,075 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

Brookhaven National Laboratory's (BNL) vision is to produce discovery science and transformative technology to power and secure the Nation's future. The Lab's mission is to deliver expertise and capabilities that drive scientific breakthroughs and innovation for today and tomorrow.

Primarily supported by the U.S. Department of Energy's (DOE) Office of Science, Brookhaven Lab is a multi-program laboratory with seven Nobel Prize-winning discoveries and more than 70 years of pioneering research. Established in 1947, BNL brings unique strengths and capabilities to the DOE laboratory system and is the only multi-program Laboratory in the Northeast. BNL carries out its mission safely, securely, and environmentally responsibly, with the cooperation and involvement of local, state, national, and international communities.

With a long-standing expertise in accelerator science and technology, BNL conceptualizes, designs, builds, and operates major scientific facilities in support of its DOE mission. These facilities serve DOE's basic research needs and reflect BNL/DOE stewardship of national research infrastructure critical for university, industry, and government researchers, including in response to national emergencies, e.g., recent COVID-19 research. Despite the pandemic, the Relativistic Heavy Ion Collider complex, the National Synchrotron Light Source II, the Center for Functional Nanomaterials, and the Accelerator Test Facility served close to 3500 scientists in FY 2020.

BNL is managed by Brookhaven Science Associates (BSA), a partnership between Stony Brook University and Battelle, and six core universities: Columbia, Cornell, Harvard, MIT, Princeton, and Yale. Stony Brook and Battelle work together to advance BNL's strategic initiatives, from basic research to the commercial deployment of technology. BSA and its partners underpin BNL's growing impact in the Northeast, especially its vital relationship with New York State.

Core Capabilities

Fifteen existing and two emerging core technical capabilities underpin all activities at Brookhaven National Laboratory (BNL). Each one is comprised of a substantial combination of facilities, teams of people, and equipment that has a unique and often world-leading component and relevance to national needs, as well as to the education of the next generation of scientists from grades K – 12 through graduate school. They arise from long-standing strengths (and synergies) in fundamental nuclear and particle physics, in energy, environmental, and data sciences with applications to current day problems, in developing and operating major user facilities, and in targeted applications in national security. These core capabilities enable BNL to deliver discovery science and transformative technology that is relevant to the Department of Energy (DOE)/Department of Homeland Security (DHS) missions. All together, they make BNL unique.

In FY 2020, BNL was assigned two new core capabilities in Computational Science and Applied Mathematics that were previously "emerging." This year, BNL is proposing two additional emerging core capabilities. The first, in Nuclear Engineering, encompasses the Lab's strengths in three major areas: Materials for Nuclear Energy Applications, Nuclear Systems and Structural Analysis, and Nuclear Data. The second is in Power Systems and Electrical Engineering, where BNL conducts research to advance the deployment and grid integration of renewable energy systems and the development of new technologies to enable the next generation smart grid

Accelerator Science and Technology

BNL has long-standing expertise in accelerator science and technology development that has been exploited in the design of best-in-class accelerators, beginning with the Cosmotron in 1948, to today's Relativistic Heavy Ion Collider (RHIC) and National Synchrotron Light Source II (NSLS-II). The Laboratory is now preparing for Critical Decision 2 (CD-2) for the Electron-Ion Collider (EIC) and is focused on developing an upgrade program for NSLS-II to provide major increases in brightness for its user community. The Accelerator Test Facility (ATF) provides a platform for development of advanced accelerator concepts that will deliver new capabilities to serve the nation's needs. Many widely-used technologies were developed at BNL including the strong-focusing principle and the Chasman-Greene lattice, which were transformational developments for modern accelerators and synchrotron light source facilities, respectively. Each of the Laboratory's accelerator facilities focus on delivering accelerator performance that exceed the current state of the art.

NSLS-II continues to provide reliable, high-brightness beams for its user community. An ongoing accelerator improvement plan will deliver another factor of 1.8 in brightness above today's levels. Looking to the future, the NSLS-II team and its user community are identifying the most compelling decadal science needs and the potential source upgrades required to address them, as discussed in section 4.2.4. Supported by BNL's Laboratory Directed Research and Development (LDRD) program, NSLS-II has established several upgrade options that would provide a 10-fold increase in brightness at 1 keV and 100-fold increase at 10 keV. This large leap in performance will be enabled by a new concept of magnetic optics developed at NSLS-II. The Complex Bend concept provides a compact ring magnet design to deliver ultra-high brightness radiation sources. Implementation of this concept can be accomplished via an R&D program in collaboration with other U.S. light source facilities and the Magnet Division (MD) at BNL. These accelerator R&D highlights were summarized in a proposal submitted to DOE earlier this year.

The EIC will provide the microscope that lets scientists explore how the properties of matter arise out of the fundamental constituents and forces of Quantum Chromodynamics (QCD). The project is currently ramping up with the strong engagement of Jefferson Laboratory and other participants in the accelerator design. BNL's core strengths in hadron cooling, superconducting radiofrequency (SRF), energy recovery linac (ERL) technology, and high-brightness electron storage rings provide a strong foundation for delivering the EIC. The project also draws heavily on the RHIC hadron beam complex, which continues to produce unique measurements for the nuclear physics community. Current RHIC operations focus on providing low-energy collision data to understand the phase transition between the protons and neutrons present in the matter around us into free quarks and gluons. This experimental campaign relies on the bunched-beam cooling techniques developed and commissioned by the Low Energy RHIC electron Cooling (LEReC) project, which is currently delivering outstanding luminosity using collisions of gold ions. LEReC represents one of numerous fundamental accelerator advancements that have been achieved as part of the RHIC program. Over its history, RHIC has achieved nearly 50 times design luminosity in Au+Au collisions through the rapid implementation of cost-effective and novel stochastic cooling for high-energy bunched beams. RHIC accelerator physicists pioneered acceleration of spin-polarized proton beams to high energy using Siberian snakes, thus making RHIC the only machine capable of exploring the polarization of quarks and gluons inside the proton. The RHIC injector complex also supports a broad range of secondary beams for users and applications at the Tandem Van de Graaff, NASA Space Radiation Laboratory (NSRL), and the Brookhaven Linac Isotope Producer (BLIP). RHIC accelerator physicists also support the Lab's Medical Isotope Research Program (MIRP).

BNL's MD, which is now part of the Laboratory's newly formed Advanced Technology Research Office (ATRO), played a central role in the early development of superconducting magnets for high-energy colliders, thus enabling RHIC construction. The excellent performance of the MD-supplied ring magnets directly contributed to the success of the RHIC physics program. The MD contributed to key RHIC advances through the helical coil magnets it provided for the polarized proton program and the precision solenoids it built for the RHIC electron lens system. A unique capability is its computer-driven "direct wind" technology – a specialized resource that has produced complex multi-function magnets for the interaction regions of colliders world-wide. This capability has also provided the unique magnet capabilities needed for recent measurements on antimatter by the ALPHA experiment based at CERN. The MD delivered magnets for the Large Hadron Collider (LHC) at CERN and continues to have a major role in constructing and testing magnets for the High Luminosity Upgrade of the LHC. Work at the MD to develop conductor and magnets for very high field magnets based on high-temperature superconductors is supported by the U.S. Magnet Development Program and supports the long-term needs of the world-wide high energy physics community. The MD's cable test capabilities are also in regular use by the compact fusion reactor community as well as conductor manufacturing companies. The MD is growing a strong partnership with the green energy sector in addition to supporting Laboratory efforts for the EIC project and the NSLS-II upgrade.

The ATF, also now part of ATRO, is the flagship user facility of the DOE Accelerator Stewardship Program in the Office of Accelerator R&D and Production (ARDAP). It supports a broad range of user-driven research in beam physics, novel radiation sources, and advanced accelerator technology and provides hands-on training for next-generation accelerator physicists. A unique feature is its combination of high-power pulsed lasers and high-brightness electron beams, which can be used individually or in combination. ATF's long wavelength infrared CO_2 laser system recently demonstrated five-terawatt operation in a single 2.3 picosecond pulse. Further planned upgrades to deliver sub-picosecond pulses with peak powers well over 10 terawatts, together with its electron beam capability, will enable a world-class research program in laser-matter interactions and plasma-based acceleration of electron and ion beams. The ATF also supports R&D towards improved MeV-class ultrafast electron diffraction (UED) and new ultrafast electron microscopy (UEM) capabilities.

BNL's strength as a world-class accelerator laboratory provides the foundation of the Lab's and DOE's research programs. The Lab is pursuing stronger integration of its Accelerator Science and Technology (AST) efforts across directorates to foster cross-fertilization of the R&D efforts for an EIC with R&D at the ATF and R&D for advanced synchrotron light sources. AST drives, both internally and externally, the projects currently envisioned to sustain the Laboratory. This includes collaboration with industry and academia on topics such as improved ion beam therapy facilities and the demonstration of a prototype multi-pass high-current ERL with large energy acceptance. BNL's AST efforts are closely integrated with developing the future leaders of the field through mentoring of students, lectures at leading universities, engagement with the joint BNL-Stony Brook University (SBU) Center for Accelerator Science and Education (CASE), and, most recently, the establishment of the Ernest Courant Traineeship in the Accelerator Science and Technology program. Roughly ten Ph.D. students conduct accelerator research at BNL under the auspices of CASE.

The Offices of Nuclear Physics (NP), Basic Energy Sciences (BES), High Energy Physics (HEP), as well as DOE's newly formed Office of Accelerator R&D and Production are the primary DOE sources of funding for AST. Additional funding is provided by SBU, the New York State Energy Research & Development Authority (NYSERDA), Laboratory Discretionary Funds, and partnership engagements with other government agencies and industry.

Advanced Computer Science, Visualization & Data

BNL science is defined by the operation and support of data-rich experimental, observational, and computational facilities, such as RHIC, ATLAS, the planned EIC, Belle II, NSLS-II, the Center for Functional Nanomaterials (CFN), cryogenic Electron Microscopy (cryo-EM), the Systems Biology Knowledgebase (KBase), U.S. Lattice Quantum Chromodynamics (USQCD) collaboration, and the Exascale Computing Project (ECP). Driven by their requirements, BNL has long-standing research, development, and operational programs in advanced computer and data science methods, applied mathematics, algorithms, tools, and infrastructures — making it one of the largest data science Labs in the DOE complex.

BNL operates one of the top ten archives in the world, with over 200 PB of actively managed data and 800 PB annually analyzed. Data traffic has reached up to 10 PB/month from data centers across the world and continues to grow as new facilities reach maturity. Data processing is supported by a variety of high-throughput and high-performance compute resources, amounting to ~6 PF of compute capacity, supported by 90 PB of disk capacity. BNL provides these capabilities 24/7 with 99.5% guaranteed availability.

A core focus of BNL's Computational Science Initiative (CSI) is the continued research and development of novel, extreme-scale data analysis paradigms that support discovery at research facilities.

CSI has built an extensive research program in machine learning (ML) and artificial intelligence (AI) that focuses on scalable, robust, and streaming ML algorithms beyond deep learning, including causal analysis, manifold learning, and natural language processing. The program integrates computer science, applied mathematics, and domain knowledge to develop new ML libraries (e.g., ECP ExaLearn and the Office of Advanced Scientific Computing Research [ASCR]-funded extreme scale spatio-temporal learning, the Scientific Discovery through Advanced Computing (SciDAC) Institute for Computer Science and Data - called RAPIDS), and Exascale Privacy Preserving AI (ExaPPAI). This program is complemented by research into AI explainability and reproducibility, using visual analytics, mathematical concepts, and provenance. These capabilities are utilized in a broad portfolio of projects supporting the Offices of Biological and Environmental Research (BER), BES, HEP, Electricity (OE), Energy Efficiency and Renewable Energy (EERE), the National Nuclear Security Administration (NNSA), and other sponsors, and in support of BNL facilities/programs, such as NSLS-II, CFN, cryo-EM, the Deep Underground Neutrino Experiment (DUNE), LHC-ATLAS, and RHIC.

The AI and ML program is supported by CSI's research into programming models, runtime systems for ML, and new performance portability approaches that provide a capability to enable the effective use of novel architectures. CSI researchers are developing programming models that allow code developers to test different optimization strategies quickly to help reduce overall development time. An associated effort is providing scientific users with an application layer agnostic of the hardware details, allowing for the use of as many computing resources as are available to maximize scientific productivity. Compiler optimization for performance portability improves the state of the art by finding quality transformations that achieve superior or equal computational performance. This work automatically transforms code to optimize for locality and parallelism (e.g., ECP SOLLVE) and allows developers to concentrate on the core science.

Many computational science applications today are run as part of complex workflows, rather than as classic standalone applications. CSI is advancing a "building block" approach to workflows and data-intensive software systems known as RADICAL-Cybertools. These allow for different points of integration with existing workflow tools, which eliminates some of the reasons for workflow systems proliferation. Building blocks facilitate performance portability and optimization of workflows/workflow systems. The tools were researched and tested in a number of projects, such as the ECP CANDLE and ExaLearn and the ASCR Production and Distributed Analysis (PanDa) for ATLAS. RADICAL-Cybertools are also used as the workhorse of the National Virtual Biotechnology Laboratory (NVBL) therapeutics response to the coronavirus disease of 2019 (known as COVID-19), creating some of the most scalable and sophisticated discovery pipelines, as well as for AI-driven multi-scale High Performance Computing (HPC) workflows, including the winner of the Association for Computing Machinery's Gordon Bell Prize for COVID-19. Recognizing the importance of workflows as an exascale programming model, and necessary building-blocks for workflows, the ECP initiated Phase II of the ExaWorks project, for which the CSI serves as the co-lead. The work is complemented by joint research with the University of Oregon on real-time workflow performance analysis and recall as part of the ASCR Integrated Product and Process Development (IPPD) and the ECP Co-Design Center for Online Data Analysis and Reduction at the Exascale (CODAR) project.

In a growing collaboration with the Instrumentation Division, CSI is delivering a comprehensive research program focused on testing and exploration of novel devices and architectures and their suitability for data-intensive workloads in open science and national security. The research includes development of edge computing devices and processors (e.g., neurotrophic chips); novel architecture testbeds for high-end computing and experiments; design space exploration for materials, devices, and systems for data-intensive computing via measurement and performance modeling; and development of new methodologies and tools for performance, power, and reliability modeling. Areas under investigation or active planning also include optical networks, specialized architectures for ML, quantum computing, and quantum networking.

The primary sources of funding are from ASCR, HEP, NP, BES, BER, OE, EERE, NNSA, New York State, Other Government Agencies (OGA), and Laboratory Discretionary Funds.

Applied Materials Science and Engineering

BNL engages in a broad range of activities related to energy storage and the electric grid, including materials synthesis, characterization and functional electrochemical evaluation, high energy density cell technology, evaluation of thermal stability and functional limits of battery materials, fundamental studies of charge and discharge mechanisms and the associated material-structure evolution, as well as irradiation services.

BNL has established expertise and capabilities for in situ characterization of energy storage materials by X-ray methods. New approaches for probing the mechanisms under operando conditions are being developed and demonstrated where spatio-temporal measurements with enhanced resolution are now possible. The advances in characterization are enabling understanding of the fundamental mechanisms under steady state conditions, and into the kinetics of functioning systems. Integrating these studies with electron microscopy provides additional structural insight. BNL is applying its expertise and capabilities as a partner in the Battery 500 consortium to develop practical lithium-ion battery cells with 500 Wh/kg energy density, more than double current commercial cells.

BNL continues to build its portfolio of electric grid research projects and has become an important player in performing research to enable grid modernization. BNL's research focuses on the deployment and grid integration of renewable energy systems and the development of new technologies to improve the resilience and reliability of the next generation smart grid. Two of the key areas studied are the application of energy storage systems to address the challenges of increased penetrations of renewable energy generation, and grid simulation and modeling to develop and evaluate innovative new control and operational technologies for grid modernization. BNL has significant expertise in power system modeling and simulation, as well as in transmission and distribution system design, operation, and planning, which can be used to analyze such systems and determine their appropriate use as solutions for grid integration of renewable generation. BNL also has capabilities for the development of control algorithms that can be applied to the operation of energy storage systems for applications to renewable integration.

BNL has capabilities to study materials in extreme environments for nuclear applications. BNL has developed a specialized robotic system at NSLS-II for the rapid characterization of radioactive materials, such as samples of pressure vessel steel and nuclear fuel. BNL is using this capability to provide industry with unique information on the performance of advanced materials for nuclear applications. BNL has also developed and continues to develop a unique suite of environmental cells for the in situ characterization of reactor materials and molten salt samples that are air and water sensitive, highly corrosive, and at high temperature. These cells are used to gain new insights on accelerated corrosion of advanced cladding materials for nuclear applications. In addition, BNL has installed X-ray diffraction computed tomography at the X-ray Powder Diffraction beamline at NSLS-II, which enables three-dimensional (3D) imaging of the microstructure of engineering-scale samples.

As part of the RaDIATE international collaboration, the 200 MeV proton beam of the Linac and the BLIP target facility are used extensively to investigate radiation damage by high-intensity proton and neutron beams of beam collimators, beam windows, and high-power targets.

The primary sources of funding are: BES, the EERE Vehicle Technologies Program, OE, the Office of Nuclear Energy (NE), New York State, and Laboratory Discretionary Funds.

Applied Mathematics

Over BNL's long history of achievements in experimental physics , BNL's mathematics research traditionally has focused on areas distinctly relevant to HEP, NP, synchrotron science (BES), and accelerator physics. In the 1970s, Brookhaven pioneered the first numerical simulations of quantum field theory that paved the way for the huge success of applying lattice QCD methods to predict properties of fundamental particles in nature. Along the way, novel numerical methods were developed, including improved linear and eigensystem solvers, smart Monte Carlo sampling methods, and error-reduction techniques. From the 1990s through the mid-2000s, Brookhaven researchers made significant distinct mathematical contributions to areas such as magnetically confined fusion, accelerator physics, peta- and tera-scale simulation tools, diesel injector design, nuclear fission reactors, and multiphase flows. Through the mid-2000s, Brookhaven also maintained a significant uncertainty quantification (UQ) capability that influenced many UQ efforts within the NNSA and subsequent DOE-sponsored ASCR and SciDAC programs.

Applied math continues to be essential to all BNL science. Since its inception, CSI has rebuilt a distinct applied math research program aligned with the changing needs of the BNL science directorates and DOE. As a result, in 2020, BNL was formally awarded a core capability in Applied Mathematics. This effort is focused on the specific needs of its constituent user community; CSI is emphasizing: 1) optimal experimental design under uncertainty and broader optimization of complex systems under uncertainty; 2) multiscale modeling that addresses the bridging of scales and integration of data and simulation. Initial focus areas are nuclear physics, climate, and chemical processes; and 3) applied math for scalable AI and machine learning that will provide key foundations needed for BNL's AI research program. An added focus will involve exploring how to achieve AI explainability through foundational applied mathematics work.

BNL is pursuing a new effort that integrates all of the above topics – namely Optimal Decision Making and Experimental Design in Multi-Stage, Multi-Fidelity Automated Scientific Workflows. This effort aims to address applied mathematics and scientific computing challenges that arise when seeking to automate discovery science for grand challenge DOE mission problems. Challenges in developing optimally designed and automated scientific workflows lie at the intersection of multiple computational and applied mathematics fields, including decision theory, operations research, UQ, model reduction, and scientific machine learning. BNL is concentrating on the setting where the workflow takes the form of multiple computational stages, potentially feeding outputs from one stage to inputs of another in a directed graph structure, with options to acquire additional simulation or experimental data at multiple fidelities and modalities. BNL scientists are developing a solid mathematical formulation for the optimal design and operation of such multi-stage, multi-fidelity workflows. BNL aims to model the flow of information, uncertainties, and dependencies between a heterogeneous set of interconnected processes, and to globally co-design an end-to-end workflow that uses such models to make decisions about what information to acquire and which resources to allocate in a resource-constrained setting. The expected project outcomes will have direct impact on diverse scientific computing applications driven by DOE HPC facilities, including design of novel functional materials, climate predictability and resiliency, drug discovery, and many others.

The Lab is a partner in ASCR's new Mathematical Multifaceted Integrated Capabilities Center, called Advances in Experimental Design, Optimal Control, and Learning for Uncertain Complex Systems (AEOLUS). The Center works toward a unified optimization-under-uncertainty framework for learning predictive models from data and optimizing experiments, processes, and designs — all in the context of complex, uncertain systems. Further, BNL leads the BER Optimal Experimental Design of Biological Systems project and partners with the CFN and NSLS-II in an LDRD project, which develops new optimal experimental design concepts in autonomous systems. BNL also serves as lead of ECP's co-design center, ExaLearn, which is cultivating and deploying exascale machine learning technologies. These include deep neural networks; reinforcement learning algorithms; and ensemble, kernel, and tensor methods. Some features of the ML methods being developed in ExaLearn include explainability and UQ. CSI has also extended its BNL collaborations to include researchers at the Nuclear Physics facilities RHIC and EIC.

Support comes primarily from ASCR, BER, New York State, and Laboratory Discretionary Funds.

Biological Systems Science

The goal of BNL's program is to develop a systems-level understanding of complex biological processes relevant to the DOE mission with respect to energy and the environment. BNL's expertise creates and integrates computational and experimental platforms. These generate and test hypotheses using approaches that include molecular biology, biochemistry, structural biology, computation, imaging, and metabolic engineering. Ultimately this work will lay the foundation for desired manipulations of growth rates, biomass accumulation, resistance to stresses, and the accumulation of desired feedstocks for bioenergy and bioproduct production in organisms relevant to the BER mission. This program is synergistic with programs in physical biosciences (funded by BES, Core Capability [CC] 6).

BNL's Quantitative Plant Science Initiative (QPSI) Science Focus Area addresses the grand challenge of "Enabling predictive biology" by accelerating the discovery of gene and protein function. The initial focus of QPSI is on genes that contribute to micronutrient resilience for the design of high-yielding, low-input bioenergy crops for growth on marginal lands. A genotype-to-phenotype discovery platform enables genome-wide screening to define the roles of genes in metal homeostasis. This capability is synergistic with integrated multi-omics approaches that make extensive use of BER genome resources in poplar and sorghum. QPSI staff collaborates with researchers at Argonne National Laboratory, the University of Wisconsin-Madison, and Cold Spring Harbor Laboratory to execute its science plan. QPSI makes use of the world-leading structural/imaging and analytical capabilities of NSLS-II and the CFN, and the computational capabilities of CSI to probe molecular structure and dynamics. Using NSLS-II, cryo-EM, and fluorescence resonance energy transfer, BNL researchers will perform structural analysis on complex biological systems at scales ranging from angstroms to the whole plant level.

The bioinformatics and computational biology capabilities are integral to the BNL biological systems science program and the data from these efforts contribute to KBase development (led by Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories).

BNL also contributes to two Bioenergy Research Centers, i.e., the Center for Advanced Bioenergy and Bioproducts Innovation (CABBI) and the Joint BioEnergy Institute. For both centers, BNL's efforts are focused on reducing lignin content of bioenergy crops to increase their saccharification efficiency. Within CABBI, the Lab's effort is principally devoted to developing strategies to accumulate triacylglycerols (TAG) i.e., oil in the stems of sugarcane, miscanthus, and sorghum.

In addition, BNL participates in three Biosystem Design projects: Systems biology With Increased TAG in Chromochloris zofingiensis (SWITCh) led by Berkeley; the Biological Design of Lemnaceae aquatic plants for biodiesel production led by Cold Spring Harbor Laboratory, and the Renewable Oil Generated with Ultra-productive Energycane (ROGUE) project led by the University of Illinois at Urbana-Champaign.

BNL researchers are also partnering in the newly initiated Systems Biology For Sustainable Bioenergy Crop Development program in Enhancing Camelina Oilseed Production with Minimum Nitrogen Fertilization (ECON) led by Montana State University.

Researchers at NSLS-II work closely with members of the Biology and Physics Departments and the CSI on the Quantum Enabled Bioimaging and Sensing Approaches to Bioenergy program for the development and use of a Quantum Enhanced X-ray microscope, in addition to X-ray crystallography and cryo-EM.

NSLS-II continues to expand its science program for molecular characterization and imaging, with the support of both BER and the National Institutes of Health (NIH). The instruments being developed to resolve hierarchies of structure and function for biological and environmental sciences will be further developed for ease of use and reliability. Through a collaborative effort between NSLS-II and Instrumentation Division staff, BNL is developing a novel Full Field Fluorescence Imaging detector to enable rapid imaging of metal distribution in complex biological systems, such as plant root/microbe systems.

Imaging of molecules by the cryo-EM capability complements the world-leading performance of the X-ray diffraction and scattering programs. The cryo-EM facility, with operations supported by BER, issues user calls on a regular basis and will function as a non-designated user facility in the near future. The unique combination of spatial, chemical, and molecular imaging capabilities of NSLS-II will be further enhanced by cryo-electron tomography. To continue integration into BER sciences, Lab researchers have established a pilot program with the Facilities Integrating Collaborations for User Science (i.e., FICUS) to enable X-ray imaging as part of their research portfolio. New capabilities will enable examination of rhizosphere and plants under realistic conditions. New collaborations with BER researchers will develop new structural biology themes. All the developments will be supported through targeted training and dissemination.

BNL's biological systems science activities are supported by: BER, the Joint Genome Institute Community Science Programs, the Environmental Molecular Sciences Laboratory's user program, FICUS, ASCR, and the NNSA/Advanced Scientific Computing ECP. Additional support comes from New York State, NIH, a Cooperative Research and Development Agreement (CRADA), and Laboratory Discretionary Funds.

Chemical and Molecular Science

BNL's chemical and molecular sciences conduct fundamental research to support rational design of chemical and biological processes for DOE mission goals, focused on sustainable energy and chemical conversion and on chemistry in extreme environments. The emphasis in sustainable energy research is on heterogeneous catalysis of C1 chemistry for fuels, light capture, and catalytic conversion by molecular systems for solar fuels, and carbon capture, conversion, and storage in plants. The program on chemistry in extreme environments uses ionizing radiation for fundamental mechanistic studies of charged and radical species in condensed phase and studies of fundamental properties of high temperature molten salts, including effects of ionizing radiation, as foundations for advances in future nuclear energy systems. The research closely integrates core program expertise with BNL's leading user facilities (NSLS-II and CFN) and the divisional Accelerator Center for Energy Research (ACER) electron radiolysis facility.

BNL expertise and unique capabilities in thermal heterogeneous catalysis are being applied to improve understanding of catalysts for conversion of difficult-to-activate small molecule feedstocks, such as abundant methane or CO_2 to synthesize fuels and higher value chemical intermediates, with a focus on synthesis and study of highly active nanostructured metal-oxide and metal-carbide interfaces. Research in catalysis combines leading capabilities in operando studies of powder catalysts, in situ studies of model nanocatalysts, and quantum chemical computation. Operando and in situ research exploit high-brightness beamlines at NSLS-II for time-resolved studies of catalysts by X-ray scattering and spectroscopy, and state-of-the-art electron microscopes at the CFN for in situ and atom-resolved imaging of catalysts. Capabilities for studies of catalytic surfaces under reaction conditions include ambient pressure spectroscopy and scanning tunneling microscopy in the Chemistry Division for characterization of catalytic active sites and their interaction with reaction intermediates.

BNL catalysis scientists lead the Synchrotron Catalysis Consortium (SCC), which provides expert training and support to expand the use of synchrotron methods in catalysis science. The SCC has supported more than 100 unique groups from universities, industry, and other National Laboratories during its 16 years of operation and is in its third year at NSLS-II beamlines (Tender X-ray Absorption Spectroscopy and Quick X-ray Absorption and Scattering). Recent expansions of capabilities include combined X-ray and optical (Infrared/Raman) spectroscopy for simultaneous characterization of catalysts and reactants under reaction conditions.

The physical biosciences program focuses on fundamental understanding of plant regulatory and metabolic mechanisms related to the capture, conversion, and storage of carbon with emphasis on highly-reduced (i.e., energy-dense) forms of carbon, including lipids and phenylpropanoids. The program exploits synergistic team capabilities that include biochemical genetics, physical biochemistry, mass spectrometry, advanced metabolic modeling, computational chemistry, molecular imaging, and structural biology, together with multiple aspects of NSLS-II and CFN. The close interactions with BNL's membrane protein structural biologists and the commissioning of cryo-EM provide opportunities to deepen the understanding of the structure and dynamics of biosynthetic complexes.

BNL's program in solar photochemistry has world-recognized expertise in the design, synthesis, and characterization of inorganic molecular catalysts and chromophores to understand and improve chemical processes for solar-to-fuels conversion in artificial photosynthesis (AP). Research focuses on key AP reactions of water oxidation and CO_2 or proton reduction. A recent focus on the science of integrating molecular AP units into functional sub-assemblies has led to flexible and rapid synthetic methods for interfacial AP assemblies with unprecedented durability and performance. Research exploits unique capabilities of ACER for mechanistic studies of key oxidation and reduction reactions. The capabilities of this program are expanding with its partnership in the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) for research on liquid solar fuels, particularly in expanding research on integration of molecular catalysts at light-absorbing semiconductor interfaces and in developing strategies for cascade catalysis as novel routes to liquid fuels.

The radiation chemistry program develops and applies advanced pulse radiolysis capabilities at ACER. Within ACER, the Laser Electron Accelerator Facility provides world-leading capabilities for ultrafast pulse radiolysis; a Van de Graaff accelerator supports kinetics studies on slower timescales; and two ^{60}C sources enable irradiation studies. Time-resolved infrared spectroscopy uniquely probes specific chemical mechanisms in pulse radiolysis studies. This is enabling new investigations of chemical reaction pathways in radiation chemistry and artificial photosynthesis and providing new insights into processes of molecular charge generation and transport.

ACER is also a foundation for growing BNL capabilities in chemistry of extreme environments. The Molten Salts in Extreme Environments Energy Frontier Research Center (EFRC) builds on ACER capabilities in radiation chemistry and is adding capabilities in handling, irradiation, and characterization of high temperature molten salts and their interactions with materials, including in situ studies at NSLS-II.

Fundamental chemistry and physical biosciences programs are funded by BES, New York State, and Laboratory Discretionary Funds.

Chemical Engineering

BNL has a small but high-impact effort in applied chemistry research that translates scientific discovery into deployable technologies.

Electrocatalysis research builds on expertise in synthesis and characterization of nanostructured core-shell metal, metal-oxide, and metal-nitride nanostructures for design of cost-effective, durable electrocatalysts for electrical-chemical energy conversion in fuel cells and electrolyzers. BNL developed innovative electrocatalysts with the potential to solve problems of low energy-conversion efficiency and high platinum loading in fuel cells. These catalysts contain smaller amounts of precious metal than conventional ones and improve durability, facilitating commercial applications of fuel cells in electric vehicles. The BNL program is participating in the newly-funded five-year program to develop high performance, high durability fuel cell systems for heavy vehicles in the Million Mile Fuel Cell Truck (M2FCT) Consortium funded by the EERE Hydrogen and Fuel Cell Technologies Office (HFTO). BNL is also a partner in L'Innovator, a partnership between BNL, Los Alamos National Laboratory, and the National Renewable Energy Laboratory to demonstrate the incorporation of Lab expertise into a new high temperature fuel cell with funding from HFTO and in partnership with Advent Technologies. Scale-up of other electrocatalyst materials is also underway with additional industry partners.

These programs are funded by BES, the EERE HFTO, and through Strategic Partnership Projects and CRADA efforts with industrial partners.

Climate Change Sciences and Atmospheric Science

BNL's atmospheric and terrestrial ecosystem science efforts develop process-level insight into the role of aerosols, clouds, and ecosystems in a changing climate through its long-standing expertise in measurement science and climate theory. BNL scientists study fine-scale processes that have a global impact on climate. A dedicated effort to build fundamental physical understanding and to scale that knowledge to the global domain is required to overcome the persistent climate projection uncertainties that impact planning and policy implementation for the nation's energy future. BNL envisions building a unified program for advancing climate observations at fine scales that will transform modeling capabilities for a range of climate applications and solutions.

BNL researchers are advancing the understanding of interactions along the aerosol-cloud-precipitation continuum and their impacts on climate for the Atmospheric Systems Research (ASR) Program through a joint Science Focus Area with Argonne National Laboratory "Process-level AdvancementS of Climate through Cloud and Aerosol Lifecycle Studies." This research is driven by data gathered from the Atmospheric Radiation Measurement (ARM) User Facility; studies of the lifecycle and radiative properties of clouds and aerosols; and developing cutting-edge retrievals of cloud properties and processes from remote sensing observations. The Terrestrial Ecosystem Science and Technology group plays a central role in the BER Next Generation Ecosystem Experiments (NGEE) in the Arctic and Tropics – ecosystems that are poorly understood, sensitive to global change, and inadequately represented in models. NGEE research focuses on improving the representation of ecosystem processes in Earth System Models and understanding what drives uncertainty in model structure and parameterization of these regions. They use state-of-the-art techniques to study ecosystem processes across a wide range of scales and biomes.

Scientific staff support the ARM observatories and data archive as instrument mentors and as data science specialists and contribute to the design and interpretation of ARM measurements. Climate modeling scientists support the Energy Exascale Earth System Model (E3SM) and the Large Eddy Simulation (LES) ARM Symbiotic Simulation and Observation (LASSO) project through their expertise in component development, model evaluation, and strong observational data analysis.

As computing resources grow and models achieve higher resolution, observations must also push current resolution boundaries. BNL staff are bringing novel measurement methodologies, instrumentation, and Laboratory facilities to bear on this problem through collaborations with BNL's Instrumentation Division. In partnership with the CSI, BNL's climate modelers are building capabilities for very high-resolution and data-driven simulations of the atmosphere and climate that will be developed through the insights gained from new high-resolution measurements. This unified observational-modeling framework will work to reform the ad hoc nature of measurement and model development in an approach that is directed at the largest uncertainties in representing atmospheric processes relevant to climate change.

Leveraging long-standing support by BER's Climate and Environmental Science Division and recent BNL investments in the CSI, BNL developed new capabilities in support of BER's needs in environmental data analysis, development of innovative measurement platforms and instrumentation, uncertainty quantification, and high-resolution atmospheric modeling. Through the Center for Multiscale Applied Sensing (CMAS), BNL has also established a mobile remote-sensing platform to support research in characterization of renewable energy resources, urban system studies, and national security applications. The application of BNL's long-standing Perfluorocarbon Tracer (PFT) technology is also coordinated through CMAS and used to conduct urban dispersion studies.

Funding comes from BER, EERE, DHS, and Laboratory Discretionary Funds with projects also supported by the New York Police Department, NYSERDA, NASA, and the Defense Advanced Research Projects Agency (DARPA).

Computational Science

Computational science, both numerical modeling and data analytics, is essential to enabling advanced scientific discovery at BNL's facilities – RHIC and EIC (NP), the BLIP (Office of Isotope Production); ATLAS, Belle II, and the ATF (HEP); NSLS-II and CFN (BES); cryo-EM and ARM (BER) - and supporting science programs. CSI has built a broad portfolio of projects that encompass multidisciplinary teams of computer scientists, applied mathematicians, and domain scientists across BNL directorates, other National Labs, and universities to support these and other DOE efforts. The teams are together expanding on state-of-the-art and inspiring new fundamental research, while delivering the tools for new scientific discoveries. The projects touch most DOE ASCR, BER, BES, HEP, NP, EE, EERE, NNSA, multiple agencies within the Department of Defense, and other federal agencies.

Collaborations around numerical modeling applications benefit in particular from CSI's ECP-funded research into performance portability (SOLLVE), ML-enabled surrogate modeling (ExaLearn, SciDAC RAPIDS), and LDRD-funded applied math for multiscale modeling and inverse problems. Examples are ECP lattice QCD, computational chemistry (NWChemEx), and the HEP Center for Computational Excellence that supports the ATLAS and DUNE experiments. The ASCR-funded IPPD project in this context focuses on the optimization of data analysis workflows at NSLS-II. CSI has also made significant advances in enhancing existing numerical modeling solutions with AI, ML driven-solutions for predictive modeling. Examples include climate modeling (E3SM), solar power, and load forecasting.

CSI's growing computational science capabilities are also manifested in close collaborations with domain scientists to apply state-of-the-art HPC techniques to accelerate scientific computing. Highly impactful applications range from image reconstruction for NSLS-II, fast calorimeter simulations for ATLAS to cloud-particle modeling for climate science, which benefited greatly from the use of GPU accelerators and/or massively parallel computers. Efforts to prepare mission critical, traditionally non-HPC applications for exascale and other novel computing architectures are ongoing, drawing from BNL's expertise built through the ECP projects. Examples include RHIC and the future EIC, direct numerical simulations (DNS) for climate, and more.

CSI has built a significant program across all BNL directorates and their user communities focused on advanced data analytics. AI, ML, Applied Math, and novel architecture testbeds are combined with domain knowledge. New ML libraries are developed and applied to domain science challenges in BES, BER, HEP, and EERE through projects such as ECP ExaLearn, the ASCR-funded ROBUST, and the SciDAC Institute for Computer Science and Data-RAPIDS. New analytical capabilities were successfully applied in ECP projects (ExaLearn, CODAR, and NWChemEx); the joint ASCR-Veteran Affairs project where BNL's contributions include advanced ML predictive models for prostate cancer prediction; ASCR funded research in PPAI; a BER Predictive Genomics project; BES efforts for Dynamics and Control of Magnetic and Charge Order in Complex Oxides; an HEP/ASCR SciDAC center Accelerating HEP Science; projects for EERE, OE, and NNSA; and joint LDRD projects with NSLS-II and CFN, cryo-EM, and RHIC. In collaboration with the Instrumentation Division, the Scientific Data and Computing Center (SDCC), and facilities such as NSLS-II, cryo-EM, and CFN, BNL's new Center for Advanced Technologies for Artificial Intelligence (CAT-AI) co-designs new experimental capabilities that integrate advanced imaging technologies with high powered edge computing devices and streaming ML and AI.

New efforts will focus on the development of digital twins as part of the new initiative in AI and Data Science, where advanced modeling and simulation capabilities will be employed to help design, guide, and improve experimental setups and workflows. A digital twin that simulates the physical experiments will be able to respond to environmental changes quickly and learn from past experiments. This will require the integration of HPC and AI, as well as advanced mathematical modeling methods.

The primary sources of funding come from ASCR, HEP, NP, BES, BER, New York State, OGA, EERE, OE, and Laboratory Discretionary Funds.

Condensed Matter Physics and Materials Science

BNL conducts frontier research in Condensed Matter Physics and Materials Science, focusing on new and improved complex, nanostructured, and correlated-electron materials for renewable energy, energy storage, quantum information science (QIS), and energy efficiency. This is accomplished through interdisciplinary and tightly coupled programs in materials synthesis, advanced characterization using a range of experimental techniques, both lab and facility based, and theoretical approaches.

A unique tool, known as OASIS (that integrates <u>o</u>xide molecular beam epitaxy, <u>a</u>ngle-resolved photoemission, and <u>s</u>pectroscopic <u>i</u>maging <u>s</u>canning tunneling microscopy), is fully operational and had a productive year with eight papers published in FY 2020. OASIS brings together in one system the ability to fabricate thin films and examine their properties in situ using scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES). In the past year, for the first time, OASIS has grown films of the cuprate known as DBCO and performed subsequent characterization of these films using STM and ARPES. In this same time period, OASIS has also provided definitive evidence on the nature of the cuprate superconducting order parameter, an exotic phase of matter known as a pair density wave.

Abhay Pasupathy now leads the OASIS effort. Under his guidance, OASIS will continue to study superconducting cuprates but is expanding its scope to include two-dimensional (2D) materials and heterostructures that can support topological excitations. As a complement to the current OASIS STM, a second scanning probe microscope is being installed. This microscope will be able to operate at both sub-Kelvin temperatures and finite magnetic fields and has a magnetic force microscopy capability.

As described in the Condensed Matter Physics and Materials Science (CMPMS) Division's strategic plan, to different degrees, all the groups in the Division are engaged in NSLS-II activities. New capabilities in X-ray scattering and angle-resolved photoemission exploit the opportunities offered by NSLS-II, and BNL scientists have led several proposals for new NSLS-II beamlines. Two of these proposals have begun their first phase of development.

BNL has a number of capabilities for performing ultrafast electron diffraction. The BNL MeV UED facility is in operation, which is complemented with a newly installed laser-free electron pulser (LFEP) device capable of “tabletop” UED. BNL has also advanced the design of a compact MeV-ultrafast electron microscopy capability, supported by LDRD funds. The LFEP and UEM efforts were recognized as significant advances in ultrafast electron science by the community, garnering multiple awards. These UED activities are complemented by a new ultrafast X-ray research program that focuses on the unique science that can be performed at ultrafast X-ray Free Electron Laser facilities around the world, particularly the Linac Coherent Light Source at SLAC National Accelerator Laboratory. This program has had a change in leadership this past year with Mark Dean becoming its scientific lead.

BNL’s Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy is developing software that will allow prediction of properties of strongly correlated materials. The computer programs, freely available to the scientific community, are expected to tie in into the activities of NSLS-II users and to be upgraded periodically by BNL, where they will permanently reside. The Center was renewed in the past year for a second four-year period.

Within CMPMS, there is a new focus on QIS that will take advantage of in-house strength in high T_C superconductivity and chiral materials. Regarding the latter, there is a sustained effort within CMPMS to learn how to optimize and manipulate the near-dissipationless currents that chiral materials support.

BES and Laboratory Discretionary Funds are the primary sources of funding for these ongoing efforts.

Large-Scale User Facilities/R&D Facilities/Advanced Instrumentation

As a key part of its mission, BNL develops and operates user facilities that exceed the funding and expertise available at individual institutions. Despite the pandemic, in FY 2020, BNL served over 3500 users at its DOE designated user facilities, i.e., ATF, RHIC (NSRL and the Tandems), NSLS-II and CFN, as well as additional users at the RHIC-ATLAS Computing Facility (RACF) and U.S. ATLAS Analysis Support Center. BNL plays a significant role in the globally-deployed ARM User Facility for climate research, which serves more than 1000 users annually.

NSLS-II is completing its sixth year as a User Facility, having hosted over 1350 unique users in FY 2020. All 28 beamlines switched to some form of remote operations in 2020 to accommodate the user program despite COVID restrictions. In 2020, NSLS-II had a record 557 publications with 38% of them published in journals with an impact factor greater than 9. NSLS-II has real strengths in imaging and dynamics and has world-leading R&D programs in nano-focusing optics and nano-precision engineering. There is a strong partnership with the CFN, running four end stations together. Partnerships with the BES neutron sources in the areas of small angle scattering and powder diffraction facilitate the work of researchers using both X-ray and neutron techniques on a single problem. NSLS-II plays a leading role in next-generation data acquisition software (BlueSky), which is the de facto standard for new beamlines across the complex, and in coordinating areas of common interest among the DOE light sources, particularly in data, optics, and detectors. Looking to the future, NSLS-II has proposed a further development of the beamline portfolio to complement the existing suite and provide much needed capabilities in high thruput scattering, spectroscopy, and imaging.

The CFN has completed thirteen years of user operations and in FY 2020 supported the research of 546 unique users, 113 of them remotely as the facility rapidly increased capabilities for remote user engagement in response to COVID-19 challenges. The more than 365 peer-reviewed publications acknowledging use of CFN facilities in 2020 is the most research impact ever in a single calendar year. CFN continues to upgrade its portfolio of nanoscience capabilities to maintain leading-edge status, especially in instruments for synthesis and characterization of nanomaterials created by assembly from nanoscale components, and tools for in situ and operando nanoscience. This year, the major CFN instrument installations included a first-of-its-kind robotic platform for automated design, synthesis, and characterization of nanomaterials from component libraries; a state-of-the-art dual-beam scanning electron and focused ion beam microscope for transmission electron microscope sample preparation; and an electron energy loss spectrometer for the aberration-corrected environmental transmission electron microscope.

BNL continues to expand the scientific reach of RHIC for its community of more than 1000 users by investing in detector and accelerator upgrades. The recently completed STAR iTPC upgrade and the Low-Energy RHIC electron Cooling upgrade enable a world-unique program of precision exploration of the QCD phase diagram. The upcoming forward region upgrades of the STAR detector will keep the QCD Spin Physics community engaged by providing unique capabilities in this field. The sPHENIX upgrade, in progress, will enable measurement of rare probes of the internal structure of the quark-gluon plasma .

BNL will host a new user facility, the Electron-Ion Collider, that builds on the RHIC user facility. It will support a new generation of users who will use high-energy electron-ion collisions to study cold nuclear matter at extreme gluon densities and enable precision measurements of the structure and properties of protons and complex nuclei at the quark-gluon level.

BNL operates the ATF for the advanced accelerator science and technology community as part of the Accelerator Stewardship Program managed by the Office of Accelerator R&D and Production. This facility is unique in terms of the breadth of advance accelerator and laser experiments that it supports.

BNL makes key contributions to international facilities – the LHC, SuperKEKB, and such future facilities as a Long Baseline Neutrino Facility (LBNF)/DUNE and the Rubin Observatory, which is under construction.

The ARM User Facility is a multi-Laboratory facility that supports basic understanding used in developing next generation predictive climate models. Its observational infrastructure is complemented by ARM's large data archive that manages nearly thirty years of observational data. BNL continues to innovate in their operation of instrumentation for aerosol, precipitation, cloud dynamics, and atmospheric radiation, the LASSO process modeling program, and data product development that support the archive. BNL scientists were chosen to lead the next five-year ARM deployment to the Southeast U.S.

BNL's new cryo-EM facility is up and running. The Laboratory for Biomolecular Science (LBMS) operates with funding from BER, supporting BER users and the General user community, including BES-funded researchers. It currently operates under the auspices of NSLS-II and has produced its first significant result – solving the structure of a SARS-CoV-2 membrane protein bound with the human protein PALS1, an interaction believed to be important in severe COVID-19 cases. It is anticipated that it will operate as a "Non-designated User Facility" in due course. The building has bays for three additional microscopes.

The Long Island Solar Farm (LISF) is a privately owned 32-megawatt solar photovoltaic power plant built through a collaboration including BP Solar, the Long Island Power Authority, and the Department of Energy. BNL instrumented the plant and data collected from the LISF is being used for research on utility-scale solar plants in the U.S. (solar insolation, weather, power, and power quality), enabling studies on the impacts of renewable generation on the power grid and the development of advanced solar forecasting models to support grid operations.

The Northeast Solar Energy Research Center (NSERC) at BNL serves as a solar energy research and test facility for the solar industry. NSERC includes a solar PV research array for field testing existing or innovative new technologies under actual northeastern weather conditions.

BNL's Instrumentation Division develops cutting-edge technologies for the Lab's major scientific user facilities and national security applications enabled by state-of-the-art detectors, electronics, and optical and laser systems. From concept through construction, major contributions have been made to instruments and experiments at BNL and other accelerator- and reactor-based facilities worldwide. The Division is known for its leadership in noble liquid detector technology, low-noise and cryogenic electronics, application-specific integrated circuit design, state-of-the-art silicon and neutron detectors, development of high brightness electron sources, and design of metrology systems. Major efforts are underway to develop advanced photocathodes for RHIC and EIC applications, to demonstrate and then develop experiments based on new QIST technologies, and to develop CdZnTe, diamond, and germanium detectors for advanced synchrotron applications, and detector concepts for nuclear reactor monitoring.

This core capability is strongly tied to CC 1, 13, 14, and 15.

Nuclear & Radio Chemistry

BNL's nuclear science programs span the range from applications in medicine to national security.

The Brookhaven Linac Isotope Producer uses the high-energy linac and target processing facilities for the production of isotopes not commercially available, mostly for nuclear medicine. Facilities are used to produce Sr-82, the parent of Rb-82, for evaluating cardiac viability and coronary artery disease in 300,000 patients annually. BNL participates in a collaboration with Los Alamos and Oak Ridge to produce Ac-225 in sufficient quantities to support clinical trials for cancer. Ac-225 is an alpha emitter that is limited in supply and has demonstrated reduced toxicity and improved cure rates in clinical trials. Work is ongoing on refurbishing and upgrading facilities and on installing a rastered beam to enable higher production yields. The 2015 Nuclear Science Advisory Committee-I report further recommends doubling of beam current and installation of a second irradiation site to increase output in the future. The irradiation facilities are also used to conduct radiation damage studies and support the RaDIATE project comprised of six international organizations that are evaluating new materials for reactors and accelerators. BNL hosts the Nuclear and Radiochemistry summer school that provides 12 undergraduates with hands-on experience in nuclear and radiochemistry lab studies and exposure to world-renowned lecturers. DOE is interested in expanding this highly successful program to grow the pipeline in nuclear sciences.

BNL's expertise in accelerator development has led to a patent for a Rapid Cycling Medical Synchrotron and for low-mass beam delivery gantries, viewed as technologies of choice for the next generation of proton- and ion-based cancer therapy centers.

BNL has leading expertise in the application of ionizing radiation for diagnosis and treatment of cancer. The effects of ionizing radiation on living systems are studied at NSRL, a flagship international user facility supported by NASA. The NSRL facility also provides the unique capability to study the effectiveness of using carbon or other ion beams for cancer therapy.

The Lab's nonproliferation and national security programs offer a wide range of skills that include scientific and technical participation in the NNSA Radiological Assistance Program (RAP), which is the regional arm of the NNSA Nuclear Emergency Support Team. RAP provides the nation with an agile, scalable, and rapidly deployable federal response capability in support of radiological/nuclear crisis operations and consequence-management events, including both accidental and deliberately caused emergencies. RAP relocated to a renovated, state-of-the-art training, staging, and office facility. BNL also assists NNSA and DHS efforts to test and evaluate candidate hand-held and unattended systems for prevention of, and response to, nuclear and radiological events, domestically and abroad, and is creating a repository for storing test data for NNSA. BNL has a new NNSA project to apply novel science and technology combined with intelligence to the nonproliferation domain.

BNL has extensive expertise in nuclear nonproliferation and international nuclear safeguards that includes more than forty years of program management delivered by the International Safeguards Project Office (ISPO), which provides technical and administrative management of the U.S. Support

Program (USSP) to International Atomic Energy Agency (IAEA) Safeguards. ISPO is responsible for coordinating all U.S. technical and personnel support provided through the USSP to the IAEA's Department of Safeguards.

Brookhaven also develops curricula and provides safeguards implementation training for IAEA inspectors and officials from other countries where IAEA safeguards are applied and provides input to technical and policy papers for the NNSA and other sponsors. BNL uses its expertise in machine learning to develop algorithms for analyzing IAEA surveillance data and delivers an annual training course in complementary access and design information verification for research reactors to IAEA inspectors.

BNL's nonproliferation and national security activities benefit from Lab wide expertise. A new course for IAEA inspectors on the proliferation considerations associated with accelerator facilities is under development. CSI contributes its data analysis and algorithm development expertise to projects related to surveillance review, proliferation detection, and data storage. The National Nuclear Data Center's (NNDC) expertise in curating and analyzing nuclear data is being used for NNSA Defense Nuclear Nonproliferation efforts. NSLS-II supports forensic analysis for NNSA and other sponsors. The Instrumentation Division also leads multiple NNSA Defense Nuclear Nonproliferation efforts to advance near-field and far-field detection.

BNL staff members have twenty years of experience in nuclear security analysis and technology from their involvement in the NNSA Materials Protection Control and Accounting program. This capability is now in demand by other countries, where there are similar nuclear material security concerns.

Funding comes from sources that include NP, the Department of State, NASA, NNSA, DHS, and a CRADA.

Nuclear Physics

BNL conducts pioneering explorations of the most fundamental aspects of matter governed by the strong nuclear force. Heavy-ion collisions at RHIC probe matter at temperatures and densities representative of the early universe, mere microseconds after its birth. RHIC experiments discovered that matter under these conditions, called the quark-gluon plasma, is a nearly perfect liquid that flows more easily than any other material. The RHIC results have led to profound intellectual connections with other physics frontiers. RHIC also probes the spin structure of protons by colliding polarized protons with each other – a capability that is unique in the world.

RHIC offers a synergistic environment for collaboration with universities, other National Labs, and industry. It has approximately 1000 users from over 20 countries. To date, the RHIC program has produced more than 300 Ph.D. nuclear physicists. Nuclear theory efforts at BNL and throughout the international theory community guide and stimulate planning and interpretation of RHIC experiments.

Experimental, theoretical, and computational research is enhanced by the presence of the RIKEN BNL Research Center (RBRC). In addition to its contributions to the RHIC research program and its role in facilitating scientific collaboration with Japan, the RBRC continues to have a major role in the development of the nuclear science workforce by seeding faculty positions at leading U.S. research universities.

BNL develops advanced software and computing facilities for applications in nuclear physics experiments and theory. Key expertise has been developed in the management and processing of petabyte-scale data sets generated at high rates and distributed computing for analysis, facilitated by the RHIC Computing Facility, a component of BNL's SDCC. Lattice QCD simulations utilize high performance computing facilities at BNL and national leadership class computing facilities to study the

QCD phase diagram.

The addition of an electron accelerator and storage ring will be a major component in the plan to transform RHIC into an EIC. The EIC will facilitate a rich science program based on collisions of high-energy electrons with RHIC's heavy ion and polarized proton beams to precisely image the quark-gluon structure of the proton and complex nuclei and to explore a novel regime of extreme gluon densities predicted to be present in all atomic nuclei. BNL scientists, in collaboration with the Thomas Jefferson National Accelerator Facility scientists, are leading an international effort to develop the science agenda and technical design of the U.S.-based EIC facility.

Development and enhancement of RHIC accelerator facilities benefit from BNL's strong program of advanced accelerator R&D, while enhancement of the RHIC detector capabilities benefits from the support of the BNL Physics Department and the Instrumentation Division. Important upgrades of the RHIC accelerator complex and the RHIC detectors are either recently completed (RHIC electron cooling, STAR iTPC) or are in progress (sPHENIX, STAR forward upgrades), while the RHIC experimental program continues.

BNL maintains a world-leading nuclear theory group whose research is focused on the dynamics of relativistic heavy ion collisions and properties of QCD matter under extreme conditions. BNL was named as lead institution for two Topical Collaborations in Nuclear Theory, called "Coordinated Theoretical Approach to Transverse Momentum Dependent Hadron Structure in QCD" and the "Beam Energy Scan Theory Collaboration." Both efforts had outstanding mid-term reviews.

BNL operates the NNDC, an international resource for the dissemination of nuclear structure, decay, and reaction data that serves as the focal point for the U.S. Nuclear Data Program (USNDP) and reactor design. The USNDP provides current, accurate, and authoritative data in pure and applied areas of nuclear science and engineering through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. The program also addresses gaps in the data, through targeted experimental studies and the use of theoretical models. Last year, there were over five million data retrievals from the NNDC websites.

Support is provided by NP as well as RIKEN and Laboratory Discretionary Funds.

Particle Physics

BNL has a key role in developing and operating particle physics experiments that seek answers to seminal questions about the composition and evolution of the universe, i.e., the source of mass, the nature of dark matter and dark energy, and the origin of the matter-antimatter asymmetry in the universe. BNL's major efforts are: host institution for U.S. contributions to the ATLAS detector at the LHC, including managing the U.S. ATLAS Operations Program and the upgrade projects; leadership in neutrino oscillation experiments, including a leading role in the DUNE Technical Coordination; leading roles in the short-baseline experiments at Fermi National Accelerator Laboratory (FNAL) (MicroBooNE, ICARUS, and the Short Baseline Near Detector [SBND]); hosting computing facilities for the Belle II experiment at KEK; and commissioning and operations of the Rubin Observatory cosmological survey. These roles are enhanced by BNL high energy physics theory efforts and by BNL's sustained leadership in detector and advanced accelerator research and development, which is also critical for the next-generation of high energy physics experiments and accelerator facilities.

BNL's high energy theory effort has made distinct impact on the field in phenomenology of collider physics, precision electroweak calculations, long-baseline neutrino physics program, flavor physics, dark sector physics, and the development of lattice gauge theory and its applications, such as the calculation of the muon g-2.

BNL develops advanced software and computing facilities for applications in high energy physics experiments and theory. Key expertise in high throughput computing has been developed in the management and processing of multi-petabyte-scale data sets generated at high rates and distributed computing for analysis, facilitated by the RHIC and ATLAS Computing Facility and the Particle and Nuclear Physics Software group. BNL's software and computing capability have also been applied to the Belle II experiment, successfully storing raw data from the experiment. Particle physics software and computing development for both experiment and theory benefit strongly from synergies with RHIC facilities funded by the DOE Office of Nuclear Physics and with the RBRC, funded by the Japanese RIKEN Institute. Lattice QCD simulations utilize high performance computing facilities that include those at BNL's CSI and at DOE's computing facilities.

Thanks to major BNL contributions to construction and operation of the LHC accelerator and ATLAS detector, analysis of the data, and computing capabilities, the ATLAS experiment continues to be an effective tool for exploration at the energy frontier. BNL scientists pioneered the design and event reconstruction techniques for liquid argon (LAr) Time Projection Chambers (TPC). These were successfully demonstrated in MicroBooNE at FNAL and protoDUNE at CERN. On the cosmic frontier, BNL developed and constructed the focal plane array for the Rubin Observatory camera, which is in commissioning and will become a premier tool for the exploration of dark energy.

Development of new detectors for elementary particles and data collection and storage systems are key for present and future particle physics experiments. BNL has key expertise and leadership in this area and participates in various workshops and planning exercises in the U.S. and world-wide.

Funding for this work comes from HEP as well as RIKEN and Laboratory Discretionary Funds.

Systems Engineering and Integration

Summary: BNL solves problems holistically and across multiple disciplines on several levels in order to design and construct Large-Scale Facilities and Advanced Instrumentation that employ forefront technologies and perform at a world-leading level. Individual facility components (accelerators, detectors, beamlines, etc.) that are conceived, designed, and implemented at BNL are complex entities, requiring broad integration for their successful performance and, in turn, for their coupling with other systems. BNL's approach applies not only to engineering at the various stages of a single project, but also to developing cutting-edge technologies that fuel multiple large projects at the Laboratory.

A recent example is the highly successful construction of NSLS-II and its X-ray beam lines. NSLS-II has executed perhaps the fastest ever ramp up of capabilities of a green field site and is now delivering high impact science at a world-leading level. State-of-the-art technologies integrated into NSLS-II include novel RF and X-ray beam position monitors, high heat-load front-end components, novel X-ray optics and detectors, and a state-of-the-art open source python-based data acquisition, management, and analysis software stack. In addition, NSLS-II staff are providing their beamline and accelerator expertise to the Advanced Light Source, Advanced Photon Source and Linear Coherent Light Source upgrade projects.

Another example is the RHIC accelerator complex, the largest accelerator and the only collider complex in the Americas. The cutting-edge technologies developed at BNL and employed at the complex include high-intensity proton and ion sources, a high-power proton target for medical isotope production, rapid cycling synchrotrons, advanced stochastic and electron beam cooling techniques, and superconducting accelerators to produce high luminosity heavy ion and polarized proton collisions. Developing the EIC will require a strong systems engineering and integration approach, which includes all of the above as well as production of high intensity polarized electron beam and integration of AI/ML in the operation of the accelerators and detectors.

A third example is BNL's development of noble liquid detectors from concept, through demonstration, to implementation in major particle physics experiments, with continuing R&D aimed at developing the very large LAr TPCs that form the DUNE experiment and the liquid Xenon (LXe) TPC for the proposed next Enriched Xenon Observatory (nEXO) experiment. The cold electronics developed at BNL for LAr TPCs in the MicroBooNE, SBND, and ProtoDUNE experiments have been used in research and development of various modifications of TPCs. These developments include complex combinations of cryogenics, power supplies, application-specific integrated circuits (ASICs), readout electronics, and computing.

Further, BNL's nuclear energy experts support sustainment of the current nuclear reactor fleet and development of next generation reactors through research on alternative fuel cycles, materials in extreme environments, and assessment of the role of nuclear energy in our Nation's energy future. BNL performs research for the Nuclear Regulatory Commission's (NRC) multi-year program on the licensing of non-light water reactor policy and provides technical guidance. BNL staff serve as the Light Water Reactor Computational Analysis Technical Area Lead in the Fuel Cycle R&D program within NE. BNL also uses state-of-the-art computer tools to analyze nuclear reactor performance and safety as well as fuel cycle designs for DOE, NRC, and the National Institute of Standards and Technology (NIST).

The major sources of funding are from BES, HEP, NP, BER, NE, NIST, NRC, and Laboratory Discretionary Funds.

Nuclear Engineering (Emerging)

BNL's nuclear engineering capability encompasses three major areas: (1) Materials for Nuclear Energy Applications, (2) Nuclear Systems and Structural Analysis, and (3) Nuclear Data.

In the area of materials for nuclear energy applications, BNL researchers develop synchrotron characterization techniques explicitly for the investigation of materials for nuclear energy systems, including using robots for handling radioactive samples, X-ray diffraction tomography to investigate material degradation, and high temperature in situ experiments for the annealing, corrosion, and molten salts. A joint BNL-Idaho National Laboratory project is studying the formation of gas bubbles within alloys and uses synchrotron techniques to measure the strain induced by this process. Synchrotron-based Bragg coherent diffraction Imaging and 2D nano-diffraction are utilized to investigate self-organization of radiation induced defects and to perform quantitative strain mapping for materials in radiation environments.

BNL leads an EFRC on Molten Salts in Extreme Environments (CC 6). This EFRC conducts basic science research to advance our understanding of properties of bulk salts and their chemistry at interfaces. BNL serves as a resource or data on molten salts and the unique experimental capabilities developed for in situ measurements of local molten salt structure, oxidation state, corrosion, and interfacial phenomenon. The primary mission is basic science research that explores the properties of bulk salts and their chemistry at interfaces. BNL serves as a resource for data on molten salts and the unique experimental capabilities developed for in situ measurements of local molten salt structure, oxidation state, corrosion, and interfacial phenomenon.

BNL is developing designs for a new dedicated synchrotron facility, the Materials in a Radiation Environment (MRE) Facility, to provide the nuclear research community with a secure, separate, and shielded beamline at NSLS-II to examine radioactive materials. Currently, there is no U.S. facility dedicated to the study of radioactive materials with the high spatial and temporal resolution, superb chemical sensitivity possible at NSLS-II. This beamline will complement and be compatible with irradiation tests and post irradiation examination infrastructure for materials characterization and sample preparation currently available in the U.S. The information on materials in radiation environments derived from this beamline will be used to improve the reliability, sustain the safety, and extend the life of current reactors, and support development of new advanced reactors.

In the area of nuclear systems and structural analysis, BNL has experience with all phases of the design and assessment/evaluation of advanced nuclear systems, such as reactors and accelerator-driven-systems (ADS) and fuel cycles, resulting from decades of support to the NRC and the DOE. State-of-the-art NRC and DOE-developed computational tools are utilized for the full scope neutronics and thermal hydraulics analyses of reactor performance and safety characteristics. These analyses can be performed with increasing levels of detail from fuel rods/assemblies up through full 3D coupled neutronic/thermal hydraulic core models. Transient analyses are performed to evaluate safety and licensing issues. BNL also has considerable expertise in the development of safety analysis/evaluation reports and technical specifications for light-water reactors, research, and test reactors as well as advanced reactors.

BNL has a leadership role in the Gen IV International Forum (GIF) Proliferation Resistance and Physical Protection (PR&PP) Working Group since its inception twenty years ago. Through engagement with this multi-national group, BNL has developed expertise in evaluating the robustness of advanced nuclear energy systems (reactors and fuel cycle facilities) against postulated acts of proliferation or malicious attacks, including diversion, misuse, clandestine operation, breakout, sabotage, and theft.

BNL conducts risk modeling, that is, probabilistic risk analysis and consequence estimates that are used to provide quantitative information to estimate the potential risk and consequences of technological designs, including cyber-security threat assessments. BNL also provides technical assistance to nuclear regulatory organizations in countries that have plans to develop nuclear power to reduce the likelihood of any nuclear accident. BNL applies human factor analysis to ensure that the human-system interface in nuclear plants and other industrial facilities contributes to the overall safety of operations. Leveraging its capability in performing perfluorocarbon-based tracer studies, BNL routinely performs control room infiltration tests for commercial nuclear power plants.

In the area of nuclear data, BNL hosts the National Nuclear Data Center (CC 12, 13), which is also the lead unit of the USNDP and BNL chairs the Cross Section Evaluation Working Group (CSEWG). BNL's NNDC is a DOE Office of Science Public Reusable Research Data Resource. BNL's nuclear data research supports a variety of national and international efforts in reactor physics, the nuclear fuel cycle, defense, nuclear non-proliferation, and isotope production. As such, the NNDC both manages and produces comprehensive evaluations for the Evaluated Nuclear Data File (ENDF) library, which is the core reaction and decay library for codes, such as Monte Carlo N-Particle Transport (MCNP) and Standardized Computer Analysis for Licensing Evaluation (SCALE); and the Evaluated Nuclear Structure Data File (ENSDF) library, the definitive resource for all nuclear structure related data.

The NNDC has decades of experience in performing high-precision gamma-ray spectroscopy experiments, including using the U.S. major spectrometers Gammasphere and Gamma-Ray Energy Tracking In-beam Nuclear Array (known as GRETINA). In-house capabilities are currently being developed, through the construction of an alpha-beta-gamma spectrometer dedicated to improving decay data relevant to isotope production, non-proliferation, and reactor applications.

To support ENDF, the NNDC has vast expertise in nuclear reaction modeling, transport theory, nuclear data formats, and processing (chairing also the Nuclear Energy Agency [NEA] Expert Group on the Generalised Nuclear Database Structure and editing the ENDF Formats Manual), nuclear reaction evaluation, and fission yield and nuclear reactor antineutrinos spectrum evaluation. These capabilities are built on a strong history of data curation in both the Nuclear Science References database and the EXchange FORmat (EXFOR) experimental reaction database and web and journal dissemination. The

NNDC houses a GitLab server supporting collaborative USNDP and CSEWG projects as well as a sizeable computing cluster useful for running the export-controlled codes MCNP, SCALE, and VERA (CC 13).

These programs are funded by NE, NP, NNSA, NRC, and Laboratory Discretionary Funds.

Power Systems and Electrical Engineering (Emerging)

BNL focuses on research to advance the deployment and grid integration of renewable energy systems and the development of new technologies to enable the next generation smart grid. BNL has significant expertise in power system modeling and simulation, as well as in transmission and distribution system design, operation, and planning, that can be used to analyze the systems and determine their appropriate use as solutions for grid integration of renewable generation. BNL also has capabilities in the development of control algorithms that can be applied to the operation of energy storage systems for applications to renewable integration.

BNL has successfully developed a portfolio of grid modernization research projects and will continue to build capabilities in this area. Previous and ongoing R&D projects at BNL that are related to the research areas funded by the DOE Office of Electricity include the development of a probabilistic technique for sizing energy storage systems, development of probabilistic techniques for transmission system planning, formal analysis for dynamic stability assessment, and a deep learning based online platform for critical anomaly detection and emergency control to enhance grid reliability and resiliency. BNL has invested LDRD funds for investigation of the use of energy storage systems to improve grid inertial response that are broadening these efforts. Further, as evidence of regional importance and interest, programs are also funded by New York State, including the evaluation of grid impacts from utility scale solar generation on sub-transmission and distribution systems and the use of Radar in real-time damage forecasting and response for restoration of electric utility systems.

In addition to expanding its research portfolio, over the next year, BNL will continue to pursue the establishment of the Grid Innovation Center (GIC) on the BNL campus. This new facility will provide a venue for collaboration with New York stakeholders on grid modernization research, including energy storage systems and increasing the deployment of clean energy generation, including wind and solar. The GIC will enable simulation and validation of innovative new technologies to address the challenges for integrating renewables and energy storage systems on the grid and reduce the risk to utilities of deploying these new technologies.

New York State, OE, and Laboratory Discretionary Funds are the primary sources of funding.

Science Strategy for the Future/Major Initiatives

The Laboratory's high-level, enduring science and technology (S&T) priorities define and distinguish Brookhaven National Laboratory. They fall broadly into the following areas:

- Discovery Science and Technology to address national needs
    - Nuclear and particle physics to gain a deeper understanding of matter, energy, space, and time
    - Energy and climate science with recognized strengths in advanced materials, catalysis, bioenergy, and environmental systems
    - Advanced and emerging technology with demonstrated strengths in instrumentation, magnet, accelerator, and laser S&T
    - Data science.
- Transformational user facilities that position the Laboratory and the Nation for continued leadership roles in science and technology. These facilities are enabled by advanced accelerator science and technology.

- Application of the results of the Lab's work to address new opportunities, including isotopes, national security solutions, and national emergencies.

To achieve the Laboratory's vision and mission requires simultaneous excellence in all aspects of BNL's work – from science and operations, to external partnerships with the local, state, and national communities, and beyond. This is enabled by safe, efficient, and secure operations; by an unwavering commitment to a diverse, equitable, and inclusive environment; and by a strong focus on renewed infrastructure, including Discovery Park that drives regional (and national) outreach and partnerships to address national needs.

Infrastructure

Overview of Site Facilities and Infrastructure

BNL's scientific vision is structured around the achievement of six initiatives as described in Section 4. Safe, efficient, and secure operations, a diverse, equitable, and inclusive environment, and a focus on renewed infrastructure enable and ensure delivery of the research mission. The Lab's strategy for mission readiness will provide a revitalized physical plant to improve scientific productivity, promote the attraction and retention of the scientific work force, including the significant BNL user population, and assure the safe, reliable functioning of BNL's major scientific facilities.

BNL is in Upton, New York in central Suffolk County approximately 75 miles east of New York City. The BNL site, former Army Camp Upton, lies in the Townships of Brookhaven and Riverhead and is situated on the western rim of the shallow Peconic River watershed. The marshy areas in the site's northern and eastern sections are part of the Peconic River headwaters. Approximately 25% of BNL's 5,322-acre site is developed.

At the end of FY 2020, there were 2678 BNL staff assigned on site in 314 buildings totaling 4,812,662 square feet (sf) and 9,220 sf in 20 real property trailers. However, due to COVID, many were temporarily teleworking with the number of on-site staff averaging under 1,000 per day. BNL does not lease any facilities and the average age of all non-excess buildings is 47.5 years with 61 buildings (718,211 sf) used by the Army during World War II (WW-II) dating back prior to the establishment of BNL in 1947. Major science (or science support) facilities, including the Research Support Building, Interdisciplinary Science Building (ISB), NSLS-II, RHIC, and CFN, were constructed during the last twenty years. The remainder of the research facilities were built predominantly in the 1950s and 1960s. Repurposing and renovation of existing facilities was a priority exemplified by the Renovate Science Laboratories (RSL)-I/II SLI projects completed in 2013 and 2015, respectively. The Core Facility Revitalization (CFR) Project, scheduled to have beneficial occupancy in FY 2021, will repurpose a majority of the former NSLS facility (Building 725), converting it into a contemporary central computing facility. Facility and utility condition, status and utilization statistics with analysis can be found in Appendix A.

The CFR project re-tasked 156,205 sf of underutilized space in FY 2019. In addition, ~31,000 sf of underutilized space was declared excess in FY 2020 and an additional 51,989 sf was declared excess in FY 2021. By consolidating staff and excessing Inadequate facilities, the percent Inadequate will decline. This trend will accelerate with the completion of the Science and User Support Center (SUSC) building, and the proposed Integrated Site Operations & Maintenance Facility, which will further reduce Inadequate space later in the planning period. At the end of FY 2020, there were 29 excess buildings and trailers, comprising 161,502 sf, and 23 buildings and trailers totaling 317,307 sf in Standby status.

Subject to availability of funds, the Office of Environmental Management (EM) will remain responsible for the decontamination and decommissioning (D&D) of contaminated excess facilities, including Building 491 (Brookhaven Medical Research Reactor [BMRR]), Building 701 (Brookhaven Graphite Research Reactor [BGRR]) and Building 750 (High Flux Beam Reactor [HFBR]) as identified in the EM-1 memorandum to SC-1 "EM Transfer Decisions for SC Excess Facilities and Materials," dated February 20, 2009 and in accordance with the HFBR Record of Decision (ROD). EM funded the removal of EM OSF asset ST0705 (HFBR Reactor Stack), which was demolished and removed from FIMS in February 2021. This represents the completion of a major milestone in the ROD between the NY State Department of Environmental Conservation (NYSDEC), the U.S. Environmental Protection Agency (USEPA), and DOE. The demolition of SC asset Building 650 (known as the "Hot Laundry") was funded in FY 2021 and demolition is complete. This demolition also represents the retirement of a significant ES&H risk at BNL.

The BNL Land Use Plan can be found at: https://intranet.bnl.gov/mp/webfiles/LandUsePlan.pdf.

Campus Strategy

Modern science is enabled through capable and reliable infrastructure. A renewed and well-operated physical plant improves scientific productivity; promotes the attraction and retention of the scientific workforce, including the significant BNL user population; and along with the Lab's operational excellence, underpins the capability of its scientific facility portfolio.

The planned infrastructure investments will promote and support the scientific initiatives and the wide range of facilities that enable BNL's core capabilities. It is recognized that a commitment to a sustained overhead investment is critical to assure routine maintenance and infrastructure stewardship is effectively practiced. In addition, the Laboratory's world-class research facilities support the recruitment and retention of premier staff.

BNL has tailored its campus strategy to support the programmatic scientific initiatives, thus enabling the Lab's research mission. The resulting strategy consists of five major elements:

1. Focus limited DOE investment in critical core buildings and infrastructure to enable the scientific agenda
2. Make research safe and cost effective by downsizing the campus and demolishing old buildings
3. Ensure scientific reliability through targeted investments in buildings and utility infrastructure
4. Ensure critical infrastructure and buildings are resilient against severe environmental, climate, and weather conditions
5. Support the growing population of scientific users through an innovative concept called "Discovery Park."

Element 1 - Investment in Critical Core Buildings and Infrastructure

Since many science buildings are 50+ years old, they require reconfiguration and substantial sustainment and recapitalization investments in mechanical and electrical systems and architectural elements to meet the demands of modern research. Research labs merit renewal and modernization to include new fume hoods and casework. In addition, many research labs need state-of-the-art upgrades, including stringent environmental and vibration controls and "clean" environments. BNL has identified those "permanent" facilities that will form the platform for current and future core capabilities. To ensure facilities are mission ready, BNL has formulated a multi-pronged strategy of consolidation and rehabilitation. Facilities would be rehabilitated using a combination of indirect funds including Institutional General Plant Projects (IGPP), Deferred Maintenance Reduction (DMR), and DOE direct funds (SLI, GPP). Additionally, supporting the Lab's strategy are Other Infrastructure Projects (OIP), which include alterations and non-capitalized betterments.

The most significant infrastructure issue facing the scientific organizations relates to computing and data management. Near-term computing needs will quickly eclipse the existing computing infrastructure. To address this, the CFR project, under construction, will provide a contemporary computing facility and infrastructure that will meet the rapidly expanding scientific needs of the Laboratory. This investment will make cost-effective use of existing infrastructure by repurposing most of Building 725 (the former NSLS), which is slated for beneficial occupancy in FY 2021. A transition to scientific operations will take effect later in 2021.

The most significant issue facing the mission support organizations is that many are still located in Inadequate WW-II era wood buildings. To address this, the SUSC, an SLI-funded project, will fulfill three key mission needs by providing efficient science user and visitor processing capability, collaboration and conference space for the research community, and modern, efficient office space to enable operational efficiencies through staff co-location and footprint consolidation.

A similar issue is the scattered locations of BNL's craft resource shops and maintenance, operations, and emergency management control facilities, also located mainly in WW-II era buildings, which are Inadequate due to condition and configuration. A centralized facility, the Integrated Site Operations & Maintenance Facility, is proposed for an FY 2025 start to increase energy and operational efficiency through co-location, elimination of repair needs and modernization costs, and centralization of craft training. In addition, the facility will allow the consolidation and co-location of maintenance management and building control systems.

An additional issue is the build-out of the laboratory/office buildings associated with NSLS-II to support the needs of the expanding number of multi-program operational beamlines. Recent changes in IGPP rules have required BNL to develop new strategies for funding the build-outs.

Element 2 – Optimizing the Campus Footprint

An important element of the overall infrastructure strategy is elimination of excess facilities and footprint reduction to realize operational efficiencies, improved facility safety, and improved utilization and quality of space. BNL is committed to reduce the Lab's building footprint by more than 5% over the planning period. The Infrastructure Investment Table and Integrated Facilities and Infrastructure (IFI) crosscut (Enclosure 4) indicate the annual overhead investments needed to eliminate existing or anticipated future non-contaminated excess facilities, albeit over an extended period, and the requests for direct DOE funding for the costlier contaminated facility projects. A request for direct funds to accelerate the removal of noncontaminated facilities is also included in the table. Over the planning period, the BNL Demolition Plan estimates that ~225,000 sf of net excess space will be eliminated, the majority of which are WW-II-era buildings. However, an additional 200,000 sf could be eliminated with the assistance of direct funds, which are requested in the Investment Table.

To meet these infrastructure challenges, BNL has formulated a strategy to address the mission and operational needs based on the constraints and strengths of the various funding sources. Capital projects and other requested funding are shown in the Infrastructure Investment Table and indirect expensed projects, such as DMR, are reflected in funding plans shown on the IFI Crosscut. In addition, non-capitalized betterment and alteration projects and infrastructure studies, i.e., OIP, not requested as part of Enclosure 4, round out the Lab's investment strategy. Consistent with BNL's Mission Readiness approach, funding for the various categories of indirect funds (DMR, OIP, and IGPP) can vary from year to year based on the projects selected.

As part of the continuing consolidation planning to right size the campus, two buildings totaling 10,840 sf were demolished at the end of FY 2020. In FY 2021, a multi-year project to demolish Building 197 (51,988 sf) was started. The demolition of Building 650 (6,453 sf) is complete.

Element 3 - Targeted Investment in Building and Utility Infrastructure

While BNL's utilities are currently reliable, they are aging and issues impacting reliability and capacity are increasing. In FY 2011, BNL completed a baseline study, which evaluated its utilities and recommended strategies to address critical needs. The study identified significant short-term needs confirming that the aging water, electric, chilled water, and steam distribution system components need replacement. Recapitalization resources to renew and replace BNL's utility infrastructure have been limited by historically tight operating budgets. In recent years, as the Laboratory growth strategy has begun to take effect, additional overhead resources have gradually been provided to operating budgets. However, progress was made with the installation of new chillers to increase the Central Chilled Water Facility (CCWF) capacity and reliability to support growing science process cooling needs. In addition, a project was completed in FY 2018, replacing the 28-year-old wood cooling tower at the CCWF. The proposed Critical Utilities Rehabilitation Project (CURP) SLI line item will address replacement of one of the three 1,200 Ton electric centrifugal chillers, original to the central plant and beyond its useful life. The project also includes two critical potable water projects: one to rebuild Potable Water Well No. 12, expected completion FY 2021, and another to replace the WWII-era 300,000-gallon elevated water storage tank with an upgraded 500,000 gallon tank expected to be completed in FY 2023.

The aging utility distribution systems present additional utility needs. Sections of the central steam distribution system date back to the 1950s. Leaks, mostly in the condensate return piping cause system inefficiencies that need localized repairs. Over the past several years, with an increasing number of water main breaks in the old "transite" (asbestos cement) piping, several sections are in critical need of replacement. Selective replacement and reinforcement of the 13.8 kV primary electrical distribution system are also needed, including an additional feeder to provide backup to the CCWF and NSLS-II. Deficiencies associated with these distribution systems will be addressed in the CURP line item and later in the planning period by the Critical Utilities Revitalization and Enhancement (CURE) project.

Element 4 – Resiliency

The utility-related projects as well as building designs and major renovations include provisions to improve resiliency against severe weather and climate and other unforeseen events. These include ensuring chiller and boiler plant capacities support N+1 operation, and steam and electrical systems have redundant feeds to mission critical facilities.

The plan for improving asset condition is multipronged and does not solely rely on maintenance investment, which was 1.0% of Replacement Plant Value for 2020 for non-excess and non-OSF 3000 assets. Continuing to consolidate out of those assets not worth maintaining, followed by cold and dark, and ultimately by their demolition is key to BNL's strategy. Continued space consolidation efforts will be enabled by renovation and alteration of underutilized buildings and through new proposed buildings, such as the SUSC and the proposed Integrated Site Operations & Maintenance Facility, allowing a major consolidation from Inadequate WW-II-era buildings. In addition, there are proposed GPP projects that would help jumpstart recapitalization of key mission critical building systems, such as HVAC, electrical, and roofing, in mission critical assets and through mission-enabling renovation of key laboratories.

From an environmental sustainability perspective, three emerging contaminants of concern, which affect groundwater quality are a key driver for this element of the Lab's strategy. This issue involves perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA), and 1,4-dioxane. This is a high visibility topic within the State and on Long Island. Testing shows these substances are present in the groundwater at BNL as a result of past releases of firefighting foam and the solvent 1,1,1-trichloroethane (TCA). Additional context is provided in Section 6.4.

Element 5 – Advancing the Innovative Public-Private Partnership Concept Called "Discovery Park"

The Discovery Park concept is a key component of BNL's infrastructure renewal plans and continues to make excellent progress. Discovery Park will repurpose approximately 60 acres of federal property at the entrance to BNL to enable joint federal and private development that replaces aging infrastructure and user housing and enables mission-enhancing technology transfer opportunities. An Alternatives Analysis conducted for Discovery Park and reviewed with the Office of Science determined the preferred development pathway for Discovery Park is a mix of federally funded and privately funded development. The initial focus of development are federally owned facilities in the Upton Square area of the Discovery Park site to include the SUSC, housing, and the Grid Innovation Center (GIC), potentially a New York State funded/DOE owned joint partnership facility. Design of the federal component is underway with initial occupancy of the federal facilities envisioned in the FY 2024 timeframe. Development of the first-privately financed facilities is contingent on approval of ground leases and will follow initial federal development.

Investment Strategy

The investment strategy relies on the following direct and indirect funding sources:

DOE SLI funds: Will be used to perform major building system revitalization or replacement in support of state-of-the-art research facilities that can readily support current and future missions. Over the planning period, BNL has proposed projects to improve the condition of existing buildings and re-task underutilized space that will help to achieve mission needs identified as part of its Site Master Plan process. The fully funded CFR project, along with proposed projects, will revitalize several existing permanent facilities and will be more cost-effective than construction of new facilities and demolition of others.

- **Core Facility Revitalization (CFR)** (TPC $74.85M, FY 2017 start) is repurposing two-thirds of the first floor of Building 725, a 156,000-sf building constructed in 1981 with additions in 1988 and the 1990s. It contains significant office and high bay space. This project is critical to the ongoing support of the mission need to provide computational and data storage support to current and planned experiments at RHIC and the U.S. ATLAS effort at CERN. The space will support the planned growth of computing resources for the existing SDCC as well as Belle II, NSLS-II, CFN, and other Laboratory users. The extensive underutilized high-bay space is well-suited for conversion to computing use (see Figure). The scope of the project includes select revitalization of the building envelope, HVAC, and other building systems, interior finishes, and building configuration as required to perform its new mission. The project received CD-0 in FY 2015, CD-1 in April 2017, CD-2/3a in October 2018, and CD-3b in January 2019. CD-3 was approved in May 2019, and construction has commenced and is expected to be substantially complete by July 2021. The CD-4 completion date is October 2023.
- **Science and User Support Center (SUSC)** (TPC $86.2, FY 2019 start) will include construction of a federally funded office and support building, which will range from 70,000 to 120,000 sf in Upton Square at the Discovery Park site to enhance user support capability, address major DOE and BNL infrastructure needs, and as an added advantage, serve as a magnet for further development. This building (see Figure) will enhance operational efficiency by consolidating approximately 200 BNL support division staff, currently dispersed in several buildings, into a single modern office building meeting DOE sustainability goals. It will also enable further consolidation of other staff, ultimately allowing the demolition of ~43,000 sf of WW-II-era space with a combined backlog of maintenance and modernization needs of $7M. In addition to the efficiency gained by co-located staff, the facility's location at the BNL main entrance will enhance public access for education and commercial outreach for BNL outward facing

organizations (such as Stakeholder and Community Relations, Human Resources, and the Guest, User, Visitor Center, among others), while supporting BNL core functions. A new visitor center, designed as a highly efficient one-stop user access portal, will be the front door of the SUSC structure and will enhance BNL's role as a major user facility laboratory. Scientific collaboration will also be enhanced through a new highly configurable and accessible conference center, the third major element of the SUSC facility. The project received CD-0 in December 2016, CD-1 in December 2018, CD-2/3 is planned for FY 2021. Construction is planned to commence early FY 2022. The CD-4 completion date is 2026.

- **Critical Utilities Rehabilitation Project (CURP)** (TPC $92.8M, FY 2020 start) will replace and rehabilitate key utility systems required for operation of mission critical research facilities. Significant portions of the utility systems are well beyond their useful life with some in service since WW-II, including portions of the sanitary system. This project will: 1) Replace central chilled water system(s), constructed in 1990, that are beyond their useful life and no longer reliably serving critical facilities, such as CFN, ISB, SDCC, NSLS-II, and Building 911 Collider-Accelerator Center; 2) Replace portions of the underground steam and condensate piping system and select manholes, some dating back to the 1940s that are failing due to extensive corrosion, leaks, and deterioration; 3) Refurbish equipment in the central steam facility, first constructed in 1949, which will assure reliable steam service to the site; 4) Replace, repair, or reline the old asbestos water main first constructed in 1941, rebuild the facility housing Well 12, and replace the Elevated Water Storage Tank, constructed in 1941; 5) Repair and refurbish deteriorated sanitary lift stations and sanitary lines; and 6) Refurbish and replace electrical feeders and switchgear with modern, safe, reliable electric equipment and systems that will reduce arc-flash hazards.
- **Critical Utilities Revitalization and Enhancement (CURE)** (TPC Estimated Range $350-$400M, FY 2024 start) will replace and rehabilitate additional key utility systems required for operation of mission critical research facilities. Some, such as portions of the sanitary system, are over 100 years old. The project will: 1) Replace the remaining original 1200 Ton electric chillers in the CCWF; 2) Replace portions of the old underground steam and condensate piping system, first constructed in 1941, and select manholes that are failing due to extensive corrosion, leaks, and deterioration; 3) Replace, repair, or reline the old asbestos water main, some dating back to 1941; 4) Replace, repair, and refurbish deteriorated sanitary lift stations and reline or replace sanitary piping and associated manholes; 5) Refurbish and replace electrical feeders and switchgear with modern, safe, reliable electric equipment and systems that will reduce arc-flash hazards; and 6) Replace key utility plant infrastructure to ensure operational control, efficiency, and reliability including electrical system and instrumentation components. This project is scalable to match available funding profiles.
- **Integrated Site Operations & Maintenance Facility** (TPC Estimated Range $70-$95M FY 2025 start) will replace and demolish approximately 107,000 sf of Substandard or Inadequate buildings, trailers, and OSF assets. The project (see Figure) will co-locate maintenance and operation resources that are spread out across 16 buildings and 19 trailers, located in five separate areas of the site, increasing operational efficiency. Most of the buildings are WW-II era wood buildings, which have an Overall Asset Condition of Inadequate. It is anticipated the project will reduce at least 20% of administrative and shops space and 30% of storage space, as well as a significant amount of common space, such as bath and locker rooms, breakrooms, and training space. In addition, the facility will enable enhanced operations by centralizing the control areas for the computerized maintenance management and building management control systems. Due to co-location, the use of shared facilities will allow more effective staffing and supervision, improved communications (e.g., lessons learned and staff feedback), and greater building energy efficiency, resulting in an increase in operational efficiency. The building will include a central location for F&O stock and material kitting, which will allow workers to

receive their assignments and work kits in one location. In addition, the facility will improve workforce development by having dedicated space that will be used to develop the next generation of craft, as well as the co-location of Subject Matter Experts to provide technical guidance. Included will be space for training and for modern remote conferencing with external vendors, such as Trane, Carrier, etc., to support staff development, troubleshooting, and remote instruction. The facility will also provide testing and assembly space for hands on mockups for areas such as electrical protective device maintenance and safety, fire alarm systems, and value maintenance. The building will contain a center for real-time operations performance monitoring to allow issues and improvement opportunities to be identified and implemented efficiently.

- **Building 911 Renovation for Accelerator Science Center** (TPC Estimated Range $50-$75M, FY 2024 start) will renovate approximately 50,000 sf of the 106,000 sf in the three-story structure, built in 1956 with a major addition in the early 1960s that is currently occupied by approximately 290 staff. Work will include updating mechanical and electrical systems, reconfiguring space to improve efficiency and enhance utilization, improve sustainability, and modernizing interior and exterior finishes to reflect a world class research facility.
- **Building 463, Replace Biology Building** (TPC Estimated Range $80–$110M, FY 2029 start) will replace the WW-II era portions of the building (1945) referred to as phases I & II. Other portions of the building constructed in the mid-1960s and the 1980s would remain and have been partially renovated using IGPP, DMR, and GPP funds. The project will demolish approximately 64,000 sf of space and reconstruct in its place a similar amount of lab, office, and greenhouse space to support BES and BER biological science programs. The new facility will re-link the newer east and west wings that total approximately 45,000 sf, leveraging the prior IGPP and GPP investments in those portions. This project should eliminate most of the current $30M in repair and modernization needs and bring the building from Substandard to Adequate.

As part of the Lab's mission readiness effort, BNL is executing a FY 2021 Notable Outcome to articulate and document the Laboratory's ten-year vision for the DOE Isotope Program. As an element of that effort, BNL is exploring a concept for a Radiochemical Processing Facility (with a notional cost estimate of $45-$60 M). Under this approach, BNL would repurpose Building 870 to support dedicated radiochemical processing of accelerator targets to provide Curies of radionuclides to meet the growing unmet demand for clinical evaluation of drugs containing Ac-225.

GPP (DOE SLI) via the Infrastructure Crosscut: BNL continues to evaluate where DOE GPP level investment will complement and accelerate BNL indirect investment. Several major recapitalizations and other needs to provide mission ready facilities and infrastructure were identified and prioritized. These cover several improvements to address the most urgent gaps including:

- Per- and Polyfluoroalkyl Substances (PFAS) Source Area Groundwater Characterization & Remediation ($10.9M, FY 2020)
- Mission Critical Building Upgrades: HVAC ($8.7M, FY 2021 funded, FY 2022 request), Electrical Distribution ($9.0M, FY 2023 request), and Roofing ($8.8M, FY 2025 request).

Excess Facilities Disposition (EFD): In concert with the related infrastructure crosscut call for GPP, BNL proposed several high impact demolition projects for DOE direct funding. A long-range plan for low impact, lower cost demolitions funded from indirect operating funds was developed and will be prioritized with other indirect-funded infrastructure needs. In addition, BNL seeks direct DOE support to accelerate the demolition of the growing list of excess facilities with a proposed project ($9.3M, FY 2025). EM committed to incorporating several SC assets including Building 491 (BMRR) and Building 701

(BGRR) into its cleanup program for disposition, but the timeline is uncertain, and they may not be accepted by EM until 2030. EM funded the D&D of Building 650 in FY 2020 and the demolition is complete.

Indirect Funding: The Laboratory anticipates increasing overall infrastructure spending over the ten-year period. Infrastructure funds are for maintenance, including dedicated DMR projects, IGPP, and OIP. OIP projects are not part of the Investment Table but fund alterations, non-capitalized betterment projects, demolition, and infrastructure studies. These OIP projects totaled ~$7.7M in 2020 (41% of the overall indirect infrastructure project budget, known as the Consolidated Unfunded Requirement List [CURL]) and are forecast at ~$5.8M (45%) in 2021.

Collectively, this indirect funding is enabling the execution of the Lab's space consolidation plans, which when coupled with demolition, will help right-size the BNL footprint, and reduce operations and maintenance costs. The strategy for use of indirect funds for non-major recapitalization and sustainment needs is as follows:

- Prioritize all proposed investments in infrastructure and ES&H and program them to maximize the value of BNL's infrastructure, reduce risk, reduce deferred maintenance, and support the Science & Technology programs
- Defer major investments in 70+-year-old wood buildings, while performing minimum maintenance to keep these buildings safe and operational. When opportunities arise, consolidate staff from these structures and demolish them.

Non-Federal Funding: As described previously, BNL is pursuing an innovative public-private partnership concept called Discovery Park as an opportunity to enhance BNL's DOE mission capability, address infrastructure deficiencies, promote user access, and contribute to local and regional economic development. The proposed privately and non-federally funded development technology partnership facilities will be complementary to the SUSC SLI line item project.

Discovery Park is a potential model approach for Laboratories of the Future and will repurpose the existing BNL Apartment Complex and adjacent area into a publicly accessible research park. This area is contiguous to BNL's federal research core but is easily configured to be outside the security area. Its location, which is adjacent to the Laboratory entrance and the William Floyd Parkway, presents a unique opportunity for public/private development in the interest of the DOE. The initial development in Discovery Park is comprised of the SUSC, housing, and the potential GIC. The SUSC, housing at Upton Square, and GIC will become an entry portal, a user housing community, and a location for scientific collaboration. The balance of the Park allows for co-location of complementary joint institutes, private companies, or other private, State, or federal scientific facilities.

In short, Discovery Park is envisioned as a joint land use partnership that will leverage key "points of intersection" with external partners and enhance the DOE's investment and assets at BNL to provide:

- Sustainable Laboratory revitalization with the SUSC and renewed privately built (and operated) housing
- An enhanced guest and user portal for growth and sustainment of the scientific user community and user facilities
- Unique facilities for energy science, education, technology transfer, and Discovery to Deployment industrial partnerships.

The development and operating model being pursued will allow for flexibility in the widest variety of funding sources and ownership while maintaining appropriate synergy with BNL's mission. The concept has received significant New York State and local support, including matching utility grants, and has served as the focal point to enhance regional, national, and international connectivity through New York State investment in a relocated railroad station.

Utilization of non-federal funding at BNL was demonstrated through a $12.7M Utility Energy Savings Contract (UESC) project that was completed in 2015. The project included both utilities (a new 1,250 Ton chiller) and building system improvements. It has consistently achieved between 95 and 101% of the originally estimated annual energy and green-house gas savings. Based on the success of this project, BNL and the Brookhaven Site Office began developing a second UESC project. Due to marginal economics and other concerns, this effort was put on hold. Other financial options are being evaluated.

Site Sustainability Plan Summary

BNL continues to be on-track to meet or exceed most of the Site Sustainability Plan goals. Many of the older buildings continue to be demolished and replaced with new, efficient facilities that meet the High-Performance Sustainable Building (HPSB) criteria. BNL is re-evaluating assets that met the prior Guiding Principles for HPSB criteria against the new 2020 Guiding Principles for HPSB and expects some additional work will be needed to ensure full compliance. Energy intensity reduction continues to be challenging and the Lab's historical success in lowering its energy intensity by approximately 60% partially accounts for this. Other issues contributing to this challenge are BNL's relatively low energy rates and high construction costs that make cost-effective projects difficult to identify. Regardless, BNL continues to maximize the use of UESCs, which continues to be a major component of the Lab's sustainability efforts.

BNL meets the Renewable Energy and Clean Energy requirements through a combination of on-site solar PV generation at the Northeast Solar Energy Research Center and the purchase of Renewable Energy Credits (RECs). Historical and projected REC purchases are shown in the Figure below. As BNL prepares for the EIC, future electricity usage is projected to vary appreciably over the next several years (Figure 1) with the planned schedule for RHIC operations and EIC construction, testing, and phased operations.

FERMI NATIONAL ACCELERATOR LABORATORY

Lab-at-a-Glance

Location: Batavia, Illinois
Type: Single-program Laboratory
Contractor: Fermi Research Alliance, LLC
Site Office: Fermi Site Office
Website: www.fnal.gov

- **FY 2020 Lab Operating Costs:** $523.03 million
- **FY 2020 DOE/NNSA Costs:** $522.184 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $0.85 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 0.2%

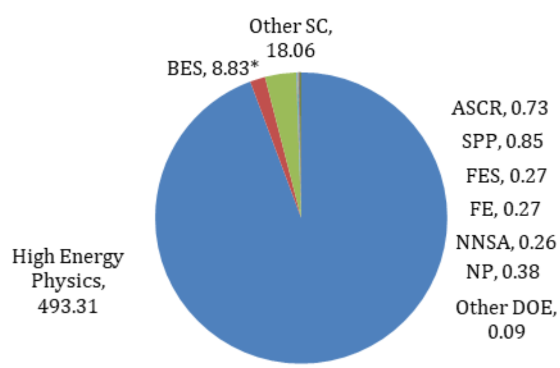
Physical Assets:

- 6,800 acres and 365 buildings
- 2.464 million GSF in buildings
- Replacement Plant Value: $2.64 B
- 28,913 GSF in 10 Excess Facilities
- 22,155 GSF in Leased Facilities

Human Capital:

- 1,818 Full Time Equivalent Employees (FTEs)
- 26 Joint Faculty
- 95 Postdoctoral Researchers
- 7 Graduate Student
- 19 Undergraduate Students
- 2,014 Facility Users
- 1,629 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



*BES number reflects funding of $4.921M provided by SLAC for LCLS-II work and $3.485M for LCLS-II HE work.

Mission and Overview

Fermilab's mission is to be the frontier laboratory for particle physics discovery. Thousands of scientists, engineers, technicians, users, and students from around the globe contribute with their unique talent, expertise, and motivation to push the boundaries of particle physics knowledge and its unique and complex enabling technologies. Fermilab takes pride in being a laboratory that builds and operates world-leading accelerator and detector facilities and looks to the future, performing pioneering research, and advancing technologies beyond the state of the art, ensuring leadership in particle physics discovery over the next several decades. The ambitious goal, endorsed by the 2014 Particle Physics Project Prioritization Panel (P5), is for Fermilab to be the worldwide leader in accelerator-based discovery neutrino science, which is enabled by employing unique accelerator and detector technologies. The construction of the Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE), along with the world's most intense neutrino beams made possible by the Proton Improvement Plan II (PIP-II project), is the first international mega-science project based at a DOE national laboratory. The laboratory has deployed project leadership teams with exceptional depth and experience.

Fermilab's major initiatives include leading one of the five DOE National Quantum Information Science (QIS) Research Centers. The Superconducting Quantum Materials and Systems Center (SQMS) has the concrete and ambitious goal to develop, build, and deploy the first quantum computer at Fermilab. The SQMS Center and other Fermilab efforts are producing high-impact results in quantum computing, networking, and sensing and growing collaborations with universities, laboratories, and industry leaders in QIS.

Fermilab's accelerator complex is the only one in the world to produce both low- and high-energy neutrino beams for science and also enable precision science experiments such as Muon g-2 and Mu2e. The laboratory's unique infrastructure and expertise make Fermilab a world leader in particle accelerator and detector technologies, enabling new particle accelerators for discovery science in many fields, including the Linac Coherent Light Source II High Energy (LCLS-II HE) project, ensuring continued U.S. leadership in photon science. Fermilab is the leading national center for data analysis, data handling, and detector and accelerator development for science at the Large Hadron Collider (LHC). Fermilab hosts several world-leading efforts exploring the mysteries of dark matter and dark energy and is partnering to launch Cosmic Microwave Background Stage-4 (CMB-S4), a major cosmic initiative.

Fermi Research Alliance, LLC (FRA), an alliance of the University of Chicago (UChicago) and the Universities Research Association, Inc. (URA), manages and operates Fermilab for the DOE and provides guidance, advocacy, and oversight. The corporate parents bring considerable operational and intellectual assets to the oversight of the laboratory.

Core Capabilities

Fermilab has unique and powerful infrastructure, essential to advancing particle physics discovery, including the nation's only accelerator complex dedicated to particle physics along with a suite of particle detectors. Scientific research around the world is supported by Fermilab's facilities for design, fabrication, assembly, testing, and operation of particle accelerators and detectors; its expertise and facilities for computing; and a talented workforce with globally competitive knowledge, skills, and abilities. The laboratory is thus uniquely positioned to advance the DOE/SC mission in scientific discovery and innovation with a primary focus on high-energy physics and capabilities that address mission needs for advanced scientific computing research (ASCR), particle accelerators for light sources (BES), nuclear physics (NP), and workforce development for teachers and scientists (WDTS). Fermilab's science mission aligns with the U.S. particle physics community's goals as outlined in the 2014 Particle Physics Project Prioritization Panel's (P5) report. Fermilab has four core capabilities: **Particle Physics; Large-Scale User Facilities/Advanced Instrumentation; Accelerator Science and Technology**; and **Advanced Computer Science, Visualization, and Data**. The laboratory is primarily funded by the DOE Office of High Energy Physics (DOE/HEP).

Particle Physics

Particle physics is the heart of Fermilab's science mission. It is defined by five main science themes—neutrino science, collider science, precision science, cosmic science, and detector R&D — supported by theory, facilities, and workforce development.

Neutrino Science

Fermilab is the only laboratory in the world that operates two accelerator-based neutrino beams simultaneously, the Neutrinos at the Main Injector (NuMI) beamline and the Booster Neutrino Beamline (BNB). These two intense neutrino sources illuminate an important collection of experiments studying neutrinos over both short and long distances, allowing Fermilab's neutrino program to address questions such as whether additional (sterile) neutrinos exist and whether neutrinos violate matter-antimatter (CP) symmetry. The NOvA experiment operates on the high-energy NuMI beamline and explores the parameters of neutrino flavor transformation. This exploration will become comprehensive with the operation of the Deep Underground Neutrino Experiment (DUNE) in a new beamline created as part of the Long-Baseline Neutrino Facility (LBNF) and powered by the Proton Improvement Plan II (PIP-II) accelerator upgrades. The Short Baseline Neutrino (SBN) program on the low-energy BNB searches for sterile neutrinos through a suite of three experiments: the MicroBooNE detector that began operating with beam in 2015, the ICARUS detector that is now in the commissioning phase, and the Short-Baseline Near Detector (SBND) that will follow in 2023. Experience with these liquid-argon detectors will also inform the future flagship international LBNF and DUNE program. This succession of neutrino experiments is prescribed by the P5 report and is being executed by collaborations of scientists enabled by the capabilities that exist at Fermilab.

Collider Science

The Large Hadron Collider (LHC) at CERN, the European center for particle physics, is the world's highest energy particle accelerator/collider. Operating at a center-of-mass-energy of 13-14 TeV, the LHC explores the energy frontier and probes the laws of nature by recreating the conditions of the early universe. Fermilab serves as the host laboratory for more than 800 university-based U.S. scientists and students working on the Compact Muon Solenoid (CMS) experiment, one of two large multipurpose detectors at the LHC. Fermilab is the leading U.S. center for LHC science and second-largest world center after CERN. The laboratory’s globally distributed computational capabilities for the CMS experiment are unparalleled. Laboratory scientists are engaged in physics analyses of LHC data including studies of the Higgs boson, precision measurements of the Standard Model, and searches for new phenomena such as supersymmetry, extra dimensions, and dark matter.

Initiated in 2012 and completed in 2019, the first significant upgrade of the CMS detector allows collection of high-quality data at event rates and radiation levels three times higher than those recorded in the LHC’s first run. Fermilab was responsible for project management of the U.S. contributions to this upgrade project, which was jointly funded by DOE and NSF and includes upgrades of the forward pixel detector, the hadron calorimeter, and the trigger system. The project included 30 partner universities (all part of the international CMS collaboration) that accounted for 80 percent of labor and M&S expenditures and contributed to the project’s success through their unique expertise. The project was successfully completed ahead of schedule, under budget, and was recognized with a DOE Project Management Achievement Award.

A skilled and talented workforce of scientists, engineers, and technicians leverages Fermilab’s accelerator and detector R&D programs and unique facilities to continue contributing essential developments, improvements, and upgrades to the CMS detector and the LHC accelerator. Fermilab is leading the High-Luminosity (HL)-LHC CMS Upgrade Project, the HL-LHC Accelerator Upgrade Project, and U.S. CMS Operations.

Precision Science

Fermilab’s precision science theme includes experiments that attempt to reveal gaps in current understanding of the laws of physics by testing predictions to the highest accuracy and searching for phenomena either extremely rare or forbidden by current theories. Deviations from expectations are possible indications of new particles and new interactions. Fermilab has reconfigured accelerator components to create muon beams, which began to deliver beam to the first experiment at the Muon Campus, Muon g-2, in 2017. The beams will increase in intensity over time, culminating in delivery of the world’s most intense muon beam to the Mu2e experiment in 2024.

The Muon g-2 experiment has presented first results on the positive muon magnetic anomaly, and the tension with the theory calculation has increased to 4.2 standard deviations. This result strengthens the evidence of New Physics and has prompted a wide set of theoretical interpretations and explanations. As improvements are made to the theoretical calculation and new lattice QCD techniques are pioneered, it will be critical to provide a window into the potential New Physics by pushing the experimental precision as far as possible. The Mu2e experiment will search for the spontaneous conversion of muons to electrons. The experiment will be sensitive to new physics manifesting itself in rare processes and with mass scales several orders of magnitude higher than those achievable at the LHC, thereby complementing collider experiments' searches for new particles and new interactions.

Cosmic Science and Detector R&D

Fermilab is a key partner in several world-leading cosmic science experiments and is performing innovative R&D toward new dark energy, dark matter, and cosmic microwave background (CMB) experiments. Fermilab researchers built the Dark Energy Survey (DES) camera and are leading the DES science collaboration. Fermilab is partnering with other DOE laboratories to build three new large cosmic survey projects, including DESI, Rubin Observatory, and CMB-S4. The laboratory is engaged in world-leading searches for particle dark matter, by leading the ADMX experiment and fulfilling major responsibilities for the construction and operation of SuperCDMS SNOLAB. Fermilab plays a critical role in the design of CMB-S4 which will establish the world's most sensitive constraint on the sum of neutrino masses and help explore the phenomenon of cosmic inflation.

DES is the world leader in exploring the mysterious phenomenon of dark energy. Fermilab manages the operation and leads the analysis of this unprecedented optical survey. The survey finished its sixth and final year of data taking in January 2019 and met or exceeded all survey metrics. The observations from the full six seasons have been processed and a new Y6 catalog, containing over 691 million objects, was released to the DES Collaboration in October 2019. So far, DES has produced 231 scientific papers that have been accepted or published. Currently, most DES analyses focusing on cosmology are working with the catalogs based on the Y1-Y3 observations. Fermilab scientists play critical roles in understanding potential systematic errors and the development of cross-checks for galaxy cluster cosmology with this dataset. Additionally, Fermilab scientists lead the Y6 DES data production and data quality effort, and they lead studies of dark matter dominated dwarf galaxy satellites in order to constrain dark matter particle properties. As DES cosmology analyses continue to advance, Fermilab scientists are preparing to play critical roles in Rubin Observatory Legacy Survey of Space and Time (LSST) operations. Fermilab staff have roles in observatory operations, data production, and system performance. In addition, Fermilab scientists are taking on leadership positions in survey simulations, dark matter science, and collaboration operations within the LSST Dark Energy Science Collaboration. Fermilab is committed to efficiently transferring expertise developed on DES into critical roles on the Rubin Observatory LSST.

Fermilab's detector R&D program has supported many cosmic science efforts. Fermilab leveraged its DES experience to pioneer the use of charge-coupled devices (CCDs) as low-threshold detectors in the DAMIC experiment. Fermilab researchers supported by the detector R&D program, an LDRD award and 2018 early career award developed even lower-noise CCD readout, enabling the detection of single electrons and opening a new window on possible ultra-light dark matter particles. The SENSEI project has now produced world leading results in electron-recoil dark matter searches using these sensors. Recently the DOE awarded the collaboration funding to design a next-generation skipper CCD dark matter experiment (OSCURA). Fermilab has continued R&D towards next-generation detectors for cosmic science by developing an underground cryogenic test stand (NEXUS) for the characterization and calibration of cryogenic solid-state detectors with sensitivity to sub-GeV dark matter, such as that developed by the SuperCDMS collaboration. An award made through the new National Quantum Initiative will enable Fermilab researchers to study how the backgrounds that plague dark matter detectors are limiting qubit coherence times. A second underground test stand (QUIET) will be constructed for this effort. See Section 3 for more information about the detector R&D program.

Dramatic improvements in quantum sensing will be one of the first products of the ramp-up of the National Quantum Initiative and Fermilab is at the forefront of the effort to apply novel quantum sensors to the detection of dark matter, including the QCD axion. While current generation experiments are limited by the standard quantum limit in readout noise, future experiments probing higher axion masses and frequencies in the 2 GHz – 10 THz range will rely on new quantum techniques to bypass this constraint, utilizing superconducting technologies including Josephson junctions and microcalorimeters. Supported by a combination of grants awarded through the new DOE QuantISED program, LDRD funding, the DOE Dark Matter New Initiatives program, the National Quantum Initiative, and private foundation funding, Fermilab is leveraging its capabilities in accelerator science and sub-Kelvin electronics to study high-quality-factor resonant cavities, single microwave photon detectors, and highly multiplexed readouts to enable future searches for bosonic dark matter.

Cosmic science provides a showcase for the benefits of broad collaboration among DOE laboratories and universities. As noted in the P5 report, particle physics drivers are intertwined, and cross-project expertise is required to extract the most science from the data. Fermilab scientists are leading these efforts. For example, the observations by DES have led to world-leading constraints on dark matter, and joint analyses of the DES and SPT data sets have shown correlation of cosmic voids in the DES data with regions of reduced lensing of the CMB. Development of new quantum sensors is enabling rapid progress in direct dark matter searches and simultaneously driving progress in quantum information science. Over the coming decades, Fermilab will act as a central platform and host for understanding cosmic science data, maximizing the scientific output of experiments across the field.

Theory, Facilities, and Workforce Development

Fermilab's Theory and Theoretical Astrophysics groups perform research at the confluence of these themes. Fermilab theorists often work with experimentalists to better interpret existing data and to better plan for future experimentation. The laboratory's accelerators and particle detectors, and its fabrication, assembly, testing, and computing facilities provide unique capabilities within DOE and for particle physics research. For example, the Fermilab Test Beam Facility is in high demand for R&D of advanced particle detector technologies. The Office of Education and Public Engagement and the Office of Equity, Diversity, and Inclusion support students and faculty in STEM education and the DOE WDTS mission.

The Fermilab workforce benefits considerably from support provided by UChicago and the Joint Task Force Initiative (JTFI). For example, UChicago provides the Strategic Laboratory Leadership Program at its prestigious Booth School of Business, as well as other professional development opportunities including the Leadership Academy for Women in Science and Engineering. The Fermilab community benefits from three awards given annually by Universities Research Association (URA) to recognize superior academic achievements and to encourage young scientists. URA also sponsors a visiting scholars program and hosts and supports the annual Fermilab users' trip to Washington D.C. The 2020 trip was held virtually, and 71 participants met with 303 congressional offices.

Particle Physics is funded primarily by DOE/HEP with additional funding from DOE/BES (and DOE/SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).

Large-Scale User Facilities and Advanced Instrumentation

Fermilab's Large-Scale User Facilities/Advanced Instrumentation core capability encompasses the Fermilab Accelerator Complex, a DOE/SC user facility, and CMS at Fermilab. The laboratory has the human capital and infrastructure essential to developing, designing, constructing, and operating large-scale user facilities and advanced instrumentation.

Fermilab Accelerator Complex

The Fermilab Accelerator Complex is the nation's only accelerator complex dedicated to particle physics and the second-largest particle physics accelerator complex in the world. Research at this user facility has led to many significant discoveries over more than 40 years of operation, including the top quark, bottom quark, tau neutrino, determination of the properties of charm- and bottom-quark systems, and numerous precision measurements, including the discovery of new matter-antimatter asymmetries in kaon decays.

The Fermilab Accelerator Complex comprises seven particle accelerators and storage rings with particle-beam capabilities found nowhere else in the world. Future upgrades of the accelerator complex enabled by the PIP-II project will provide megawatts of beam power to LBNF and DUNE. Currently, Fermilab uniquely supplies two very intense neutrino sources (the low-energy BNB and the high-energy NuMI beam) that enable the physics programs of the NOvA and MicroBooNE experiments. The BNB will deliver neutrinos to all three detectors of the SBN program. Beams of muons are being delivered to the Muon g-2 experiment following successful reconfiguration and upgrades of the accelerator complex. Fermilab will become the world center for the study of muons when high-intensity muon beams are delivered to the Mu2e experiment. The Fermilab Test Beam Facility is the only U.S. location enabling detector R&D tests with high-energy hadron beams. It is used by more than 200 international researchers annually.

CMS at Fermilab

For almost two decades, Fermilab has served as the host laboratory for the more than 800 scientists and students from approximately 50 U.S. universities who work on the CMS experiment at the LHC in Geneva, Switzerland. Fermilab also leads the HL-LHC CMS Detector Upgrade Project, the HL-LHC Accelerator Upgrade Project, and U.S. CMS operations. Researchers using Fermilab's CMS facilities played leading roles in the 2012 Higgs boson discovery, and ongoing research promises to further revolutionize our understanding of the universe.

CMS at Fermilab consists of the LHC Physics Center (LPC), CMS Remote Operations Center, and the U.S. CMS Computing Facility. The LPC is designed to engage members of U.S. CMS institutions distributed across the country in physics analyses of LHC data and in CMS detector upgrades. The LPC creates a thriving environment for collaboration among participating institutions by facilitating remote participation, conferences, classes, and providing visit opportunities. Through the Distinguished Researcher, Guest, and Visitor programs, collaborators are supported to spend significant time at the LPC, and the CMS Data Analysis School draws more than 100 participants each year. The Remote Operations Center enables physicist participation in remote operations and monitoring of the CMS detector and keeps scientists, students, and technicians connected to operations activities at CERN without the time and expense of European travel. The U.S. CMS Computing Facility at Fermilab is the largest and most reliable Tier-1 computing facility (after the CERN Tier-0 center). As part of a worldwide grid computing capability, this facility is available to qualified CMS researchers around the world.

The LPC enables close communication between CMS scientists and members of the Fermilab theory group. The theory group is deeply involved in advancing LHC new physics phenomenology and improving modeling of Standard Model processes through precision QCD and electroweak calculations.

Fermilab theorists participate in LPC events, share new ideas with the experimental colleagues, and collaborate on analysis projects. Several new ideas leading to CMS and phenomenology publications originated through these close interactions.

Advanced Instrumentation

An experienced and talented Fermilab workforce conceives and develops state-of-the-art particle detector technologies and uses them to construct detector systems. Achievements include the development of very-low-mass silicon detectors for particle physics collider experiments, CCD detectors for the Dark Energy Camera, scintillator detectors used for a wide variety of particle physics experiments, and liquid-argon time-projection chambers used by current neutrino experiments and the future flagship experiment, DUNE. Fermilab's advanced instrumentation capability is used to develop and construct upgrades for the CMS detector at the LHC, including innovative silicon trackers, a silicon-based calorimeter, readout electronics, and R&D for precision timing detectors.

Large-Scale User Facilities/Advanced Instrumentation is funded primarily by DOE/HEP (and DOE/SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).

Accelerator Science and Technology

Fermilab's Accelerator Science and Technology core capability includes five core competencies, strategically aligned with the 2015 HEPAP Accelerator R&D sub-panel recommendations: high-intensity particle beams; high-power target stations; high-field superconducting magnets; high-gradient and high-quality-factor SRF cavities; and accelerator science and technology training. These core competencies are enabled by unique accelerator and beam test facilities and world-leading expertise that sustain Fermilab's leadership role in high-intensity and high-energy accelerator applications. Fermilab has established strategic partnerships in accelerator science and technology with leading universities including Northern Illinois University, Illinois Institute of Technology, Northwestern University, Cornell University, and the UChicago. Fermilab's Illinois Accelerator Research Center (IARC) is uniquely positioned to cement partnerships with industry and universities to increase strategic partnership projects and to advance DOE's accelerator stewardship program.

High-Intensity Particle Beams

Fermilab operates the world's most advanced high-intensity proton accelerator complex dedicated to particle physics. The PIP-II project and future complex upgrades will maintain Fermilab's international leadership and support the next generation of neutrino and precision science experiments. PIP-II leverages laboratory capabilities in accelerating and transporting high-intensity beams in circular and linear accelerators. It is needed as the next step to achieving a beam power of more than 2 MW for LBNF/DUNE and beyond. Results from Fermilab accelerator R&D support the flagship neutrino science program and influence how U.S. and international accelerators are designed, constructed, and operated. Fermilab has achieved more than 700 kW beam power to the NOvA experiment through PIP and is running approximately $2x10^{17}$ protons per hour from the proton source to support the SBN program and the Muon g-2 experiment.

High-Power Target Stations

Fermilab operates three high-power target stations: the 700+ kW NuMI beam (now capable of accepting 1 MW); the BNB; and the muon-production target station for the Muon g-2 experiment. A fourth target station is under construction for the Mu2e experiment. A fifth target station is under design for DUNE, capable of 1.2 MW and upgradeable to 2.4+ MW. Each of these stations include specialized targets with capabilities up to 1.2 MW of beam power, specialized focusing devices (magnetic horns, lithium lenses, graded solenoids), shielding, instrumentation, beam windows, remote handling, and other systems. Fermilab maintains this core competency through the development of these facilities and continuous improvement of its devices and processes. Fermilab also executes a high-power targetry (HPT) R&D program directed at future multi-MW target facility challenges. The laboratory leads the international RaDIATE collaboration researching materials and technologies compatible with high radiation and thermal shock. The HPT R&D program is launching a targetry materials science and technology initiative to create the needed infrastructure (expertise, equipment, and facilities), to ensure Fermilab's core competency in targets evolves to enable multi-MW operation.

High-Field Superconducting Magnets

Fermilab has a long history of developing, fabricating, and delivering advanced superconducting magnets, including the world's first superconducting dipole magnets deployed in a circular collider (the Tevatron). The laboratory's core competency in high-field superconducting magnets, including novel superconducting materials and magnetic components, electromechanical magnetic designs, and technologies, is essential to the luminosity upgrades of CERN's LHC accelerator. This core competency is also critical to enable upgrades of the LHC for operations at higher energies, which require further increases in the maximum magnetic field achievable in accelerator-quality magnets. Infrastructure supporting Fermilab's magnet work includes a superconducting strand and cable testing facility, cable making and coil winding machines, collaring and yoking presses, reaction ovens, a cryogenic vertical magnet test facility for cold masses, a cryogenic horizontal magnet test facility for magnets in cryostats, and cryogenic infrastructure.

High-Gradient and High-Quality-Factor SRF Cavities

Fermilab's SRF expertise and infrastructure comprise a globally renowned core competency in the fabrication and testing of SRF technology. Laboratory staff members play an important role in the design and planning of linear and circular accelerators around the world that depend on SRF technology. This core competency enables Fermilab to be a key partner in the construction of the superconducting linear accelerator for SLAC's LCLS-II free electron laser, the highest-priority construction project in the DOE Office of Science. Fermilab's experienced staff and extensive infrastructure led the way in the design of SRF cryomodules and cryogenic infrastructure for LCLS-II and extended the state of the art for SRF cavity performance. By working with SLAC National Accelerator Laboratory and Thomas Jefferson National Accelerator Laboratory to establish LCLS-II as a world-leading facility, Fermilab is contributing its unique infrastructure and expertise to the broader scientific endeavor while simultaneously enhancing in-house capabilities for future projects like PIP-II. This infrastructure and expertise also position the laboratory to contribute to potential future accelerators and colliders. SRF infrastructure includes chemical processing and high-pressure rinsing of cavities, processing and brazing furnaces, cleanroom assembly facilities, inspection and testing capabilities for both bare and dressed cavities, cryomodule assembly stations, and a complete cryomodule test facility. The laboratory's core competency in SRF technology, including design and production of non-elliptical cavities such as those needed for PIP-II, are also essential to the luminosity upgrades of CERN's LHC accelerator through the application of crab cavities for luminosity control and levelling and to the high energy upgrade of the LCLS-II (LCLS-II HE).

Beam Test Facilities

The Fermilab Accelerator Science and Technology (FAST) facility hosts a unique program of advanced accelerator R&D centered around its Integrable Optics Test Accelerator (IOTA) ring. As the world's only facility focused on intensity-frontier R&D in storage rings, the FAST research program will address key technological and scientific challenges in the realization of next-generation, high-power accelerator facilities. The FAST facility also houses a state-of-the-art, high-brightness SRF electron injector, which principally serves the IOTA program but also facilitates a range of R&D programs with outside collaborators. Furthermore, as the only operational SRF accelerator at Fermilab, the FAST injector also comprises a valuable R&D platform for SRF systems integration and operations.

Accelerator Science and Technology Training

Fermilab is making significant contributions to the nation's accelerator science and technology workforce training. The laboratory hosts the United States Particle Accelerator School (USPAS), which has trained over 4,500 students since its inception in 1981 and has undergone a restructuring that re-establishes the USPAS as a Fermilab-managed program. Fermilab also maintains a renowned joint university/laboratory doctoral program in accelerator physics and technology, and several undergraduate summer internship programs in collaboration with Argonne National Laboratory.

Accelerator Science is funded by DOE/HEP with additional funding from DOE/BES (and DOE/SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission (SC 1, 4, 21, 22, 24, 25, 26, 33, 34, and 35).

Advanced Computer Science, Visualization, and Data

Fermilab's expertise in advanced computer science, visualization, and data enables scientific discovery. This core capability complements theory and experiments to increase scientific knowledge through data collection, storage, reconstruction, simulation, and scientific analysis. Fermilab has a remarkable history of developing, delivering, and deploying computing technologies for the scientific community and has been instrumental in the success of the ProtoDUNE experimental program through contributions to data acquisition (DAQ), data processing, event reconstruction and data analysis. Fermilab will continue to play a critical role in supporting the success of the ProtoDUNE II experimental program.

Fermilab is recognized for expertise in designing, developing, and operating distributed computing infrastructures and facilities, exascale scientific data management, and scientific workflows for data recording, processing, and analysis. The laboratory provides access to large-scale computational and data-management facilities for the CMS experiment at CERN, the LHC Physics Center, neutrino science and precision science experiments, the Dark Energy Survey, computational cosmology, lattice QCD, and accelerator simulations.

The laboratory is a leader in active mass storage and distributed computing, which has evolved to satisfy the rapidly expanding data and computational needs of energy frontier and intensity frontier experiments. Fermilab scientific computing facilities provide active access to exabyte-scale data storage. In addition, Fermilab has developed and is now operating the HEPCloud platform, which provides a unified portal technology for accessing and sharing resources for data processing, storage, and analysis across heterogeneous facilities and platforms. HEPCloud capabilities provide Fermilab computing users [cost] optimized access to DOE/ASCR HPC centers, internationally partnered facilities, university-supported computing clusters, and commercial cloud resources. HEP Experiments including CMS, DUNE, Mu2e, and NOvA are exploiting Fermilab's HEPCloud capabilities to accelerate their scientific discoveries.

Due to the collaborative nature of particle physics research, Fermilab does not develop scientific software or computing capabilities in isolation. The laboratory partners with all DOE/SC laboratories and international laboratories such as CERN, DESY in Germany, and KISTI, the Korean Institute of Science and Technology Information, to work on projects that include accelerator modeling, computational cosmology, and particle physics simulations. Fermilab's strategy is to leverage DOE/ASCR expertise where appropriate to respond to computational challenges presented by the DOE/HEP program through the judicious use of partnership programs such as DOE's Scientific Discovery through Advanced Computing (SciDAC) program, as well as periodic DOE/ASCR calls for proposals.

Fermilab's data center is the single largest U.S. high energy physics computing center with 70,000 processing cores, 45 petabytes of disk storage, and over half an exabyte of data storage capacity on robotic tape systems. State-of-the-art computational facilities enable the laboratory to develop new capabilities to support the DOE scientific mission. Fermilab plays an essential role in developing software and hosting scientific computing projects and three major computing facilities for the science community: a CMS Tier-1 Center; Lattice QCD Computing; and FermiGrid. All these on-site facilities will be accessible through HEPCloud in the institutional cluster model mentioned in Section 3.3.

CMS Tier-1 Center: The CMS experiment uses a distributed computing model in which data distribution, processing, and delivery is handled by seven international Tier-1 centers together with university- and laboratory-based Tier-2 computing and storage facilities. This computing model satisfies the needs of particle physicists by providing data storage and processing power on an extreme scale, interconnected by the strongest networks. The CMS Tier-1 Center at Fermilab is the most powerful worldwide (after CERN's Tier-0 center) for the 3,000-member, 41-country CMS experiment.

Lattice QCD Computing: QCD is the theory that describes how quarks and gluons interact via the strong force and predicts the properties of hadrons such as the proton, neutron, and pion. QCD calculations involve numerical simulations performed on a lattice of space-time points (known as Lattice QCD) that can be extremely computationally intensive. Fermilab operates large computer clusters for such calculations as part of DOE's national Lattice QCD computational infrastructure. The institutional cluster that has been deployed for Lattice QCD calculations will further align the laboratory with a path towards developing HPC-optimized science applications and provide additional computing capacity for non-Lattice QCD science.

FermiGrid: Fermilab is the host laboratory for several neutrino and precision science experiments. It provides computing facilities for these experiments including reliable resources for data recording and processing (the equivalent of the CERN LHC Tier-0 for neutrino and precision science). FermiGrid is the primary HEP facility for non-LHC computing and provides computing and storage resources that are shared among these experiments.

Advanced Computer Science, Visualization, and Data is funded primarily by DOE/HEP with additional funding from DOE/ASCR (and DOE/SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission (SC 1, 4, 5, 6, 21, 22, 23, 24, 25, 26, 27, 29, 33, 34, and 35).

Science and Technology Strategy for the Future/Major Initiatives

As America's premier particle physics and accelerator laboratory, Fermilab is moving forward with new experiments, international engagements, and R&D programs that support all science drivers identified by the U.S. particle physics community in its consensus Particle Physics Project Prioritization Panel (P5) report. A major initiative in the coming years is serving as the host laboratory for the Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE). DUNE is powered by megawatt beams from an upgraded and modernized accelerator complex made possible by the Proton Improvement Plan II (PIP-II) project. Additional key initiatives include solidifying existing and attracting new international engagements and advancing accelerator, detector, and quantum science and technology. Fermilab's scientific vision builds on six strategic goals:

- Be the international hub for neutrino science
- Be the frontier laboratory for particle physics discovery
- Be the world leader in accelerator science and technology
- Drive innovation in particle detector technology
- Advance the forefront of large-scale data analytics and storage
- Develop and host unique national facilities for quantum computing and sensing

Infrastructure

Overview of Site Facilities and Infrastructure

Fermilab's 6,800-acre site and conventional infrastructure network provides the foundation for the laboratory's scientific research and development (R&D). The Fermilab Accelerator Complex is DOE/SC's national science user facility at the laboratory. Fermilab employees and users include scientists and engineers from around the world who use the laboratory's scientific infrastructure for research. The infrastructure is evolving to support the significant requirements of the international LBNF, DUNE, and PIP-II projects and future R&D.

All Fermilab real property in Batavia, Illinois is used and owned by DOE and much dates from the 1960s and 1970s. In addition to the Illinois campus, DOE has a 22,155 gross square footage (GSF) real-property lease with the South Dakota Science and Technology Authority (SDSTA) at the Sanford Underground Research Facility (SURF) in Lead, South Dakota. In FY 2020, there were no new real estate actions, leases, renewed leases, leased disposals, gifts, or third party financed projects. Planning is underway for a future hostel on the Batavia site supported by third-party financed projects. The total Replacement Plant Value (RPV) for conventional facilities is $1.42B. The total RPV including programmatic accelerator and tunnel assets (OSF 3000) is $2.64B. Property use predominantly serves R&D and administrative functions. Other land is preserved for future science by maintaining it as restored prairie, tilled agriculture, or woodland.

Fermilab provides oversight of DOE real property at SURF in both leased space and non-leased (SDSTA-owned) space as part of the LBNF/DUNE Project. The laboratory is working with SDSTA to improve infrastructure and construct underground detectors and support systems for LBNF and DUNE.

The Fermilab Campus Master Plan[2] supports the laboratory's strategic plan and major initiatives and requires investment in demolitions to reduce the laboratory's excess facility operating burden. While here are no demolitions scheduled in FY 2021, the laboratory has projects ready for execution if funds become available and has prioritized demolitions as part of its strategic infrastructure plan.

Fermilab's facility strategy is built on the FY 2014 Laboratory Operations Board (LOB) infrastructure assessment. In FY 2019, Fermilab revised its infrastructure planning process to better align and prioritize infrastructure investments with the science strategy. This process matured in FY 2020 to create an integrated prioritized list of infrastructure projects for execution as funding becomes available. The list includes over 110 infrastructure projects that directly support and/or enhance the following: the laboratory's scientific mission, lifeline infrastructure (e.g., water, sewer, and electrical distribution) reliability, workspace modernization, and laboratory security.

During FY 2020, the laboratory made progress in implementing several new initiatives including:

[2] https://fess.fnal.gov/master_plan/

- Advancing Fermilab’s pilot program of centralized facility management (CFM)
- Establishing a $314M Utilities Infrastructure Project (UIP), building on the 2018 $36M Utilities Upgrade Project
- Defining a project to completely replace the accelerator controls system and associated infrastructure supporting the campus’ central experimental neural controls network (ACORN)
- Defining a significant Wilson Hall renovation project to renovate the laboratory’s central, mission-critical 16-story high-rise
- Maturing facilities condition assessment, planning, design, construction, maintenance, resiliency, and disposition procedures
- Initiating a Strategic Facility Assessment to provide detailed information regarding facility capability gaps and modernization and demolition needs

Types and Conditions of Facilities

Fermilab’s annual facilities and structures assessments reflect an increased percentage of “substandard” and “inadequate” classifications. The FIMS evaluation, utilization, and maintenance cost of existing facilities as of the end of FY 2020 is shown in the snapshot table below. It does not include the detailed facility assessment data Fermilab is gathering through a contracted initiative to assess all facilities. The initial assessment results of the first third of the facilities (140 buildings) indicates a net increase of Deferred Maintenance (DM) cost from $40M to $70M. Future increases are expected as the remaining facilities are assessed.

	Structures				Utilization				Maintenance	
Types of Facility (Usage Codes)	Adequate	Inadequate	Substandard	Total	90-100%	75-89%	50-74%	0-49%	Deferred	Annual
Laboratory/Experiment Buildings (711, 721, 723)	20	9	3	32	32				$1,553,073.00	$1,700,669.00
Accelerator (785, 3221)	53	4		57	57				$2,470,898.00	$2,775,362.00
Office Buildings (101)	16	17	11	44	42	2			$4,802,222.00	$2,037,127.00
Operations Buildings (261, 297, 551, 561, 591,601, 611, 614, 621, 641, 642, 693, 694, 6271, 6719, 7009)	30	13	9	52	50		2		$4,868,367.00	$3,952,871.00
Storage Buildings (400, 401, 410, 4010, 4020, 4171, 450, 4500, 4221)	88	36	11	135	119	6	6	4	$292,164.00	$706,530.00
Residential Buildings (300, 691)	61	1	1	63	62			1	$533,265.00	$977,292.00
Other Building Types (234, 294, 295, 298, 644, 801, 2449, 2909)	21	3		24	18	6			$71,821.00	$264,757.00
Utility Infrastructure (508, 525, 531, 595, 5171, 5569, 5789, 5906, 6919, 7261, 8129, 8131, 8171, 8329, 8549, 8561, 8629, 8719, 8929, 8939, 8949, 8979)	12	4	8	24	23	1			$22,080,806.00	$2,741,194.00
Roads and Walkways (1129, 1169, 1729, 1739, 1749, 1769, 1789)	6	4		10	10	0	0	0	$4,512,824.00	$401,045.00
Culverts, Dams, Fences (2429, 2629, 2819, 2619)	4			4	4	0	0	0	$208,546.00	$89,707.00
Total	**311**	**91**	**43**	**445**	**417**	**15**	**8**	**5**	**$41,393,986.00**	**$15,646,554.00**

The above facilities inventory indicates of the 417 structures operating at or near 100 percent utilization, 134 are inadequate or substandard. Office buildings (FIMS-101) are close to full utilization despite being in a degraded condition. Of the 44 office buildings on site, 28 are either inadequate (17) or substandard (11) with $4.8M in deferred maintenance. Laboratory and experimental spaces (711, 721, 723) reflect $1.5M deferred maintenance, and 12 of 32 buildings are in inadequate (9) or substandard (3) condition. The accelerator complex buildings (785, 3221) are proportionally better with only four of 57 being inadequate; however, they carry a balance of $2.5M in deferred maintenance. The laboratory’s infrastructure priorities align with these needs, targeting utilities and systems (Central Utility Building (CUB), UIP, ACORN), laboratory and office spaces (IERC, CAST, Wilson Hall), and general supporting infrastructure (sanitary sewer improvements).

To illustrate the ongoing usage of facilities at Fermilab, the following chart breaks down the quantity and GSF of buildings and OSF by their operational status.

	Operating		Standby		Shutdown	
	Total	GSF	Total	GSF	Total	GSF
Building/Trailer	388	3,481,245	3	5,772	10	28,913
OSF	52	-	2	-	0	-

As the laboratory completes the FY 2019-initiated site infrastructure condition assessment and completes CFM implementation, the level of substandard and inadequate facilities is expected to increase due to 1) the assessments provide a more detailed facility examination that extends beyond fault and repair history, and 2) the CFM program is expected to provide more timely and accurate facility condition reporting. These CFM planning and reporting mechanisms are consistent with the Safeguards & Security Program and are inherently reliant on the Design Basis Threat and Science and Technology (S&T) Policy requirements. The current S&T Risk Matrix review process is a fluid practice and allows for the future scalability of S&T implementation needs.

Campus Strategy

Fermilab's campus strategy will enable three objectives:

- Close infrastructure gaps associated with emerging science frontiers and existing projects including LBNF, DUNE, PIP-II, and the quantum science program
- Improve the sustainment and resiliency of existing assets
- Recapitalize or dispose of overaged, obsolete, and severely deteriorated infrastructure

Fermilab's infrastructure planning and investment strategy addresses these objectives and ensures Fermilab will continue to provide modern, world-class facilities for scientific research. Fermilab's 10-year S&T plan is the basis of the campus strategy which provides an integrated approach to achieve a campus fully supportive of current operations and future mission requirements. The strategy incorporates facility and utility strategic assessments and a program to centralize facilities management.

Planning infrastructure improvements is a major part of the laboratory's Campus and Facility Planning Board (CFPB) responsibility to support future/major initiatives identified in Section 4. The cornerstone of the campus strategy is the annual process to identify, coordinate, prioritize, and communicate infrastructure needs.

Sustainment

Fermilab has begun a multi-year campaign to ensure site infrastructure is prepared for future science missions which includes significantly increasing laboratory maintenance funding to reach the DOE target by 2024; centralizing facility maintenance and applying a risk-based approach to maintenance investment to align maintenance with overall laboratory strategy; and increasing funding on major repair and renovation projects for science missions.

In FY 2020, Fermilab began updating the facility condition assessments that will, over time, provide a more accurate measure of facility condition. In FY 2021, the laboratory initiated a Strategic Facility Assessment process. Combined with existing facility maintenance and repair records, the assessment data will be used to balance resources and improve risk-based planning and investing. One planned investment in infrastructure modernization will increase the site's digital wireless foundation to provide better coverage for Internet of Things (IoT) devices throughout campus (indoors, outdoors, and underground). This enhanced wireless network will enable real-time remote monitoring, smart metering, and communications at a scale and speed not currently possible.

In FY 2021, the laboratory will fully execute a CFM program. The program enables a lab-wide risk-based facility and infrastructure maintenance investment strategy and enables more accurate facility maintenance planning and reporting. The CFM program will enable Fermilab to more efficiently deploy advanced technologies and data analytics to improve the effectiveness of facility management efforts and investments.

Site Sustainability Plan Summary

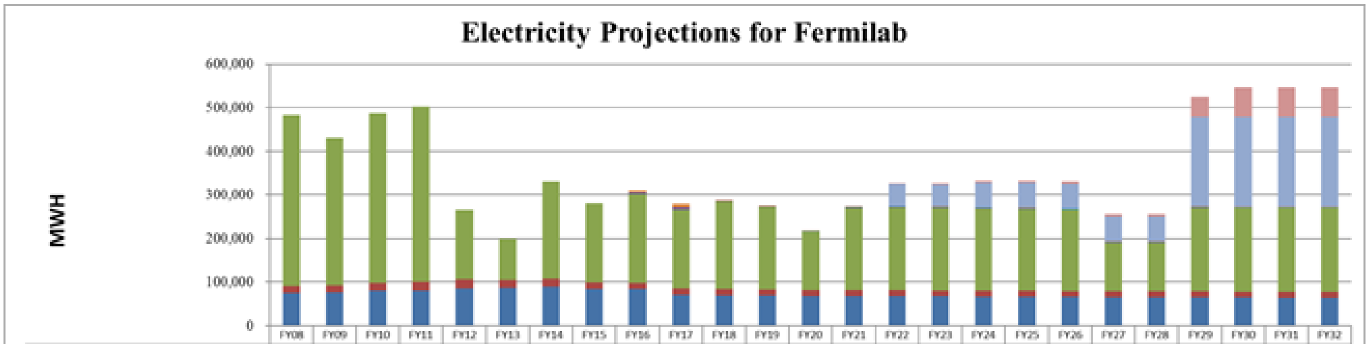
Despite significant operational challenges due to the COVID-19 pandemic, Fermilab continued to advance initiatives in support of sustainability goals. For high-performance sustainable buildings, eight of 58 eligible buildings currently comply with guiding principle requirements. As Fermilab approaches a particularly intense period of conventional facility design and construction to support LBNF, DUNE, and PIP-II projects, an additional ten facilities are projected for completion over the next five years. Additionally, two existing buildings are identified as candidates for sustainable modernization. When completed, these 12 facilities add an additional 277,238 GSF (29 percent of building count, 21 percent of square-feet) of compliant sustainable buildings to the Fermilab site.

Beginning FY 2021, Fermilab will begin a major project to improve its aged sanitary sewer system. This effort plans to repair, replace, or reline approximately 14,000 linear feet of sanitary sewer pipe and services, repair or replace 140 manholes, and repair or upgrade mechanicals to eleven sanitary lift stations. It is expected that upgrades to the sanitary sewer system will ultimately reduce sewage leak losses and improve excessive infiltration/inflow that currently occurs during periods of high precipitation that occasionally overwhelms system capacity.

A funding profile is being coordinated with DOE to execute the UIP. This project will seek to make major investments in upgrading facility utility and operational infrastructure. It is currently supported by DOE at the CD-0 level. The project is divided into three phases to facilitate execution. Phase one: Fermilab anticipates the construction of a new chilled water plant and renovation of the existing CUB. A newly constructed chilled water plant will provide for dynamic expansion as cooling demands increase resulting from upgrades to the laboratory's accelerator complex and associated experimental infrastructure. Phase two: replacement and modernization of the Kautz Road Substation. Phase three: repair and or replace significant segments of primary linear utility systems across the site including potable water, chilled water, industrial cooling water, storm sewers, and electrical distribution infrastructure.

In the area of energy management, in FY 2020, the laboratory's electrical energy consumption was just 66.6 percent of anticipated use. Most of the reduction was due to powering down the accelerator as the laboratory drastically reduced operations in mid-March in response to the pandemic. Actual and projected electricity usage is shown below.

Electricity Use and HEMFs – Actual and Projected FY08-FY32



	FY08	FY09	FY10	FY11	FY12	FY13	FY14	FY15	FY16	FY17	FY18	FY19	FY20
LBNF													
PIP-II													
SBN Near & Far Detectors									3,942	8,870	549	522	670
Mu2e (MC-2)											325	349	471
Muon G-2 (MC-1)									5,081	5,081	933	947	1,057
Existing Particle Accelerators HEMSF	391,208	337,150	390,288	402,903	160,678	94,728	224,837	182,507	203,178	179,477	200,217	189,303	133,630
Existing High Performance Computing HEMSF	16,548	17,215	17,230	19,719	19,542	18,389	16,574	14,743	14,743	15,904	15,321	14,334	13,131
Site Base	74,689	75,595	80,021	80,556	85,979	86,723	90,333	83,857	83,618	70,311	69,310	68,920	68,533

	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30	FY31	FY32
LBNF		1,000	2,000	3,000	4,000	5,000	5,000	5,000	45,552	68,328	68,328	68,328
PIP-II		51,430	51,430	56,993	56,993	56,993	56,993	56,993	205,913	205,913	205,913	205,913
SBN Near & Far Detectors	701	701	701	701	701	701	670	670	670	670	670	670
Mu2e (MC-2)	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752
Muon G-2 (MC-1)	1,057	1,057	1,057	1,057	876	876	876	876	876	876	876	876
Existing Particle Accelerators HEMSF	189,208	190,157	189,532	188,341	187,889	186,253	111,644	112,001	191,882	191,455	191,801	192,144
Existing High Performance Computing HEMSF	13,131	13,131	13,131	13,131	13,131	13,131	13,131	13,131	13,131	13,131	13,131	13,131
Site Base	68,151	67,772	67,397	67,026	66,658	66,294	65,934	65,578	65,224	64,875	64,529	64,186

Significant changes to Fermilab's projected energy consumption are anticipated over the coming decade as the new PIP-II accelerator is brought into service and the LBNF/DUNE complex is tied into the existing accelerator complex beginning in 2029. The connection of LBNF will require a one and half year shutdown that is currently scheduled to begin in 2027. Current electrical use projections reflect recent changes in schedule and differ from data provided in Fermilab's 2021 Site Sustainability Plan. The addition of the PIP-II accelerator and beam requirements for LBNF are expected to increase Fermilab's overall energy consumption by 30 percent over historic peak levels. The laboratory will continue to use renewable energy certificates (RECs) as the primary mechanism to offset greenhouse gas emissions associated with electrical consumption.

LAWRENCE BERKELEY NATIONAL LABORATORY

Lab-at-a-Glance

Location: Berkeley, California
Type: Multi-program Laboratory
Contractor: University of California
Site Office: Bay Area Site Office
Website: www.lbl.gov

- **FY 2020 Lab Operating Costs:** $959.63 million
- **FY 2020 DOE/NNSA Costs:** $862.97 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $95.67 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 10%
- **FY 2020 DHS Costs:** $0.99 million

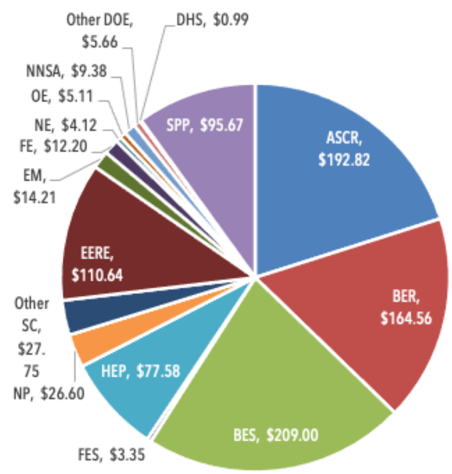
Physical Assets:

- 202 acres and 97 buildings
- 1.7 million GSF in buildings
- Replacement Plant Value: $1.49 B
- 315,471 GSF in Leased Facilities

Human Capital:

- 3,398 Full Time Equivalent Employees (FTEs)
- 1,699 Scientists and Engineers
- 245 Joint Faculty
- 513 Postdoctoral Researchers
- 332 Graduate Student
- 159 Undergraduate Students
- 13,990 Facility Users
- 1,611 Visiting Scientists and Engineers

FY 2020 Costs by Funding Source ($M)



Mission and Overview

For the last 90 years, Lawrence Berkeley National Laboratory (Berkeley Lab) has played an important and distinctive role within DOE's network of great national laboratories. Berkeley Lab delivers scientific breakthroughs over a remarkable range of science, with special focus on research addressing sustainable energy, climate resilience, environmental quality, health, and economic competitiveness. Our most important asset is our workforce, a diverse group of talented, creative researchers and professionals who have committed their careers to finding science solutions to the greatest human challenges of our time.

Berkeley Lab specializes in integrative science and technology, taking advantage of our world-renowned expertise in materials, chemistry, physics, biology, earth and environmental science, mathematics, and computing. We advance the frontiers of science and technology through three approaches: advanced instrumentation and user facilities, large team science, and core research programs led by outstanding investigators. The close integration of these three approaches optimizes the impact of the Lab's research, to the benefit of DOE's missions.

Our five national user facilities provide nearly 14,000 researchers with capabilities in HPC and data science, chemical sciences, materials synthesis and characterization, and genomic science. Our scientific impact is built upon the foundation of strong capabilities in basic and applied science and is amplified by the world-class user facilities.

We have continuing partnerships with other national laboratories on a wide range of projects from subatomic physics to quantum information, biomanufacturing, climate science, water-energy, ecosystem science, and innovative energy technologies. In 2020, we contributed as part of the network of national laboratories to the global campaign to understand the SARS-CoV-2 virus and to counteract the spread of COVID-19.

We have built strong relationships throughout California and particularly in the San Francisco Bay Area region. We partner with local industries to scale up technologies, organizations in disadvantaged communities to collaborate on energy efficient homes, and educators to provide STEM activities to students, especially those in underserved cities.

Berkeley Lab's close relationship with the nation's leading public university, the University of California, brings the diverse intellectual capital of UC's faculty, postdocs and students to bear on the pursuit of DOE's science and energy missions. The Lab's scientific strength is enhanced by its deep integration of basic and applied science and its emphasis on collaboration with the national scientific community. We continue to innovate with our world-class user facilities, capabilities, and expertise to solve the S&T challenges that define our time.

Core Capabilities

Each of Berkeley Lab's Core Capabilities involves a substantial combination of people, facilities, and equipment to provide a unique or world-leading scientific ability to support DOE missions and national needs. Each is executed safely, with minimal impact on the environment and surrounding community. This section summarizes Berkeley Lab's Core Capabilities, their targeted missions, and their funding sources.

The Core Capabilities lend an exceptional depth to our broad research portfolio, while enabling an integration of efforts to better support the DOE missions. To emphasize their strategic nature, the Lab has grouped these Core Capabilities into scientific themes: Large Scale User Facilities/Advanced Instrumentation; Basic Research in Energy; Biological and Environmental Sciences; Computing and Mathematics; High Energy and Nuclear Physics; Accelerator Science and Technology; and Applied Science and Energy Technology.

Large Scale User Facilities/Advanced Instrumentation

Since its inception as the first accelerator laboratory, Berkeley Lab has had an overarching Core Capability of designing, constructing and operating leading scientific facilities for large user communities. Among the national lab system, the Lab has the largest population of users; these researchers produce scientific breakthroughs because of their creative work at these facilities. Below are summary descriptions of the Laboratory's large-scale user facilities. Core Capabilities in other areas of this report, such as Basic Research in Energy, Computing and Mathematical Sciences, and Applied Science and Energy Technology, are key to the success of Berkeley Lab's advanced facilities and instrumentation.

The Advanced Light Source (ALS) is the world-leading facility for high-brightness soft X-ray science, with additional excellent performance ranging from the infrared through hard X-ray spectral regions. Scientists use the data they collect to understand, predict, and ultimately control matter and energy at length scales ranging from the atomic to the macroscopic. This research underpins many of DOE's Core Capability areas, including those involving chemical, material and biological systems. In FY20 the ALS had 1,816 users (1,356 of whom were onsite). ALS-based results appear in nearly 1,000 refereed journal articles annually, ~20% of which are in high-impact journals. Funded primarily by BES, it has an annual budget of ~$65 million.

The Molecular Foundry provides communities of users worldwide – 750 in FY20 (643 of whom were onsite) – with access to expert staff and leading-edge instrumentation to enable the understanding and control of matter at the nanoscale in a multidisciplinary, collaborative and safe environment. Established 15 years ago, the Foundry's reputation as a world-leading center attracts expert scientists from around the globe to do cutting edge research. The Foundry encompasses facilities specializing in characterization, made up of the National Center for Electron Microscopy, along with the Imaging and Manipulation of Nanostructures facility; Nanofabrication; Theory of Nanostructured Materials; and synthesis, focusing on Inorganic Nanostructures, Biological Nanostructures; and Organic and Macromolecular Synthesis. Funded primarily by BES, it has an annual budget of ~$31 million.

The ***DOE Joint Genome Institute (JGI)*** is a national user facility carrying out projects of central relevance to DOE missions in bioenergy, global carbon cycling and biogeochemistry. JGI is the world's largest producer of plant and microbial genomes, with programs focused in three areas: large-scale generation of DNA sequences; development of innovative DNA analysis algorithms; and functional genomics, a strategic focus that includes a growing DNA design and synthesis program and metabolomics capabilities. In FY20, JGI served 2,030 capability users and over 10,500 active data users; its FY21 budget of ~$89 million is funded primarily by BER. JGI's strategic plan lays out the I5 Strategic Framework, encapsulating guiding principles for JGI's activities (identification, interrogation, investigation, integration, and interaction) to guide its transition to an Integrative Genome Science User Facility that will integrate sequence and functional capabilities for systems-level biology. At the end of the 2-year period, 85% of the 2-year milestones are complete.

The National Energy Research Scientific Computing Center (NERSC) supports more than 7,500 users from universities, national laboratories and industry, representing the largest and most diverse research community of any DOE user facility. NERSC is the mission High Performance Computing center for the DOE Office of Science, providing resources for SC's six scientific program offices. NERSC deploys large-scale, state-of-the-art supercomputing and data storage systems, networking, and expert consulting and support services. Over the last decade NERSC's workload has been gradually changing to include a growing number of scientists using NERSC to analyze data from DOE SC's experimental and observational facilities, including light sources, sequencers, telescopes, and microscopes. This growing workload requires new capabilities, including more robust support for AI, data analytics, data management, transfer and sharing and the ability to support complex workflows that originate outside of NERSC. As such, NERSC has developed and deployed key enabling technologies for supporting this growing workload including containers that run on HPC platforms, interactive notebooks for data analysis, and scaling ML and deep learning frameworks to take advantage of HPC scale resources. New workflows are also requiring a more flexible and dynamic HPC system. The Perlmutter (NERSC-9) system, which will be available to users in FY21, will provide a significant step forward in supporting SC user workflows and will provide a boost in computing performance and capability to the user community with more than 6000 NVIDIA GPUs, an all flash file system, and TB/s gateway to ESnet's network. The system will also continue the transition to exascale era architectures by introducing GPUs to the broad SC user community. The NERSC Exascale Science Application Program (NESAP), pairs application developers, with NERSC performance engineers and vendor experts to prepare teams and optimize applications for the Perlmutter system. Thus far NESAP has enabled six key SC applications to achieve a speedup of more than 25X using GPUs on a NERSC development system, compared to performance on NERSC's Edison (NERSC-7) system. One example is a 60X speedup on the LAMMPs code used at multiple national labs and academic institutions. NERSC's scientific impact is enormous: it's cited in more than 2,000 scientific publications each year. In 2020 alone, NERSC systems provided more than eight billion computational hours to researchers. NERSC's FY20 funding was $110 million, provided by ASCR.

The Energy Sciences Network (ESnet) is SC's high-performance network user facility, delivering highly-reliable data transport capabilities optimized for the requirements of large-scale science. ESnet serves as a vital "circulatory system" for the entire DOE national laboratory system, dozens of other DOE sites, and ~200 research and commercial networks around the world—enabling tens of thousands of scientists at DOE laboratories and academic institutions across the country to transfer vast data streams, access remote research resources in real-time, and collaborate on some of the most important scientific challenges, including energy, biosciences, materials, and the origins of the universe. In essence, ESnet is a force multiplier that enhances scientific productivity and expands opportunity for discovery. In the past year, the network transported over an exabyte of data. During FY20, ESnet completed a successful CD 2/3 for ESnet6, a strategic facility project to upgrade its network to meet the increasing data needs of science. In addition, ESnet deployed and transitioned services to a new nationwide optical backbone after deploying optical equipment over 15,000 miles of dark fiber, notwithstanding pandemic conditions and restrictions. In addition, ESnet developed User Portal, my.es.net, was a finalist in the R&D100 awards. ESnet's FY20 funding was ~$90M (ASCR).

Basic Research in Energy

Chemical and Molecular Science. Berkeley Lab has world-leading capabilities in fundamental research in chemical and molecular sciences that support DOE's mission to achieve transformational discoveries for energy technologies, while preserving human health and minimizing environmental impact. The Lab has integrated theoretical and experimental Core Capabilities and instrumentation to enable the understanding, prediction, and ultimately the control of matter and energy flow at the electronic and atomic levels, from the natural timescale of electron motion to the intrinsic timescale of chemical transformations.

Berkeley Lab has expertise in gas-phase, condensed-phase and interfacial chemical physics. State-of-the-art laser systems that generate ultrashort pulses of extreme-ultraviolet light; soft X-ray sources; photon, electron and mass spectrometers; spectromicroscopy; *in situ*, *operando* and other capabilities are all used to advance the understanding of key elementary chemical reactions and excited states, reactive intermediates, and multiphase reaction networks that govern chemical transformations in realistic environments.

The Lab has deep expertise in experimentation, simulation, and theory aimed at a first-principles description of solvation and molecular reactivity confined and complex microenvironments such as interfaces and catalytic nanopores. Novel instrumentation expertise at the ALS pioneers the application of vacuum ultraviolet and soft X-ray synchrotron radiation to critical problems in chemical dynamics and interfacial chemistry.

The Lab is a world leader in ultrafast attosecond and femtosecond probes of electron dynamics, electron momentum-imaging instrumentation, reaction microscopy, and theoretical methods that probe how photons and electrons transfer energy to molecular frameworks. These capabilities are key to understanding and ultimately controlling energy flow at the atomic scale. These laser-based ultrafast X-ray sources for chemical and atomic physics contribute to the knowledge base for current and future powerful FEL-based light sources.

Berkeley Lab's catalysis capabilities span fundamental research on homogeneous and heterogeneous chemical conversions for high efficiency and selectivity. The Catalysis Facility co-locates a suite of state-of-the-art instruments for synthesis and analysis, including high-throughput dryboxes, a micromeritics analyzer, flow UV-vis spectroscopy, liquid chromatography, pressure reactors and FTIR instrumentation. The core strengths are in three pillars of catalysis: mechanisms, transformations, and environments, to elucidate fundamental principles in catalysis and chemical transformations at the molecular level. Research on both the catalytic center and its environment advance the field from discovery to catalyst design.

The Heavy Element Research Laboratory (HERL) has unique capabilities for determining the electronic structure, bonding and reactivity of compounds of the poorly understood actinides, including the transuranic elements. Our leading scientific personnel and instrumentation characterize, understand, and manipulate rare earth complexes for the discovery and separation of alternative elements and technology-critical materials, including those for energy storage, motors, solid-state lighting, batteries, and quantum information storage.

Berkeley Lab's flagship geosciences group possesses the expertise and methods to discover and model the fundamental processes controlling subsurface resources, with an emphasis on molecular-scale interfacial processes that govern couplings between chemical reaction and rock mechanics. Studies are performed with advanced laboratory methods including quantum sensing, through collaborations with the Molecular Foundry and the Advanced Light Source to develop electron and X-ray probes of Earth fluids and minerals, and through multi-scale molecular modeling and machine learning. Primarily focused on the Lab's Basic Energy Sciences mission, the geosciences group also contributes knowledge to the Lab's Earth Systems Science programs, described below.

Berkeley Lab has exceptional capabilities in solar photoelectrochemistry, photosynthetic systems, and the physical biosciences. These photosynthetic and photoelectrochemistry capabilities, together with spectroscopies and unique *in situ* imaging methods that use photons in the energy range from X-rays, in particular free-electron lasers, to infrared at high temporal resolution, enable elucidation of the structure and elementary mechanisms of biological and artificial photon-conversion systems. The in-depth understanding of artificial and natural photosynthesis forms a basis for efficiently engineered solar-conversion systems. Berkeley Lab is lead partner for the Liquid Sunlight Alliance, the DOE Energy Innovation Hub devoted to the development of new photoelectrochemical approaches to fuel production.

This Core Capability is supported primarily by BES, with important contributions from ASCR. Other DOE contractors and SPP enable this Core Capability, which supports DOE's mission to probe, understand and control the interactions of phonons, photons, electrons and ions with matter; and to direct and control energy flow in materials and chemical systems.

Chemical Engineering. At Berkeley Lab, this Core Capability links basic research in chemistry, biology and materials science to deployable technologies that support energy security, environmental stewardship and nanomanufacturing. Leading capabilities are provided in the fields of chemical kinetics; catalysis; molecular dynamics; actinide chemistry; electronic, biomolecular, polymeric, composite, and nanoscale materials; surface chemistry; ultrafast spectroscopy; crystal growth; mechanical properties of materials; metabolic and cellular engineering applied to recombinant DNA techniques that create new chemical processes within cells and vesicles; and new methodologies for genomic and proteomic analysis in high-throughput production that enable gene libraries that encode enzymes for metabolic engineering; and technologies that integrate chemistry, biology, and bio-inspired approaches into a single process or reactor design.

Other program components translate fundamental research in catalysis, chemical kinetics, combustion science, hydrodynamics and nanomaterials into solutions to technological challenges in energy storage. The Advanced Biofuels and Bioproducts Process Development Unit (ABPDU), supported by EERE and SPP, integrates biological and chemical unit operations through bioprocess engineering to understand and optimize processes for producing biofuels, renewable chemicals and proteins relevant to the industrial biotechnology industry. Berkeley Lab also has expertise in chemical biology and radionuclide decorporation, necessary for characterizing mammalian response and developing sequestering agents for emergency chelation in humans in case of heavy-element or radioactive contamination.

Berkeley Lab is a leader in materials for advanced battery technology, and develops low-cost, rechargeable, advanced electrochemical devices for both automotive and stationary applications. This effort includes numerous applied R&D programs funded by EERE VTO and the collaborative JCESR program. The related field of fuel-cell research enables the commercialization of polymer-electrolyte and solid-oxide fuel cells for similar applications.

This Core Capability is supported by BES, ASCR, BER, EERE, and SPP, including NIH, DoD, universities, and industry. It supports DOE's missions to foster the integration of research with the work of other organizations within DOE, as well as other agencies, and applies directly to DOE's energy security and environmental protection mission, including solar and biofuels.

Condensed Matter Physics and Materials Science. Berkeley Lab researchers integrate state-of-the-art, and often world-unique capabilities in synthesis, characterization, theory and computation to design and understand new materials and phenomena. These capabilities push the boundaries of materials research towards fundamental spatial, temporal and energy limits with the potential to directly and significantly impact solutions to grand challenges in energy, environment, security, and information technologies.

A key Berkeley Lab strength in this capability is in quantum materials, encompassing weakly correlated topological phases such as topological insulators and Weyl and Dirac semi-metals, and materials that exhibit novel forms of magnetic, electronic and geometric/spatial order, including 2D materials such as graphene or van der Waals heterostructures. Through its efforts within the BES core programs and the Center for Novel Pathways to Quantum Coherence in Materials, we are targeting new paradigms for the creation and control of coherent phenomena in materials. Novel states of matter can be explored in the ultrafast time regime, including when the system is driven far from equilibrium.

In addition, we have developed comprehensive capabilities for top-down and bottom-up synthesis and patterning of complex materials. A long track record of groundbreaking discoveries related to the synthesis of inorganic nanoparticles and nanowires has more recently been extended to highly complex and structurally dynamic ionic semiconductors. The Lab also has specific expertise in synthetic polymer synthesis, including sequence-defined polypeptoids, and organic/inorganic nanocomposite synthesis that can precisely and simultaneously control the nanoparticles and their spatial arrangements.

Berkeley Lab has deep expertise in theory and computational simulations in conjunction with novel synthesis approaches that rely on machine learning and AI concepts, which are critical to the discovery and design of new materials. Researchers develop models for understanding, predicting, and controlling complex materials with targeted properties. The Center for Computational Study of Excited-State Phenomena in Energy Materials develops new general software, theories, and methods to understand and predict excited-state phenomena in energy-related materials from first principles with exascale performance. Open access to analysis tools and computed information on known and predicted materials provided by the Materials Project helps the Lab to conduct computational work in high-throughput modalities.

Berkeley Lab researchers leverage the unique X-ray characterization capabilities at the ALS as well as signature electron microscopes and other instruments at the Molecular Foundry, among other facilities, to characterize properties and behavior of materials. By elucidating structure, function, and reactions, specifically at interfaces between various phases of matter, Lab researchers better understand how new materials may perform in various energy-relevant environments. Efforts rely on developing instrumentation for time-domain approaches in spectroscopy, diffraction, and quantitative microscopy. Advancing X-ray, electron beam, and scanning probe techniques, including for operation under cryogenic conditions, and *in situ* and *operando* environments with near-atomic resolution, is a key focus. Unique characterization tools include time-resolved angle-resolved photoemission spectroscopy for studies of materials far away from equilibrium as well as ultrafast electron diffraction.

The Lab is a key partner in the ANL-led Joint Center for Energy Storage Research (JCESR), which seeks to understand electrochemical materials and processes at the atomic and molecular scale, and to use this fundamental knowledge to discover and design next-generation electrical energy-storage technologies. Our understanding of materials and chemical processes at a fundamental level will enable technologies beyond state-of-the-art lithium-ion batteries.

We are addressing some of the looming challenges in microelectronics, often described as the era beyond Moore's Law, through a co-design approach, where transformative materials discoveries driven by advanced computation and property characterization are integrated with the design of device and system architectures and scale-up processing.

This Core Capability is primarily supported by BES, with important contributions by ASCR, EERE, and DoD, as well as other SPP sponsors from industry. It supports DOE's missions to discover and design new materials and molecular assemblies with novel structures and functions through deterministic atomic and molecular scale design for scientific discovery, innovative energy technology, and improved homeland security.

Earth Systems Science. Our geosciences group, the largest and most comprehensive in the DOE complex, develops knowledge and predictive models to describe the full range of complex subsurface processes and their impacts on energy and water systems as well as on aboveground infrastructure. We use diverse laboratory and field methods to probe chemical, physical, thermal, and mechanical processes under relevant subsurface conditions and on length scales from nanoscale pores to reservoirs. A particular expertise lies in the development and use of high-resolution time-lapse imaging approaches, from *in situ* X-ray tomography at the ALS and the Rock Dynamics laboratory to field-scale monitoring of dynamic subsurface processes using acoustic and electromagnetic methods. In partnership with the ALS, our geoscientists have constructed an X-ray microscope at Beamline 11.3.1 for fundamental studies of rock and materials deformation and failure. Experimental field research efforts at LBNL and across the complex benefit from the Geosciences Measurement Facility (GMF), which provides exceptional expertise and tools to design, build, test, and deploy new equipment and instrumentation, and sampling tools required for geoscience investigations, including large field scale deployments.

BES support enables researchers to discover the molecular-scale mechanisms of fluid-rock processes and to translate molecular- and nano-scale insights into larger-scale models and capabilities. Our flagship geosciences program is unique in the U.S., and unifies the disciplines and the expertise needed for mechanistic understanding of how rock-fluid systems evolve in response to stress and reactive fluids and solutes, knowledge that is required for accessing subsurface geologic resources. We develop and integrate powerful experimental methods with exceptional expertise in molecular-to-continuum scale theory and modeling. World class instrumentation is used to quantify geologic fluids, solutes and minerals under elevated temperature and pressure, including *in situ* X-ray imaging and spectroscopy and facilities. The group designs and constructs novel instruments capable of measuring the geochemical and mechanical evolution of out-of-equilibrium interfaces or rocks. The group is a leader in the use of cryogenic transmission electron microscopy of clay minerals to provide insights into the pathways for clay swelling and ion exchange, and uses complementary coherent X-ray scattering methods for dynamics. We also advance and integrate stable isotope measurements, including clumped isotope methods, to identify and interpret chemical signatures of rock-fluid interactions. Advanced experiments on geologic samples help to understand chemical-mechanical dynamics on timescales of picoseconds to millions of years. Exciting emerging computational capabilities include the first coupled geochemical-geomechanical model for chemically mediated deformation and the integration of ML and molecular simulation for efficient prediction of complex fluid and interface properties. ECRP awardee Laura Lammers is developing predictive, first-principles models for mineral formation under relevant geochemical conditions through interfacial experimental science and molecular modeling.

Translation of fundamental knowledge to increasingly accurate subsurface simulations is a cross-cutting goal and one that ultimately requires HPC. Supported by ASCR, Berkeley Lab leads the only two subsurface exascale application projects in the complex. The first project focuses on scale-adaptive approaches to simulate, from the micro- to the reservoir scale, the coupled hydrological, chemical, thermal, and mechanical processes that are critical to many subsurface energy applications, including geologic CO_2 sequestration, oil and gas extraction, geothermal energy production, and nuclear waste isolation. The second project, referred to as EQSIM, is preparing to exploit emerging DOE exascale computers for a transformational advancement in the ability to simulate earthquake processes at regional scale. Over the past three years, EQSIM has made major computational and algorithmic advancements and regional scale simulations (e.g., the entire San Francisco Bay Area) can now be performed routinely at unprecedented frequencies of engineering interest – up to 10 Hz – with computer run times on the order of 6-7 hours. This new capability is being used to improve the understanding of the complex spatially varying distribution of regional earthquake risk with ultimate broad applicability to urban, transportation and energy infrastructure systems.

The Lab's applied subsurface portfolio is primarily supported by EERE-Geothermal, FE Clean Coal, FE Oil & Gas, NE Spent Fuel and Waste Disposition, and by several significant SPPs, with other support from OE, EM, CESER and NNSA. The synergies between BES and applied geoscience programs at Berkeley Lab contribute to an understanding of how fundamental processes influence reservoir-scale processes — and how reservoirs can be manipulated for beneficial utilization while minimizing environmental risks. It is critically important to extend geoscience theory and approaches to the field scale, where research can be done under *in situ* conditions, across compartments and scales, and in the presence of natural forcings. To this end, the Lab has developed and is conducting significant research at several field-based subsurface energy test facilities. For example, our Geothermal program seeks to realize enhanced geothermal systems (EGS) and more flexible geothermal energy production. In support of this effort, the Lab leads the multi-lab EGS Geothermal Collab project, where novel stimulation and heat mining production methods are tested *in situ* in boreholes drilled from deep tunnels at the SURF facility in South Dakota.

Beyond the Collab project and related research on enhanced geothermal systems, Berkeley Lab has a significant and broad portfolio in geothermal technologies research, including discovery of conventional hydrothermal resources, direct use of geothermal for heating and cooling, thermal energy storage, and exploration of synergistic benefits such as the extraction of critical materials from geothermal brines.

For example, working with LLNL and Rice University, LBNL is leading a project using dark fiber within the Imperial Valley to investigate if distributed acoustic sensing (DAS) and distributed thermal sensing (DTS) can identify the presence of hidden geothermal resources. We are also a partner in three new research projects funded by the international Geothermica consortium: 1) SPINE, developing a new tool and protocols to conduct stress profiling in crystalline rock for improved EGS reservoir creation; 2) DEEP, developing improved seismic monitoring technologies, modeling capabilities and process understanding to reduce the risk of induced seismicity associated with EGS; and 3) DEEPEN, developing a play fairway analysis methodology for geothermal plays associated with magmatic geothermal systems. Also with funding from EERE-Geothermal, the Community Geothermal project focuses on integrating low-temperature geothermal energy and subsurface energy storage techniques directly with the needs of communities and the built environment.

The project works with internal and external teams to couple building controls and model programs with subsurface simulators to expand the services that the subsurface can provide to the built environment. It also explores new ways to combine other renewable energy resources like solar with long-duration energy storage in the subsurface to create the hybrid energy systems of the future, and to provide energy as well as heating and cooling. Researchers are exploring additional energy storage technologies, including the porous media-compressed air energy storage (PM-CAES) and subsurface hydrogen storage — activities that are well aligned with the goals set in DOE's Energy Storage Grand Challenge Roadmap. Considering the future energy revolution will depend on access to critical minerals, Berkeley Lab has initiated several activities and projects to ensure ready supplies of these elements. This includes a focus on lithium with the Lithium Resource Research and Innovation Center (LiRRIC); four Li recovery projects have already been launched with key partners as described earlier.

The Lab's FE Oil & Gas portfolio includes efforts such as investigating hydrocarbon recovery processes from shales across scales, including improved stimulation and production methods for more efficient and environmentally sustainable hydrocarbon recovery. Berkeley Lab continues to be instrumental in advancing the feasibility of gas production from gas hydrates—(1) through research projects to develop tools for assessment of production methods from hydrate resources or to evaluate production techniques for an ongoing field test in Alaska; and (2) through scientific outreach such as providing Technical assistance to India's Ministry of Oil and Natural Gas. Berkeley Lab also leads three projects in the Fossil Energy Fundamental Shale program, is a partner in field-based research at the Eagle Ford Unconventional Testbed (Texas), and leads a collaborative multi-national lab - project to evaluate shale stimulation that occurred in the Hydraulic Fracturing Test Site in the Permian Basin of Texas.

The Lab's FE Carbon Capture and Storage (CCS) research focuses on enabling geologic carbon sequestration at scale to support an effective transition from a hydrocarbon-based to a clean energy future. Key aspects of our program include evaluating carbon sequestration risks through DOE's National Risk Assessment Partnership (NRAP) program, developing advanced monitoring and accounting solutions and testing them at various demonstration sites, such as the Decatur project in Illinois, the Aquistore site in Canada, or the Otway site in Australia. In another field demonstration site in Switzerland, our researchers have pioneered and demonstrated an experimental method that allows controlled fault activation tests deep underground, providing a window into the complex processes leading to induced seismicity. The Lab is a key partner in the Brine Extraction Storage Test in Florida, developing synergistic approaches to couple CCS pressure management with brine desalination methods. We also assist the Gulf of Mexico Partnership for Offshore Carbon Storage (GoMCarb) project by carrying out novel offshore modeling (CO_2 blowout into water column) and monitoring (seafloor dark fiber) of CO_2 leakage for risk assessment and assurance monitoring. In DOE's new multi-institutional

SMART Initiative (Science-informed Machine Learning for Accelerating Real Time Decisions in Subsurface Applications), Berkeley Lab scientists are applying ML techniques to monitoring data and reservoir simulation that will contribute to development of a virtual learning environment applicable to design and management of subsurface geologic carbon sequestration sites and oil and gas applications. Further complementing its CCS activities, we are actively developing and refining a Lab-wide Carbon Negative initiative, including terrestrial and geological solutions based on enhanced mineralization of rock resources for carbon removal.

Finally, through support from NE's Spent Fuel and Waste Science and Technology Program, Berkeley Lab is developing advanced approaches to enable safe long-term geologic disposal of nuclear waste and concomitant environmental protection. Our research centers on studies of complex coupled subsurface processes — thermal, hydrological, mechanical, and chemical (THMC) — which will be triggered by perturbations from the repository construction, engineered barrier emplacement, and waste disposal. Numerical modeling methods for evaluating and predicting these coupled processes are being developed and tested against experiments conducted at multiple laboratory and field scales, from micro-scale imaging of clay swelling and clay rock damage in laboratory settings to large *in situ* experiments conducted in Underground Research Laboratories (URLs). THMC studies are critical for the evaluation of the potential long-term impacts on repository site safety. For example, temperature rise from radioactive decay may trigger an increase in pore pressure, mechanical deformations, and chemical reactions, possibly causing rock damage and mineralogical changes, which could strongly affect radionuclide transport.

Complementary to the DOE-supported research at Berkeley Lab are several significant recently awarded projects with the California Energy Commission. One project targets improved monitoring and risk assessment for underground natural gas storage (such as the risks to natural gas pipelines arising from land subsidence or seismicity). And, at The Geysers geothermal field, a second project is demonstrating how seismic and electromagnetic data can map geothermal reservoirs and create enhanced structural imaging to better target production wells. A third project is developing networked observational systems to quantify methane fluxes from energy infrastructure using aircraft, towers, and intensive ground-based sensors. These awards are in addition to those related to mineral recovery from geothermal brines mentioned earlier.

Berkeley Lab recognizes a tremendous opportunity to transform the way society designs, monitors, and maintains critical infrastructure systems via rapid advancements in computational simulations, sensors and communications, and high-performance materials. Our capabilities and involvement in research associated with critical infrastructure and natural hazards have realized substantial growth in the past years. Lab scientists have now established a significant program in this area with funding from DOE, the State of California, LDRD, local governments, and local stakeholders. In a major effort supported by the DOE Exascale Computing Program, the Office of Nuclear Safety, and NNSA, Berkeley Lab is leading development of transformational simulation tools and a new experimental testbed for earthquake ground motion simulations. This effort is closely coupled to new computational models for predicting the infrastructure damage through advanced nonlinear response simulations of soil/structure systems. Leveraging DOE's HPC ecosystem, this work will yield an unmatched fault-to-structure simulation capability that can reduce current uncertainties in earthquake processes. These capabilities will have widespread applicability to DOE sites and the vast DOE enterprise of unique, mission-critical facilities, as well as spin-off applications to other sectors (e.g., energy, water, transportation). For example, a project supported by DOE's Office of Cybersecurity, Energy Security and Emergency Response uses these advanced simulation capabilities to assess hazards and risk associated with electrical and gas transmission systems as a basis for grid resilience and energy reliability planning.

Berkeley Lab scientists are also working on exciting new characterization and monitoring methods to better constrain risk-relevant properties of natural and engineered systems. For example, LDRD support has been used to develop ultra-dense monitoring methods for subsurface parameters and ground motions. One of these methods employs unused telecom fiber optic cables, referred to as “dark fiber,” to achieve spatially unparalleled acoustic sensing and ambient noise tomography in urban settings. A new LDRD focuses on using 5G, AI and novel distributed wireless sensors to remotely detect ground movement and to investigate associated hydromechanical behaviors. Lab scientists have also developed and tested advanced optical sensor and wireless communication systems that allow, for the first time, rapid determination of potential damage in critical building structures immediately after a natural hazard event. These sensors have been installed in Berkeley Lab’s Wang Hall and are currently being designed for installation in BioEPIC. The application space of these technologies and tools is quite broad and can impact a wide range of infrastructure systems including energy facilities, industrial complexes, pipelines, levees, bridges, and buildings.

Biological and Environmental Sciences

Many of the most pressing energy and environmental challenges of our time require an ability to understand, predict, and influence environmental and biological systems. For this we need a new and deeper understanding of fundamental biology, Earth processes, and their interactions. Berkeley Lab is transforming our ability to decipher and map the vast networks of these interconnected systems, the scale of which range from nanometers to thousands of kilometers, and from nanoseconds to centuries. This enables predictions for how environmental changes impact biological systems and vice versa; to harness biology for sustainable energy and other valuable products; and to develop understanding of dynamic, multi-scale Earth systems. Our growing suite of fabricated ecosystem platforms and sensors is enabling new strategies to predictably and reproducibly establish, monitor, and perturb laboratory ecosystems at multiple scales.

Biological and Bioprocess Engineering. Our strengths in biological systems science are complemented by unique capabilities for biological and bioprocess engineering to translate fundamental science discoveries to use-inspired solutions for energy and environment. We have world-renowned capabilities in synthetic biology, technology development for biology, and engineering for biological process development. By leveraging resources such as the JGI, the DOE Systems Biology Knowledgebase (KBase), the ALS, the Molecular Foundry, NERSC, and programs like ENIGMA, we can develop the new technologies and processes needed to create renewable fuels and chemicals, remove environmental contaminants, and support capture and storage of carbon in soils and in durable products from point sources and the atmosphere.

The Joint BioEnergy Institute (JBEI) is one of the four DOE BRCs whose mission is to advance science, engineering, and technology to support the maximum possible conversion of carbon from lignocellulosic biomass to liquid transportation fuels and bioproducts. Using molecular, computational, and high throughput technologies, JBEI has successfully altered biomass composition in model plants and bioenergy crops, demonstrating that ionic liquids can deliver near-complete dissolution of plant biomass to facilitate its conversion to sugars and lignin-derived intermediates needed to produce energy-rich biofuels and advanced bioproducts. In a project funded by the California Energy Commission, JBEI scientists worked with Aemetis, the leading biofuel company in CA, to scale-up a conversion process pioneered at JBEI. This project successfully developed, optimized and scaled an innovative “one-pot” ionic liquid pretreatment technology developed to convert waste woody biomass to fermentable sugars at 83% yields. This technology was scaled-up to the pre-commercial scale, and then the hydrolysate was converted into cellulosic ethanol by *Saccharomyces cerevisiae* with an overall fermentation efficiency exceeding 90% and achieved overall carbon conversion efficiency from biomass to fuel of nearly 80%.

This process required no solid-liquid separations. Scale-up from prior lab scale (~2 liters) to a working volume of 680 liters in a 1,600 liter industrial-level fermenter was an important validation of commercial feasibility and scalability of the entire process.

The production of commodity and specialty biochemicals from biomass brings environmental and economic benefits, as well as the possibility of producing diverse, novel molecules through biological conversion pathways that are challenging or currently impossible using chemical synthesis approaches. Industry realizes the economic potential of such breakthroughs, and licensed technologies and startups from JBEI's activities are steadily coming out of the strong industrial affiliate program.

The Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) provides capabilities for scale-up of biofuels pretreatment, saccharification, and fermentation methods. In collaborations with national labs and with industry, this facility develops new and optimizes existing processes for biofuels and bio-based chemicals and materials processes. In FY21, the ABPDU team helped three companies scale-up production of new technologies that could aid in ending the COVID-19 pandemic. For CASPR bio, ABPDU optimized the fermentation process, scaled-up to 10 liters, and purified their CRISPR enzymes which were tested in rapid COVID detection tool kits. ABPDU also scaled-up technologies from Swiftscale on COVID antibodies and Digestiva on enzymes for protein digestibility to 300L. These projects were all rapidly executed within two months each. It has been instrumental in developing and optimizing new processes for bio-based chemicals and materials. ABPDU company partners have brought eight products to market as a result of the process improvements and optimizations enabled by projects with the ABPDU. Some of the ABPDU core strategic industry partners include: Bolt Threads, Checkerspot, Lygos, and Mango Materials.

Successes from JBEI, the other BRCs, and other biological engineering programs have given rise to Berkeley Lab's Agile BioFoundry (ABF), with the potential to transform manufacturing practices through advanced bioconversion technologies in support of a bio-based economy. Supported initially with LDRD, DARPA, and EERE funding, the ABF was established in FY17 as a seven-lab consortium with funds from EERE's BETO. Led by Berkeley Lab, the ABF consortium leverages capabilities across the complex; its partners include ANL, LANL, NREL, ORNL, PNNL, and SNL. The ABF integrates computer-assisted biological design, advanced metabolomics and proteomics techniques, machine learning, technoeconomic and sustainability analysis, and process integration to optimize biological process design and develop methods for predictable scaling. The ABF consortium engages with private sector stakeholders through its industry engagement team and its advisory board of experts from companies in the bio-based products and biological computing fields. In FY20, the ABF is continuing 11 projects (eight for industry, three for academia) resulting from a directed funding opportunity (DFO) in FY17 and two EERE funding opportunity announcements from FY18 and FY19. Ranging from technology integration into the ABF workflow (software, equipment) to the development of novel biological engineering technologies and pathways (biosensors, new pathways for novel products), these projects aim to solve problems of relevance to industry while building out the ABF's capabilities. The ABF has initiated an FY21 DFO to solicit additional industry and academic partner projects, and has built strong ties to industry through relationships with LanzaTech, Lygos, Teselagen, and Agilent.

BER and EERE are the primary supporters of this Core Capability, building upon capabilities and programs established with BER funding. Other key sponsors include industry and other SPP; anticipated sponsors include USDA, DoD, and the NIH. This Core Capability supports DOE's objectives by applying understanding of complex biological systems to design systems; by creating technologies for bioenergy and bioproduct production; by increasing commercial impact through the transition of national lab-developed technologies to the private sector; utilization of national lab facilities and expertise; and demonstration and deployment for the economic, energy, and national security.

Biological Systems Science. As described below, Berkeley Lab sustains leading capabilities in systems biology, genomics, secure biodesign, structural biology, and imaging at all length scales (from protein structure to ecosystems). The Lab is also a national leader in microbial biology, cell biology, plant biology, microbial community biology, environmental sciences, and computational biology. The capability is further enhanced by instrumentation at the ALS, DOE JGI, the Molecular Foundry, NERSC, NMDC, and JBEI. The Lab has the capability to characterize complex microbial community structure and function; manage highly complex biological data; visualize biological structure; and produce large-scale gene annotation.

The JGI provides a diverse scientific user base with access to state-of-the-art genomic technologies and scientific expertise to enable biological discoveries and applications in the DOE mission areas of bioenergy, nutrient cycling, and biogeochemistry. This national user facility offers a suite of capabilities that are unique in their ability and scale to advance energy and environmental science. Now well beyond a production sequencing facility, today the JGI offers users a comprehensive set of integrative genome science technologies such as state-of-the-art sequencing technologies, advanced genomics data science and informatics, epigenomics, single-cell genomics, DNA synthesis, and metabolomics. This suite of capabilities enables users to derive deeper biological insights.

JGI produces a variety of environmental omics data that requires everything from a single node to a supercomputer to process and analyze. The single-node workload is supported through personal computers, or LBNL IT resources, whilst the large-scale computing needs are well met by resources at NERSC. JGI currently has a gap in mid-range computing to support analysts and research scientists running complex workflows to explore large amounts of data where the complexity is not known a priori and facility upgrades at LBNL in IT or IGB would enable JGI to meet this need. To further address scientific productivity as well as organizational resilience, JGI has developed and deployed software and hardware infrastructure that distributes work across LBNL IT and NERSC. In FY21, JGI will expand the capabilities of this distributed computing system. JGI will maintain a central data repository at NERSC and will continue to leverage NERSC for large-scale analyses on the Cori and Perlmutter systems. JGI has also engaged in a significant effort to make all data and analysis products Findable, Accessible, Interoperable, and Reusable (FAIR). Finally, JGI will deploy a new interface to its data that will make it more discoverable by humans and machines. The design of this new interface was informed by a rigorous user-centered design approach to meet the needs of the community.

KBase is an open source, open access software and data platform designed to address the grand challenge of systems biology – predicting and designing biological function from the biomolecular (small scale) to the ecological (large scale). KBase enables researchers to collaboratively generate, test, compare, and share hypotheses about biological functions; perform large-scale analyses on scalable computing infrastructure; and combine experimental evidence and conclusions that lead to accurate models of plant and microbial physiology and community dynamics. The KBase platform has expanded to over 200 analysis tools spanning reads management, genome and metagenome assembly and annotation, basic comparative genomics, RNA-seq analysis, and metabolic modeling of organisms and their communities.

The JGI-KBase partnership is developing complementary and integrated high-performance tools to provide users with the ability and infrastructure to explore complex and diverse datasets to extract deeper biological insights. This partnership will create a JGI presence within KBase, build a diverse, engaged joint user community, and enable scientific discovery. Under the guidance of a new JGI-KBase Strategic Leadership Team, researchers have continued to work closely over the past year to develop systems within KBase, and hosted at NERSC, that allow users to execute JGI tools and pipelines on the KBase system. JGI and KBase have built production-quality genome and gene homology services that are in use by JGI's IMG system as well as KBase. In FY21 the team deployed a new search interface to JGI's public data, and plans to make private data imports more seamless in FY22. JGI and KBase have accelerated efforts to integrate JGI tools into KBase and have now integrated the JGI Web of Microbes microbial exametabolomics data into KBase.

As both JGI and KBase exist to serve a broad scientific community, our focus is on expanding user engagement and partnership with other User Facilities. KBase will establish and coordinate user working groups (UWGs) on metabolism, microbiome, and functional genomics to organize efforts to integrate the data-types, data, tools, and analyses from DOE-sponsored groups operating in each topic area into either in the KBase platform itself, or in shared infrastructure run by KBase, JGI, and other user facilities (e.g., NERSC, EMSL). Additionally, these UWGs will partner with users to generate user-driven designs, science and data standards. Together, JGI and KBase have continued to host joint outreach activities and booths, and hold workshops. JGI has encouraged users who submit proposals to their Community Science Program to utilize KBase tools for their data analyses. A JGI-KBase-NERSC call was launched in late FY18 under the Facilities Integrating Collaborations for User Science (FICUS) umbrella.

In partnership with JGI and NERSC, KBase is embarking on developing a scalable open platform for foundational genomics based on homology, taxonomy, and environmental sources of genomes and metagenomes. A prototype of the KBase Knowledge Engine (KE) computes key relationships among all public and shared data in the system and instantaneously returns the most biologically relevant data to a user's interests and analyses on the system. The KE platform is being extended with new types of relationships using results of the large-scale analyses from our JGI co-development work and new tools being generated by the KBase team. Ultimately, this engine will make increasingly sophisticated inferences of function and behaviors of genes, organisms, and communities.

JBEI is a significant contributor to this capability through use-inspired fundamental research into complex biological systems. Research at JBEI establishes the scientific knowledge needed to engineer bioenergy crops with low susceptibility to disease and drought, and that can be readily deconstructed into useful intermediates; develop feedstock-agnostic deconstruction processes that use ionic liquids; engineer microbes with efficient metabolisms to simultaneously utilize sugars and aromatics from biomass; and for the underlying technologies that can meet future research needs. One of JBEI's strengths since its inception has been deep and enduring ties with industry partners to drive the use-inspired research that will propel the bioeconomy forward, including the companies Aemetis, Novozymes, SAPPI, and Total.

The developing NMDC also provides critical support through leveraging existing resources, unique capabilities, and expertise across our four National Laboratory partners, to deliver a set of unique microbiome data science capabilities aligned with the Findable, Accessible, Interoperable and Reusable (FAIR) Data Principles. Led by Berkeley Lab, the NMDC Phase I 27-month Pilot (July 2019 – Sept. 2021) has established a collaborative framework for coordinated integration of multi-omics data generated at JGI and PNNL's Environmental Molecular Sciences Laboratory (EMSL). The NMDC develops core capabilities in metadata standards for sample and environmental descriptors; standardized bioinformatic workflows; prototype interface for data search and access; and a robust strategic engagement plan for research teams, scientific societies, funding agencies, and publishers. Further, the Pilot builds upon integral efforts underway at the JGI and KBase (described above) and HPC systems, in particular NERSC, to provide an unparalleled integration of multi-omics data for DOE mission-relevant environmental microbiome research. Following the first annual review in August 2020, the DOE extended the NMDC Pilot for an additional 12 months with support to broaden collaborative infrastructure with ESS-DIVE and NSF's NEON.

The Ecosystems and Networks Integrated with Genes and Molecular Assemblies (ENIGMA) project emphasizes achieving a multiscale, causal, and predictive understanding of microbial biology and the reciprocal impact of microbial communities on their ecosystems. This BER-funded SFA, led Berkeley Lab, is a multidisciplinary, multi-institutional research consortium with a special focus on processes that affect denitrification and metal reduction. Efforts are centered on studying subsurface microbiomes within the Bear Creek aquifer at the Oak Ridge Reservation (ORR) in East Tennessee, a site with complex contaminant gradients. The contaminants, generated by nuclear material research and production, include nitrates, uranium, and volatile organic carbon species. Their fate and complex dispersal flow paths are mediated by the activity of subsurface microbial communities. To better understand these processes, ENIGMA performs field experiments to measure natural versus anthropogenically perturbed dynamics of geochemical processes and the assembly and activity of microbial communities. Researchers infer the most predictive of these chemical, physical, and microbial interactions to estimate the ecological forces that shape microbial community function. Using laboratory studies, the team applies a unique array of culturing, genetic, physiological, computational, and imaging technologies to understand and model gene function and material flow within and among cells, and maps this back to field studies to determine the causes of environmental observations. The team also investigates how different environmental forces dynamically change geophysical and geochemical features, how these forces disperse materials across the site, and how the genomes of ORR microorganisms adapt to specific environmental conditions and the presence of other microbes. Through these studies and approaches, the ENIGMA SFA is delivering a mechanistic understanding of complex environmental bioprocesses and ecology, ultimately extracting principles that enable prediction of and intervention in functional microbiome assembly and activity in complex sediment ecosystems.

A collaborative, coordinated, and integrated mission-driven SFA, m-CAFEs (Microbial Community Analysis and Functional Evaluation in Soils) interrogates the function of soil microbiomes with critical implications for carbon cycling and sequestration, nutrient availability and plant productivity in natural and managed ecosystems. m-CAFES targets molecular mechanisms governing carbon and nutrient transformation in soil, with a focus on microbial metabolic networks, and looks at how changes persist throughout the ecosystem.

Laboratory fabricated ecosystems hold the potential to bridge the gap between highly-constrained lab experiments and field-scale experiments that are challenging to control, allowing researchers to dissect microbial community dynamics and effects in relevant environments. EcoFABs, small chambers with control of liquid flows and spatially-defined imagining capabilities, have been employed in two BER-funded projects, m-CAFEs and TEAMS (Trial Ecosystems Advancement for Microbiome Science). Currently being developed at Berkeley Lab, EcoPODs are meter-scale enclosed environments that allow direct and intensive monitoring and manipulation of replicated plant-soil-microbe-atmosphere interactions over the complete plant life cycle.

BER-funded programs benefit from substantive collaborations across the University of California campuses, e.g., JBEI partners include UC Berkeley, UC Davis, UC Santa Barbara, UC San Diego, and the UC Agriculture and Natural Resources. The JGI and UC Merced jointly established the Genomics Distinguished Graduate Internship Program. In February 2020, the NMDC formally established a microbiome data science tri-institutional partnership with UC Davis and UC San Francisco and five new research collaborations were launched. Also in the last year, the EcoFABs team partnered with UC San Diego researchers to expand the use of fabricated ecosystems for advancement of microbiome science.

BER-funded programs at the ALS support the analysis of biological systems at the atomic, cellular and multicellular scales. The IDAT program operates small angle X-ray scattering and crystallographic beamlines to allow BER researchers to understand biomolecules at atomic resolution and in solution. The National Center for X-ray Tomography uses soft X-ray microscopy to visual cells and their contents. The Berkeley Synchrotron Infrared Structural Biology (BSISB) program uses infrared spectromicroscopy to measure and visualize living systems at the multicellular level. These resources are available to all BER researchers nationally. They are complemented by several other crystallography beamlines supported by NIH, industry, and private foundations (e.g., HHMI), and LBNL's cryo-EM facilities.

In 2020, BER gave an ECRP award to Simon Roux to study viral diversity in the environment and host-virus interactions. This effort focuses on the impacts of the interactions between viruses and their hosts to understand the impacts on individual and ecosystem processes, using a combination of experimental approaches and large-scale data analysis. The project will identify the mechanisms used by soil viruses to take over and reprogram their host cell during infection, evaluate how these infection dynamics change with soil location and condition, and measure how these viral infections eventually alter global element and nutrient cycling. Berkeley Lab's strength in viral research was brought to bear in the study of virus dynamics as part of the NVBL.

In 2018, a DOE-BER ECRP project was awarded to EESA scientist Kolby Jardine, which focuses on advancing knowledge of plant cell wall chemical composition and metabolism in order to enhance biosynthesis, deconstruction, and conversion into fuels and other bioproducts. This project builds upon the Lab's NGEE-Tropics research and connects climate-relevant plant volatile emissions and their isotopic composition to chemical roadblocks of biomass deconstruction, seeking to understand their plant physiological and biochemical roles during growth/development and abiotic stress responses. Genetic manipulation of cell wall chemical composition will be used to further evaluate their biological roles and stress responses, as well as potential improvements in yield and bioenergy conversion efficiency. The project will not only provide important knowledge on the physiology and ecology of plants but will also lead to the characterization of novel volatile signatures of dynamic plant responses to environmental variables detectable at the leaf to ecosystem scales.

BER is the primary sponsor of the research in this core capability; others include EERE, NIH, DoD, industry, and other SPP. This Core Capability supports DOE's mission to obtain new molecular-level insight for cost-effective biofuels; make discoveries for DOE's needs in climate, bioenergy, and subsurface science; and coordinate bioenergy, climate, and environmental research across applied technology offices.

Environmental Subsurface Science. Watershed physical, chemical, biological and atmospheric interactions regulate the geochemical flux of life-critical elements and influence contamination mobility and migration. These interactions also influence water and energy security, including water available for energy, industry, agriculture and urban use, as well as agriculture production.

With support from BER, Berkeley Lab is developing a predictive understanding of watershed extreme hydrology and biogeochemical function — from genome to watershed scales. A focus of the Watershed Function SFA is on developing new constructs and approaches to predict how vulnerable mountainous watersheds respond to increasingly frequent perturbations, such as droughts, floods and early snowmelt, and the associated impacts to downgradient water quality and quantity. Important advances over the last year include: improved the prediction of hydroclimate impacts on downgradient water discharge; testing 4D digital watershed and functional zone approaches for tractably characterizing complex watersheds; demonstrated the first satellite monitoring of groundwater depletion at management scales; advanced ML for predicting watershed organization and functions; documented the surprisingly large role of bedrock weathering in nitrogen exports to a river; predicted influence of wildfire and snowmelt dynamics on groundwater recharge in mountainous systems; and advanced the first watershed-based documentation of the impact of wildfire on water quality. As soil-microbe-interactions play a key role in water and biogeochemical cycling, the Watershed SFA is an anchor tenant of BioEPIC. Prototype components of new BioEPIC platform technologies, such as the EcoSENSE SMARTSoils testbed, are starting to be used to enable the Watershed SFA goals in sensing-data-model integration, with a near term focus on improving estimates of evapotranspiration and nitrogen cycling.

As was mentioned earlier, with the collocation of several BER investments at the East River Colorado Site, the Watershed SFA and colleagues were deeply involved this year in developing constructs important for gaining a predictive understanding of multi-scale mountainous watershed processes across bedrock through atmosphere compartments. The SAIL team made significant progress this year as it accelerates towards a September 2021 start. They have developed detailed science and logistics plans for each instrument, hosted a community-wide campaign workshop with over 135 participants across BER and academia, and engendered a sister campaign led by NOAA.

To improve prediction of future watershed function, a range of HPC, AI and data approaches are being developed, including adaptive mesh refinement methods to enable models that can telescope into a watershed to capture fine-scale processes. Advanced simulation capabilities are being developed for watersheds through the BER multi-institutional Interoperable Design of Extreme-Scale Application Software (IDEAS) and ExaSheds projects, both funded by BER. The new ExaShed effort has made advances this year in hybrid physics and machine-learned approaches as was previously described. A recently awarded BER ECRP is investigating the impacts of streamflow disturbances such as floods and droughts on water quality using data-driven methods. The methods include a data integration tool built for the Watershed Function SFA (BASIN-3D) and several ML techniques for classification and prediction.

Expertise and capabilities associated with monitoring and predicting hydrobiogeochemical watershed dynamics developed through BER investments have been extended to address challenges associated with agriculture, and environmental remediation, the onset of harmful algae blooms, and water quality impacts from wildfire. With EM support, Berkeley Lab is developing a new AI-based paradigm for long-term monitoring of DOE's legacy contaminated sites, using the Savannah River Site as a testbed. The Lab was also chosen by EM for a project on climate resilience for environmental remediation. We continue to collaborate with the Japanese Atomic Energy Agency (JAEA), and other institutions, on advanced modeling and data analytics that support Fukushima's remediation and rehabilitation effort. BER-developed capabilities are being used and extended through the California water agency and CalFIRE support to address surface and groundwater quality in regions impacted by the recent significant California wildfires, and are providing the first watershed-based strategy for investigating wildfire impacts on water quality. Based on new developments, the scientists have been asked to engage in various wildfire-focused city, state, and Western U.S. panels. LDRD investments have extended BER-developed insights about coupled biological-environmental-climate systems to advance ML and systems approaches for predicting the onset of harmful algae blooms; and to advance approaches to estimate subsurface biogeochemical interactions using volatile organics sensed from above the ground.

Climate Change Science and Atmospheric Science. Berkeley Lab has developed an internationally recognized program in theoretical, empirical, and computational climate change and atmospheric science. The Lab continues to make major advances in understanding how atmospheric processes and climatic extremes will respond to further warming of the environment. This work is complemented by novel observations of how the terrestrial ecosystems serve as a critical carbon sink, the vulnerability of this sink to future climate perturbations, and how elevated concentrations of greenhouse gases are leading to measurable increases in the atmospheric greenhouse effect. We integrate this information to help DOE produce the most advanced models of the Earth system and to utilize those models to project the possible physical and biogeochemical impacts of further global climate change.

Berkeley Lab conducts internationally recognized research on advancing the understanding and prediction of ecosystem responses and feedbacks to climate. We lead the TES Belowground Biogeochemistry SFA, which contributes to developing a new paradigm for soil organic matter dynamics through basic research on soil carbon turnover, storage and loss. This SFA is producing new understanding and improved predictions of belowground biogeochemistry in the soil-plant-microbial system and the role of soils in global change.

Soil warming experiments are ongoing at the Hopland, Calif., field study site, and efforts are underway to develop a more extensive SFA experimental site at Point Reyes, Calif. The Lab leads NGEE-Tropics, which is advancing cutting-edge predictive representation of tropical forest carbon balance and climate system feedbacks in DOE's E3SM using a modeling-experimental (ModEx) approach that combines model development and extensive field research. NGEE-Tropics is global in scale, with tropical forests accounting for the largest terrestrial carbon, water, and energy fluxes, comprising Earth system feedbacks that are widely recognized as essential for accurate climate projections. NGEE-Tropics has also led significant regional studies, for example, utilizing airborne remote sensing campaigns before and after Hurricane Maria in Puerto Rico to quantify tropical forest hurricane impacts, in collaboration with the U.S. Forest Service, NASA, LTER, CZO, the University of Puerto Rico, and other partners. NGEE-Tropics leads the development of a process-rich tropical forest ecosystem model — the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) —which enables the representation of physiology, growth, competition, and mortality of individual plants at scales tractable for global simulations. FATES introduces a mechanistic and trait-based approach to vegetation dynamics and climate impacts on ecosystems within the DOE E3SM climate model. The Lab is also applying FATES to understand potential drought response and tree mortality in California as part of a BER ECRP, and to model wildfire and vegetation distribution in the western U.S. as part of a UC-funded collaboration. FATES development is expanding as E3SM's global dynamic vegetation model to address critical terrestrial-climate system carbon, water and energy feedbacks. Also a key partner in the NGEE-Arctic project, the Lab contributes its expertise in environmental geophysics, soil biogeochemistry and microbial ecology, and mechanistic modeling of ecosystem-climate feedbacks. The LBNL team contributed significantly to the NGEE-Arctic project over the last year. For example, the team developed a distributed temperature system and electrical-resistance tomography that have provided unparalleled insights about permafrost variability; measured CO_2, CH_4, water, and energy fluxes under harsh conditions; revealed the high temperature sensitivity of old permafrost carbon; projected that 21st century plant responses could substantially affect soil temperature, hydrology, and CO_2 and CH_4 fluxes; and forecasted that fire and 21st century climate will double deciduous plant productivity in high-latitude regions.

The five BER ECRP projects that are being carried out by Earth and environmental scientists at Berkeley Lab are emblematic of the Lab's efforts to scale from microbial mechanisms to ecosystem processes. Two ECRP awardees are focused on global change impacts on soil microbiomes and their consequences for global biogeochemical cycles and atmospheric feedbacks. One of these projects is tackling the microbial metabolic response to permafrost thaw, using microbial communities as integrators of site conditions in an effort to predict forward trajectories of biogeochemistry following permafrost thaw. The other is focused on drought in tropical systems and its impact on carbon processing and stabilization by the soil microbiome and implications for drought resilience and forest productivity. Both projects are developing advanced approaches to observe and manipulate soil microbiomes to build mechanistic understanding that directly translates to improved model process representation and parameterization. As described above in the Biological Systems Science core competency, a third project focuses on advancing knowledge of plant cell wall chemical compositions in order to enhance deconstruction and conversion into fuels and other bioproducts by microbial fermentation. Known as "the poplar esterified cell wall transformations and metabolic integration study" (PECTIN), this project builds upon research carried out in the NGEE-Tropics project, and connects climate relevant plant volatile emissions to biochemical roadblocks of biomass deconstruction. A fourth project is exploring the implications of western U.S. climate extremes, in particular, recent severe droughts on western forests using the Functionally Assembled Terrestrial Ecosystem Simulator (FATES). The objective is to use these droughts to predict the response of western forests to increasing disturbances, as well as to predict similar forest responses to the northward shift in the mid-latitude storm tracks, and the associated shifts in rainfall patterns, predicted and now observed under global anthropogenic climate change. The fifth project, described above, is an investigation of the impacts of streamflow disturbances on water quality using a data-driven framework. This study is designed around extensive application of machine-learning to understand water quality changes in the river corridors and watershed attributes that confer resilience to extreme events.

Berkeley Lab also leads the AmeriFlux Management Project (AMP), which serves the AmeriFlux network of 525 sites and the broader scientific community by producing high quality data products of ecosystem-atmosphere fluxes of carbon, water and energy that enable scientific and modeling advances. In Phase 2 of the project (2015-2020), more than 250 new sites joined the AmeriFlux network (including 47 NSF National Ecological Observatory Network (NEON) sites in the context of a DOE-NSF MOU), more than 950 peer-reviewed publications benefited from AmeriFlux Management Project site support, a new gap-filled, partitioned flux dataset was released (FLUXNET2015), and AmeriFlux site data were downloaded 114,195 times by 2,813 unique users. In June 2020, the AmeriFlux Management Project renewal proposal was approved for Phase 3, for the fiscal period 2021-2025.

AmeriFlux is making major contributions to coastal research, in alignment with BER's priority on terrestrial-aquatic interfacing systems. Its network has over 200 flux-measurement sites located within 50 miles of a coastline. The important data from these coastal flux sites, publicly accessible from AMP, were synergistic with the Year of Methane Fluxes theme which supported new community efforts, enhanced instrument suites, and led to the hosting of a new international dataset in 2020 of ecosystem fluxes from 81 inundated areas worldwide.

The 2020 California wildfires were the worst the state has experienced, easily exceeding the records set earlier this century for impacted area and destruction. There is a significant need for basic science to develop an understanding of controls and to guide policies and forest management strategies. We have been deeply involved in various aspects of wildfire research over the last year, including research to quantify wildfire impact to air and groundwater quality; developing rapid-response environmental post-fire sampling strategies; using FATES to numerically explore wildfire spread and guide forest management strategies; and using AI approaches to remotely sense wildfire. This year, we frequently contributed to wildfire-based panels and interviews to inform practitioners, policy makers, and the public.

We are advancing AI to explore many challenges associated with carbon cycling and healthy soil. In the LDRD-funded AR1K project, we have used ML to tie critical plant, soil, and weather data together to provide actionable intelligence to farmers. Application of the developed methodology to an agricultural site led to 60% reduction in chemical inputs with no statistically significant impacts on yield. The success inspired a new SMARTFARM project funded by ARPA-E that uses ML to quantify the carbon intensity and budget in farming ("Rice'n Grits"). Berkeley Lab is part of a core multi-lab organizing team to partner with BER's Earth and Environmental Systems Sciences Division to advance a new initiative on AI for Earth system predictability (AI4ESP). The AI4ESP initiative explores how AI can be harnessed — together with multi-scale mechanistic models, diverse observations, and technologies such as edge computing and exascale capabilities — to engineer paradigm-changing advancements in Earth system predictability with a particular emphasis on hydrological extremes.

Berkeley Lab is one of the primary science centers studying the atmospheric carbon cycle and land-atmosphere interactions, and currently leads several major BER projects in the Atmospheric System Research (ASR) and Atmospheric Radiation Measurement (ARM) programs. With five other National Labs, we have developed and operated the ARM Carbon Project and ARM Aerosol Observing System Infrastructure to conduct precise and accurate measurement of trace gases, to contribute to multi-agency validation of satellite-based column CO_2 estimates, and to close the gap in U.S. emissions estimates for CH_4. The Lab recently initiated the ASR Convection and Land-Atmosphere Coupling in the Water Cycle project to advance climate prediction by improving representation of land-atmosphere coupling. The specific objectives are to better understand the mechanisms that link convective triggering and organization to land-surface states, and to parameterize feedback mechanisms to better predict drought and precipitation extremes. ARM data, along with careful model diagnostics, revealed much stronger than expected coupling between soil moisture and convection triggering in a 2019 *Journal of Geophysical Research* article, suggesting new ways to improve precipitation predictions. We are also pioneering the use of digital stereo photogrammetry as a tool to observe clouds, which play a critical role in weather and Earth's radiation balance. The Lab has deployed six new cameras ringing the SGP ARM site in Oklahoma that provide a 4D gridded view of shallow clouds. These generate a 50m grid of cloudiness every 20 seconds, called Clouds Optically Gridded by Stereo (COGS). These new capabilities are providing unprecedented data on cloud sizes, lifetimes, and life cycles—critical information for developing cloud schemes for the next generation of weather models. Based on a successful proposal, the ARM mobile facility will be deployed to Colorado's East River, providing a key part of the foundation to advance an 'integrated mountainous hydrology' initiative (as was described above). In addition to addressing questions related to water cycles in mountainous systems, SAIL is also poised to support critical research on cloud microphysics and snow-radiation interactions in montane environments.

Berkeley Lab is a major contributor to DOE's flagship Earth system modeling project, continually advancing the Energy Exascale Earth System Model (E3SM) and aiding in multiple components of the first version (v1) of E3SM. The Lab's contributions to the E3SM Land Model (ELMv1) include improved biogeochemistry representation between the soil, plant, and abiotic processes responsible for constraining the global carbon budget. This work has led to an experiment to test the effects of nitrogen and phosphorus on climate-biogeochemistry interactions and the impact on land uptake of CO_2. Within ELMv1, the Lab has also developed an extensible and scalable three-dimensional hydrology and thermal module, and integrated the FATES dynamic vegetation model, which applies trait-based competitive demography for a richer representation of ecosystem responses to climate in an ESM. To account for future interactions among availability of human relevant energy, food, and water resources with climate change, we have included an integrated assessment model (IAM) component to E3SM, soon to be coupled with FATES. This will allow for future projections of U.S.-relevant carbon pathway scenarios using state-of-the-science treatments of physical, chemical, and biogeochemical processes. Lab researchers serve as members of the E3SM leadership team for the land model group and NERSC exascale applications. We are further enhancing the treatment of terrestrial ecological processes for future release in E3SM v2, developing enhanced fire-ecosystem modeling, and land-use land-cover change in FATES which will interact with E3SM's IAM component (i.e., GCAM). We are also experimenting with testing of the newly implemented continuous plant hydraulic dynamics and plant nutrient competition in FATES. Outside of terrestrial processes, the Lab has a large role in developing high-resolution ice sheet modeling using an Adaptive Mesh Refinement to accurately model the physical processes of ice sheet retreat, and high resolution cloud resolving atmospheric modeling for the success of E3SM v2/v3.

The Calibrated and Systematic Characterization, Attribution and Detection of Extremes (CASCADE) SFA aims to understand how and why extreme weather and climate events have changed in the observational record and how and why they might change in the future. CASCADE successfully synthesized the team's interdisciplinary expertise in physics, statistics, and atmospheric and computer science to tackle large scientific questions that require innovative datasets, computational tools, and statistical methods. In 2020, the Lab quantified anthropogenic, atmospheric, and oceanic drivers of hydroclimate extremes in the western U.S. via an extensive analysis of climate simulations produced for the Coupled Model Intercomparison Project version 6 (CMIP6). Several recent deliverables illustrate this success, including publication of the Toolkit for Extreme Climate Analysis (TECA) and the software tool climextRemes, both of which allow sophisticated analysis of extreme events in massive datasets.

BER is the primary sponsor of the research in the Lab's climate change and atmospheric science core capabilities. Others include DOE ARPA-E and SBIR; UC; California agencies, other SPP, and the Moore Foundation. These Core Capabilities support DOE's mission to advance predictive understanding of complex biological, environmental and climate systems and their multi-scale couplings.

Computing and Mathematics

Advanced Computer Science, Visualization and Data. Berkeley Lab has substantial expertise and research activity in this core capability. Much of this work is focused on meeting the challenges of exascale computing, including performance analysis and algorithms, programming languages, systems and tools and alternative computer architectures for increasing future computing capability. Also significant is our work on high performance parallel I/O, machine learning, and data-intensive visualization and analysis targeted at exascale computing. Not all computer science challenges are associated with exascale computing, and our development of scalable solutions for scientific data, including management, curation, quality-assurance, distribution, and analysis, troubleshooting and performance-analysis tools for complex, distributed applications will have substantial impact on the broad computational challenges faced by DOE scientists who seek to derive understanding from data produced by experiments and observations coming from environmental sensors, genomics, light sources, and cosmological observations, etc.

Berkeley Laboratory has a longstanding expertise with hardware architecture and codesign, where we are already turning our attention to enabling post-exascale HPC performance improvements through innovative architecture and algorithm codesign in close collaboration with our industry partners. LBL is pursuing three complementary approaches to achieving these goals.

Resource Disaggregation: The cost and complexity of existing interconnects prevent designing datacenter racks tailored to emerging applications such as machine learning. Resource disaggregation is a system-level approach to runtime customization of heterogeneous system elements, in which compute, memory or storage modules are flexibly combined through one-model-fits-all embedded photonic connectivity and better utilize distant resources.

Heterogeneous Integration: This approach looks at co-integrating diverse "blocks" of chip designs from vendors like Arm and government innovations to create designs tailored for high performance computing. Currently this is supported by Project 38, which is an interagency collaboration between the DOD and the DOE, focusing on a set of vendor-agnostic architectural explorations.

Custom Acceleration for Science: A complementary approach is to select a high-value application target and design a custom accelerator around that application's requirements. Over the past 2 years, we have co-designed a custom accelerator design targeting Materials Science Codes (Density Functional Theory) because those codes account for a large fraction of DOE's HPC workload. This has led to a more rigorous mathematical approach to translating procedural algorithms into a form suitable for dataflow acceleration with custom circuits, and has also demonstrated 22x speedups on CGRAs like GraphCore and SambaNova compared to NVIDIA's latest GPUs.

We leverage our longstanding work in global address space programming to provide a productive, scalable and accessible programming environment for data analytics and data-driven science. Global Address Space presents a distributed memory machine as a unified memory architecture where all memory is easily accessible via familiar language interfaces like C++ (UPC++ for the global address space version) and Python (PyGAS extensions to SciPy in the global address space case). Current applications include ExaBiome and ExaGraph/ GraphBLAS work, but is being extended into discrete event simulator frameworks for agent based modeling of transportation and the power grid.

Berkeley Lab is one of the primary developers of new capabilities in machine learning, high performance parallel I/O, storage, and data-intensive visualization and analysis. Our work on machine learning for advanced imaging has helped automate analyses and processes, e.g., via modeling and characterization of silicon fibers, cells, protein nanorods, and weather phenomena. We have developed scalable, exascale-ready, topological algorithms and abstractions, providing stable feature descriptors for automatic analysis and decision-making and to enhance machine-learning pipelines. Through the design of scalable infrastructure for in situ visualization (SENSEI), climate analytics (TECA), and others, we make our algorithms broadly accessible, enabling broad application and scientific discovery. Our R&D on scaling analytics for large simulation and experimental data exploits diverse parallel schemes and heterogeneous architectures, as well as edge computing and new technologies (FPGAs, etc.). Our work in efficient parallel I/O, querying, pattern-matching, data compression, and storage management for the evolving storage hierarchies of current and future HPC systems delivers functionality, predictability and high transfer rates for a variety of application development projects. Our object-oriented data management and HDF5 research are enabling HPC applications to efficiently store, search, retrieve, and analyze petabyte-scale data.

The Lab is a pioneer in scalable workflow solutions for scientific data, including meta-data generation, management, curation, quality-assurance, distribution, usability, and analysis. The growth in scientific data volumes has resulted in a need to scale up processing and analysis pipelines using High Performance Computing (HPC) systems. These workflows need interactive, reproducible analytics at scale. Our efforts bring together core technologies based on the Jupyter Platform to create interactive, reproducible analytics at scale on HPC systems. Berkeley Lab leads the data processing and curation aspects of the BER-sponsored AmeriFlux Management Project, described in the Climate Change Science and Atmospheric Science core capability, which focuses on distributing high quality, standardized datasets to a variety of end users. We have also developed the Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository, whose mission is to preserve, expand access to, and improve usability of critical data generated through DOE-sponsored research of terrestrial and subsurface ecosystems. We lead the work on the Neurodata Without Borders: Neurophysiology (NWB:N) data standard for neurophysiology, providing neuroscientists with a common standard to share, archive, use, and build analysis tools for neurophysiology data. We lead the Software Engineering Team for the FE-funded Institute for the Design of Advanced Energy Systems (IDAES) project that is developing a next generation modeling and optimization platform to aid in the design of novel energy systems, where are work primarily involves managing, navigating, and guiding the development of the data management framework, solvers, and user interface as well as building surrogate modeling capabilities. Deduce (Distributed Dynamic Data Analytics Infrastructure for Collaborative Environments) is focused on exploring methods of evaluating the sensitivity of data analyses and data products to changes in the underlying data used to produce the product or analysis result.

Berkeley Lab is a leader in developing software to enhance, troubleshoot and debug performance of complex, distributed scientific applications. Open source software developed by the lab has had tremendous impact worldwide. PERFormance Service Oriented Network monitoring ARchitecture (perfSONAR) application, is now deployed at over 2,000 sites worldwide in national laboratories, commercial and research networks, universities, and corporations. ESnet's On-Demand Secure Circuits and Advance Reservation System (OSCARS) technology, deployed in over 50 networks worldwide, operates like a dynamic expressway, creating uncongested paths between endpoints. Our researchers are prototyping a model-based approach to allow scientific workflows to orchestrate end-to-end network paths along with optimized data-transfer nodes via the SENSE project. The project maintains a persistent testbed that spans multiple institutions and is integrating this approach with science applications. This approach has been adopted by the ExaFEL ECP project as well as being deployed worldwide through the AutoGOLE project. In addition, we are exploring the application of machine learning techniques on network traffic prediction in order to optimize traffic engineering and routing of large scientific flows over uncongested paths, and revolutionizing measurement and monitoring of elephant data flows. We will be capable of proactively finding these performance issues by developing a nano-second precision packet telemetry system leveraging FPGAs, programmable data planes, and an innovative software processing infrastructure as part of the 'high-touch' component of the ESnet6 project. The same FPGA platform is also being leveraged for edge-computing with prototype deployment at an ALS beamline and NCEM. The first phase of FABRIC (whatisfabric.net), an NSF mid-scale project, with the goal to build a nation-scale network testbed on ESnet6 architecture to promote groundbreaking computer science research as well as innovation in implementation of science application workflows, is in process of getting deployed.

We are pursuing a comprehensive strategy for edge computing and in-situ data processing at data sources – a crucial technology to address the increasing data volumes from new experimental facilities. Our goal is to design and deploy specialized computing workflows that include new/efficient algorithms, codes, programming systems, specialized hardware and networking to enable real-time computing for streaming data in-situ with the experiment. We are working with science teams deploying sensors networks so that edge computing devices can be integrated directly onto sensors, in the field, in the network and inside the data center. These devices can range from tiny distributed sensors deployed in the environment, such as Smart Dust for wide-area edge computing, to powerful FPGA or ASIC accelerators performing data reduction and analysis for in-situ for large-scale experiments that have high-performance edge computing requirements. There is an opportunity to use novel computing devices, including neuromorphic or other non-Von Neumann processors, to maximize the data reduction and analysis performed for minimal energy.

ASCR provides the primary support for this Core Capability, with additional support from BER, EERE, IARPA, ARPA-E, LPS, NSF, and ARO, and significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners. This capability supports SC's mission to deliver computational and networking capabilities that enable researchers to extend the frontiers of science and to develop networking and collaboration tools and facilities that enable scientists to work together and share extreme-scale scientific resources.

Custom Acceleration for Science: Another approach is to pick a high-value application target and design a custom accelerator around that application's requirements. This is very similar to Google's approach with the TPU and also D.E. Shaw's Anton. Over the past 2 years, LBL CRD and Materials Scientists have co-designed a custom accelerator design targeting Materials Science Codes (Density Functional Theory) because those codes account for the largest fraction of DOE's HPC workload (>25%). This has led to a more rigorous mathematical approach to translating procedural algorithms into a form suitable for dataflow acceleration with custom circuits and also has an impact on mapping onto CGRAs like GraphCore and SambaNova which has demonstrated 60x speedups compared to modern CPUs and 22x speedups in comparison to NVIDIA's latest GPUs. We will expand and generalize this mathematical method so that the implementation cost barriers are minimized to support a broader variety of DOE application driven acceleration.

Heterogeneous Integration: This approach looks at co-integrating diverse IP blocks from IP vendors like Arm and government innovations to create designs tailored for high performance computing. Currently this is supported by Project 38, which is an interagency collaboration between the DOD and the DOE, focusing on a set of vendor-agnostic architectural explorations. These explorations are intended to accomplish the following: *Near-term goa*l: Quantify the performance value and identify the potential costs of specific architectural concepts against a limited, focused set of applications of interest to both the DOE and DOD. *Long-term goal*: Develop an enduring capability for DOE and DOD to jointly explore architectural innovations and quantify their value.

Modern deep learning (DL) pipelines rely on a combination of numerical and combinatorial approaches for solving complex real world problems. For example, modeling and designing proteins requires recurrent neural networks (RNN) for the sequence part and graph neural networks (GNN) for the structure part. Large-scale dense and sparse matrix computations are the primary workhorses of RNN and GNN training, respectively. Therefore, parallel matrix algorithms play the crucial dual roles of (1) providing a unified platform for solving complex DL problems that has both numerical and combinatorial components, and (2) scaling efficiently to large datasets on modern supercomputers. Communication-avoiding (CA) algorithms enabled unprecedented scaling for many problems in numerical linear algebra, yet many of the computational primitives that modern DL use are not optimally addressed with existing CA algorithms. The success of these emerging communication-avoiding approaches will unleash the full power of CA algorithms for modern DL.

Data volume from new experimental facilities and many research investigations collecting data from distributed sources continue to grow at rates greatly exceeding Moore's Law. Many of these projects also have requirements for near real-time processing implying demands for processing and data movement speed growing even faster than raw data volumes. To meet these demands will require large scale distributed facilities for data generation, transport, storage, and analysis which can operate as integrated units seamlessly and reliably. The successful operation of these 'Superfacilites' will depend on strategies for comprehensive collection and analysis of operational data from a diverse set of components well beyond current practice. This is a fast-growing area that is a more urgent need of advanced programming infrastructure than the already well-established simulation/modeling community.

We leverage our longstanding work in global address space programming to provide a productive, scalable and accessible programming environment for data analytics and data-driven science. Global Address Space enables a distributed memory machine look like a unified memory architecture where everything is easily accessible via familiar language interfaces like C++ (UPC++ for the global address space version) and Python (PyGAS extensions to SciPy in the global address space case). This has already begun with ExaBiome and ExaGraph/GraphBLAS work, but is extending into discrete event simulator frameworks for agent based modeling (the MOBILITI agent-based simulator) to integrate traffic models together with realtime-gathered traffic data and power grid models. It also opens up new avenues for launching tailored computing environments and DSL's more tailored to the needs of the data-driven science and data analytics community. This also intersects with research in storage systems such as HDF5 and Proactive Data Container where the PGAS abstraction is extended out to include storage as an extension of the global address space. Together with ESnet, NERSC, and partners in the experimental facilities (ALS, APS, NCEM), CRD is pursuing a comprehensive strategy for edge computing. The purpose of the edge computing activity is to design and deploy specialized computing workflows that include new/efficient algorithms, codes, programming systems, specialized hardware and networking to enable real-time computing for streaming data in-situ with the experiment. Edge computing depends upon the CAMERA effort in applied mathematics to create advanced algorithms to turn data into knowledge, high-performance code implementations done by staff in Vis & Data Analysis in the Data sciences department, advanced programming systems and specialized hardware from the CS Department, as well as high-performance/high-touch networking from ESnet, and scalable computing and storage from the NERSC facility.

As experimental and observational data is often collected at sites located a considerable distance from an available HPC center where the volume and velocity of experimental data threatens to overwhelm both the wide area network and HPC center ingest rates, even with the upgraded ESnet6 capacity. For example, a single microscope under development at the National Center for Electron Microscopy (NCEM) is already pushing the limits of what can be transferred to NERSC over the network; even though a dedicated 400Gb/s network connection was installed directly to NERSC, the detector frame rate of the electron microscopes is still limited by the available network bandwidth. Just as each experiment today frequently benefits from custom sensors and associated hardware to gather the data, the experiments of the future will benefit from custom hardware solutions to reduce, analyze and respond to collected experimental data in real time. To address the unique needs presented by the diversity of experiments, a generalized framework must be developed to allow rapid design, prototyping and deployment of edge computing devices.

We are working with science teams deploying sensors networks so that DOE-designed edge computing devices will be integrated directly onto sensors, in the field, in the network and inside the data center. These devices can range from tiny distributed sensors deployed in the environment, such as Smart Dust for wide-area edge computing, to powerful FPGA or ASIC accelerators performing data reduction and analysis for in-situ for large-scale experiments that have high-performance edge computing requirements. The creation of this framework creates the opportunity to use novel computing devices, including neuromorphic or other non-Von Neumann processors, to maximize the data reduction and analysis performed for minimal energy. The use of edge computing devices will help Computing Sciences realize this vision of ubiquitous computing seamlessly integrated throughout complex scientific workflows. The creation of new algorithmic approaches and custom computing devices will be combined with commodity hardware and integrated into complex workflows as transparently as any software-based library, enabling non-experts to design, deploy and utilize custom edge computing devices.

Applied Mathematics. Berkeley Lab has world-leading capabilities for developing mathematical models, algorithms, tools and software for addressing important scientific challenges for the DOE. These capabilities are supported by highly recognized experts in applied mathematics, many of whom are SIAM Fellows and/or members of NAS and NAE. Berkeley Lab applied mathematicians are internationally recognized for their invention of new mathematics to tackle the challenges of transforming experimental data from DOE's scientific user facilities into understanding, their ground-breaking research on modeling and simulation of complex physical processes, bringing the power of predictive simulation to a broad range of science areas, and for their leadership in the development of highly performant numerical linear algebra algorithms and software capable of harnessing the power of the DOE's leading edge scientific computing platforms. Berkeley Lab's mathematics research is a point of leverage for exascale science impact. The algorithms and models are designed for parallel scalability and to reduce expensive data movement, with special attention to the hardware features emerging in next generation systems. They are incorporated into open source software libraries and frameworks that are used at NERSC and other centers across DOE, and will enable higher resolution, more fidelity, and new models of scientific phenomena.

Berkeley Lab has unsurpassed expertise in algorithms for modeling and simulating compressible, incompressible, and low-Mach-number flows in many applications, from combustion processes, to ice-sheet formation and retreat, to atmospheric flows. Adaptive Mesh Refinement techniques pioneered at the Lab are globally recognized as a key enabling technology, and Berkeley's Exascale AMR Co-Design Center continues to improve AMReX, a software framework leveraging a variety of hybrid CPU/GPU systems that supports ECP and SciDAC scientific simulation codes for combustion, astrophysics, cosmology, accelerator technology and multi-phase flow.

New numerical methodology has been developed to model the effect of electric fields on flames and implemented in the ECP PeleLM code. This enables the study of the "ion wind" of charged particles created naturally in many flames that can be shaped and controlled with electric fields in order to reduce pollutant emissions and enhance flame stability.

In collaboration with scientists in the Lab's Physical Sciences Area, Berkeley Lab mathematicians have developed increasingly capable simulation capabilities for understanding astrophysical phenomena. Recent developments include an electromagnetic Particle-In-Cell code that self-consistently models relativistic magnetic reconnection, providing an appropriate lens to study fundamental mechanisms that dominate particle acceleration in astrophysical processes. A new algorithmic coupling has also been developed that combines the new two-moment, high-order neutrino radiation solver Thornado with the compressible hydrodynamics code CASTRO on AMReX adaptive meshes that will enable the study of dynamical neutrino-to-fluid coupling in core collapse supernovae and star mergers with unprecedented accuracy at the Exascale. A new Monte Carlo radiation transfer code, SedonaEx, allows researchers to simulate large-scale high-resolution astrophysical radiation transport problems that would not otherwise be possible in 3D.

Berkeley Lab has also made significant strides in the development of methodology for simulating the dynamics of physical systems at microscopic and mesoscopic scales. In collaboration with New York University, UCLA and San Jose State University, a new fluctuating hydrodynamics immersed boundary technique has been developed that allows efficient simulation of nanoscale electrokinetic flows near charged surfaces at sub-Debye length scales and electrolytes with low ion concentrations, thus laying the foundation for studying electrokinetic phenomena such as electro-osmosis and electro-convection with applications in nanofluidics, water desalination, biological cell separation and ion transport in batteries. With UC Merced and San Jose State, a new hybrid approach has been developed for modeling mesoscale systems where interactions between surface chemistry and bulk transport critically affect the overall system dynamics, laying the foundation for modeling heterogeneous catalysts and electrochemical cells at the mesoscale, supporting the design of technologically innovative devices at very small scales.

Ab initio molecular dynamics (AIMD) is a powerful tool for the study of chemical systems in condensed phases but is limited in applicability due to poor scaling inherent in the traditional approach. Berkeley Lab, in collaboration with UC Berkeley, have developed and implemented a new approach that combines a machine learning-based simulation protocol with HPC to push AIMD to 100 million atoms, or 100x current capabilities, and with speeds greater than 10,000x faster than current state-of-the-art. This Gordon Bell prize-winning capability is a revolutionary advance for molecular simulation.

Berkeley Lab has developed state-of-the-art methods for simulating multi-phase, multi-physics systems through their introduction of implicit mesh Discontinuous Galerkin methods, which provide highly accurate and economical modeling of coupled physics-driven interface propagations. These techniques feature in two HPC4Mfg efforts, including high speed rotary bell simulations in automotive spray painting, and predicting coating properties and uniformity in industrial painting.

The Center for Applied Mathematics for Energy Research Applications (CAMERA), an integrated, cross-disciplinary center aimed at developing and delivering the fundamental new mathematics required to support DOE user facilities, has delivered numerous advances. CAMERA mathematicians have developed two- and three-dimensional "Mixed-Scale Dense" convolutional neural networks, which are designed to work when experimental training data is limited, and optimized these methods on advanced GPU-HPC computer architectures. These methods are being applied to cryo-EM images at SLAC, and in many other applications. CAMERA has also developed a mathematical approach for autonomous driving of large-scale experiments. This tool, gpCAM, is based on Gaussian process regression, and is completely agnostic to a particular technique or experiment and can send suggestions back to the scientific user to steer data acquisition. gpCAM is now in use at multiple facilities across the DOE and in Europe and has been demonstrated to increase instrument utilization by as much as 4-fold, while reducing the required data for decision making by as much as 50-fold. In collaboration with scientists at ANL's Advanced Photon Source (APS), CAMERA scientists have developed the first algorithm capable of reconstructing ab initio 3D material structure form Coherent Surface Scattering Imaging (CSSI) experiments. Based on the Multi-tiered iterative projection technique pioneered by CAMERA, this new capability enables 3D CSSI imaging of thin materials, the focus of a featured beamline in the APS-U upgrade. CAMERA scientists have introduced the first mathematical models and numerical algorithms (M-TIES) capable of extracting rotational diffusion coefficients from X-Ray Correlation Spectroscopy Data (XPCS), which will be a prominent experimental technology resulting from synchrotron light source upgrades at the ALS, APS, and LCLS at SLAC. CAMERA scientists have introduced and delivered a package for equivariant neural networks (ENN), which encode symmetry constraints in data representations, with applications to economically representing chemical structures. In collaboration with the Advanced Light Source and Brookhaven National Laboratory, CAMERA scientists have developed a new projection matching algorithm that enables accurate registration of sample motion and deformation during exposure; this is critical for the calculation of high resolution reconstructions free of misalignment induced artifacts.

In numerical linear algebra, Berkeley Lab is the only SC lab that has expertise in large-scale eigenvalue calculations and direct solutions in sparse matrix inversion. Direct and preconditioned iterative solutions of high-frequency wave equations are critical components for many ECP and SciDAC applications, including MFEM at LLNL, accelerator modeling at SLAC, EM simulation codes at Sandia. Their fast solutions require leveraging the recently developed numerical linear algebra tool, butterfly, to exploit the low rank structures of the linear systems similarly to what is done in the classical FFT algorithm. Berkeley Lab mathematicians developed an exascale solver containing a collection of butterfly-enhanced hierarchical matrix formats and their parallelization schemes to significantly reduce solution time. This was integrated into the STRUMPACK code and benchmarked using MFEM examples, resulting in the first quasi-linear complexity multifrontal solver for high-frequency wave equations. Berkeley Lab developed the first 3D communication-avoiding algorithms for sparse LU factorization and sparse triangular solve, which have probably lower communication complexity than the state-of-the-art sparse direct solvers. These algorithms are implemented in SuperLU code, and demonstrated up to 27x faster on 32,000 processes for sparse LU and 7x faster on 12,000 processes, compared to the respective 2D algorithms. To meet the needs of DOE SciDAC partnership, DOE Computational Materials Software center, DOE Computational Chemical Science center, and EFRC projects in quantum chemistry and nuclear physics, Berkeley Lab developed better Kohn-Sham density functional theory based nonlinear eigensolvers, configuration interaction based sparse linear eigensolvers, and linear response eigensolvers. These eigensolvers are integrated with the application software tools such as Quantum Espresso, SIESTA, NWChemEX, BerkeleyGW, MFDn, Omega3P.

These capabilities and their applications are sponsored primarily by ASCR, with support from other DOE program offices and SPP. These capabilities support DOE missions in fusion energy science, biological and environmental research, high-energy physics, nuclear physics, basic energy sciences, environmental management and fossil energy. They also support the development of mathematical descriptions, models and algorithms to understand the behavior of climate, living cells, and complex systems related to DOE mission areas of energy and environment.

Computational Science. Berkeley Lab is a leader in connecting applied mathematics and computer science with research in many scientific disciplines, including biological systems science, chemistry, climate science, materials science, cosmology, astrophysics, particle and nuclear physics, subsurface science, fossil energy, environmental management, and all Core Capability areas described in this Plan. The Lab has a successful track record of effectively integrating these research areas in conjunction with HPC resources to obtain significant results in many areas of science and engineering.

Within the national lab network, Berkeley Lab plays a very visible role in the SciDAC Program, with the largest participation across the DOE Laboratory complex. We are involved in 14 of the 30 science partnership projects, providing advanced computer science methods and robust applied math techniques and algorithms for enabling and accelerating scientific discoveries. These science partnerships also benefit from the results of the two SciDAC Institutes, FASTMath and RAPIDS, where we provide senior leadership and which leverage our Applied Math and Advanced Computer Science, Visualization and Data core capabilities. LBNL has played key roles in the recent successful competition of the Institutes under the SciDAC-5 Program. Furthermore, the Lab plays key roles in 12 Application Development subprojects in the Exascale Computing Project supporting computational science development for exascale systems across many disciplines. The LBNL roofline methodology from RAPIDS has been extended to analyze deep learning workloads and emerging accelerator technologies, and has been integrated into the production vendor tools of Intel Advisor and NVIDIA Nsight Compute. Researchers from RAPIDS have enabled a two-order of magnitude improvement of data sharing (compared with disk I/O) by transferring variables directly on two BOUT++ simulations computing ELM and transport. A collaboration between FASTMath and RAPIDS researchers at LBNL has reduced communication overhead for many-body localization eigensolver by overlapping computation with communication, using mixed precision arithmetic and reducing overhead with the CSPACER runtime tool. SciDAC researchers at LBNL have improved by a factor of 2-5 the performance of an approximation algorithm for a Traveling Salesman Problem, which arises in optimizing the sparsity structure for GPU implementation of certain sparse matrix computation. Working with SciDAC collaborators, Berkeley Lab researchers in FASTMath and ProSPect have coupled the lab-developed BISICLES ice sheet model with a model of the solid earth response and demonstrated that including solid-earth feedbacks to changes in the West Antarctic Ice Sheet can be a stabilizing influence with the potential to reduce the amount of sea level rise due to ice sheet loss. They also have contributed to a community effort designed to better understand uncertainties in projections of future ice sheet contributions to sea level rise and are co-authors of an in-press paper in Nature reporting the results of that effort.

The Computational Science Dept. recently formed the Quantum Information, Science, and Technology Group (QuIST), a multidisciplinary team working on early, noisy quantum computing hardware based on superconducting electronic circuits. QuIST concentrates on all aspects of design, co-design, fabrication, characterization, operation fidelity optimization, and deployment of superconducting quantum computing processors. This group is implementing quantum protocols and algorithms that advance and push the frontiers of QIS. Further, they are interfacing with the wider QIS community through the Advanced Quantum Testbed User program, which recently initiated its first call for proposals and embarked on direct user engagements.

A multi-disciplinary team within Computational Science is working to develop a first comprehensive quantum computing software stack for DOE (aide-qc.org). The team is building novel algorithms to simulate complex systems interacting with their environment (so-called open quantum systems) and to limit quantum operations depth and the number of qubits needed to allow for larger systems to be run on quantum computers for longer periods of time. Various error mitigation approaches are being developed to increase the reliability of quantum simulations on near-term noisy hardware, and they are demonstrated on physical quantum hardware. Revolutionary new approaches are being developed to extract excited states and free energies, properties important to many DOE science problems. The advances are used to simulate scientific problems relevant to DOE in quantum chemistry and quantum materials research.

The Computational Biosciences Group brings together experts from our core capabilities of Computational Science, Applied Mathematics, Machine Learning, Data Management and Analytics, with strategic partners in the Biosciences Area to understand the dynamics and multi-scale nature of many biological problems. Recent work has focused on creating a tool to recommend molecules which meet a desired specification, along with the pathways to synthesize them, to enable molecular inverse design through machine learning.

Key collaborations connected with DOE's EFRCs and JCESR continue, targeting quantum materials, materials design and synthesis, gas separation and storage, and batteries. The mathematical methods and computational tools developed also have applications in many other scientific domains, such as improving catalysts for hydrogen fuel cells and storage.

Although ASCR is a key source of support for this Core Capability, all SC offices sponsor computational applications and software development for their respective areas of science. Other federal agencies such as NASA and DoD also benefit from and contribute to the research effort. This Core Capability supports all of DOE's science, energy, environmental and security missions. For SC's discovery and innovation mission, it provides the mathematical models, methods and algorithms to enable scientists to accurately describe and understand the behavior of complex systems.

Cyber and Information Sciences. Berkeley Lab conducts research into a broad array of cyber and information sciences including security for high-performance computing environments, high-throughput networks, "open science" computing workflows, and the power grid. Example applications include the development of RISC-V based hardware trusted execution environments (TEEs) appropriate for high-performance computing (HPC) to isolate data and computing from cyberattack, and enabling privacy-preserving analysis of and machine learning model training without exposing raw data. Ongoing, current, and future work in trustworthy hardware/software co-design for HPC, from architecture to OS and runtime, is being performed to ensure both the integrity and the confidentiality of scientific computing in the face of accidental or malicious threats, without significant cost to either usability or performance. Novel research techniques are also being used to leverage the "physical" aspects of cyber-physical systems, such as the power grid, to detect cyber-attacks against equipment controlling the power grid. Because these systems must act within the laws of physics, these properties can be exploited to detect malfeasance or failing sensors. In two current power grid cybersecurity projects, AI is being leveraged to automate the use of defensive control logic to maintain power grid stability in the face of solar inverters or grid-attached storage, with the development of the PyCIGAR software being integrated into the NRECA Open Modeling Framework (OMF). Leveraging LDRD funding, AI is also being examined for its vulnerabilities by developing means to detect and mitigate attacks on complex, automated, AI-driven systems.

In addition to Berkeley Lab's cybersecurity research, ESnet provides an integrated set of cyber security protections designed to efficiently protect research and operational data while enabling cutting edge research. ESnet's unique 100G SDN network testbed provides an international research platform for cybersecurity research at all network layers. ESnet's newly funded project from NSF, FABRIC, is also going to promote cybersecurity research at scale. The Lab leads the world in developing technologies to optimize science data transfers across local and wide-area networks. Developing the "Science DMZ" model, ESnet has championed an architecture to transfer data securely across the national and international research and education community. Work continues on developing the Science DMZ as many data sets have special privacy and security concerns. In particular, the "Medical Science DMZ" was designed to help address the concerns of HIPAA/HITECH while supporting the high performance needs of big data science.

Formerly known as Bro, the Zeek network security analysis framework started at Berkeley Lab in 1995 to monitor network traffic in open scientific environments. It is now deployed at National Labs, major universities, supercomputer centers and, particularly through the Corelight commercial spinoff, *Fortune 100* companies. Starting in 2010, Zeek went through a major overhaul to support next generation networks at 100Gbs, with one of the first production 100Gbps deployments at Berkeley Lab in 2015. Currently, ESnet is exploring novel techniques to apply Zeek on a WAN environment where geographically dispersed, asymmetric traffic breaks the assumptions of most network security monitors. New technologies in ESnet's 6th generation network will potentially provide ESnet the building blocks to solve this security challenge and more at scale. ESnet maintains leadership both formally on the Zeek management team, and with the many technical contributions back to the project.

Berkeley Lab is also a co-lead of Trusted CI, the NSF Cybersecurity Center of Excellence, where it has had key roles in recent years in leading the development of key reports on causes and mitigations of bit flips, issues in scientific data sensitivity and confidentiality, and the state of software assurance in research computing. It has also participated in numerous one-on-one engagements with developers of key software used in research computing.

ASCR, the CEDS R&D and CEDS Threat Mitigation programs in the CESER office (including GMI/GMLC), and NSF are the primary supporters of this Core Capability, as well as recent CSR and LDRD support, and with additional previous support from EERE/BTO, OE, OCIO, NNSA, NSF, and NSA/LTS. Significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners such as the DoD, the IC, and NIH. This capability supports SC's mission with disciplines, technologies and practices designed to protect, analyze and disseminate information from electronic sources, including computer systems from edge devices to HPC, computer networks, sensor networks, and network-connected scientific instruments and user facilities.

High Energy and Nuclear Physics

Particle Physics. Berkeley Lab has a long record of excellence in particle physics and cosmology, with two premier programs: one in the Energy Frontier on the ATLAS experiment, with many contributions and leadership roles over more than two decades; and one in the Cosmic Frontier, where the Lab is leading next-generation projects in both dark energy, dark matter and a future ground-based CMB polarization experiment to study inflation. In addition, the Lab has a small but focused effort in the Intensity Frontier, where we are making key contributions to the Mu2E and leading the DUNE Near Detector effort at Fermilab.

Berkeley Lab's experimental program is fully aligned with the P5 roadmap, and is enabled and enhanced by our traditional strengths in instrumentation and detector R&D, expertise in QIS, microelectronics, software and computation including AI/ML, enhanced by our proximity to NERSC and connections to the Computational Research Division, and a strong theory group in partnership with UC Berkeley. Strong connections with UC Berkeley bring faculty and students to collaborate in our experimental HEP programs as well, providing significant leverage and opportunities for enhanced funding support through fellowships and other non-DOE resources.

On the Energy Frontier, Berkeley Lab is playing leading roles in the ATLAS pixel and silicon strip tracking upgrades, computing and software systems, and physics analysis. The Lab plays a leading role in the international R&D program on pixel readout for both ATLAS and CMS, and developed the silicon strip stave concept that has been adopted by the ATLAS collaboration. The Lab leads the Strip detector and Global Mechanics upgrade in the U.S. ATLAS HL-LHC Upgrade project.

Physicists and computational scientists also play leading roles in the ATLAS software framework, and more recent efforts have focused on the applications of machine learning and quantum computing techniques, as well as more efficiently harnessing the HPC capabilities at NERSC. Over the years, Lab scientists have led all aspects of ATLAS, including as Physics Coordinator (twice), Deputy Spokesperson, Upgrade Coordinator, Computing Coordinator, Simulation Convener (twice), Upgrade Physics Working Group Convener, SUSY Working Group Convener and Higgs Working Group Convener. Lab scientists are also playing lead roles in both the pixel and strip inner tracking detectors for the HL-LHC ATLAS upgrades, serving in management positions on both the U.S.-ATLAS and the international ATLAS upgrade teams.

Berkeley Lab is a world-leading center for the search for dark matter. The Lab led the Large Underground Xenon (LUX) experiment, managed the science operations at the Sanford Underground Research Facility in South Dakota from 2012 to 2017, and is currently leading the LUX-ZEPLIN (LZ) experiment. LUX completed data taking in 2016, and produced results that are still among the most sensitive limits in the search for dark matter. The LZ experiment received CD-4 in September 2020, and installation and commissioning of the apparatus is nearing completion. The experiment will begin operations in mid-2021. Berkeley Lab played many leading roles in the LZ construction project, including the Project Director and Project Manager, and is leading the Operations phase. Berkeley Lab will continue its leadership role during the Operations phase of the experiment. More recently, Berkeley Lab has begun R&D on an upgrade of LZ that would involve freezing the xenon to trap radioactive impurities, supported by a DOE Early Career Award. We are also pursuing advanced low-mass dark matter detection techniques supported by a new QuantISed consortium grant to develop new quantum-enabled sensors and readout and the TESSERACT concept to deploy TES readout on multiple targets supported by DMNI R&D funding. In addition, LBNL designs and oversees fabrication of skipper CCDs for the SENSEI and DAMIC dark matter experiments.

The Lab led the successful design and construction of the Dark Energy Spectroscopic Instrument (DESI), a Stage IV BAO experiment to create the largest 3-D map of the universe, with over 30 million galaxies. DESI successfully passed CD-4 in May 2020 and is on track for official start of the survey in mid-2021 after re-commissioning and survey validation. The Lab has developed a detailed DESI operations plan and will continue to manage it during the five-year survey. Berkeley Lab staff have played many leading roles in DESI including Project Director, Project Manager, Project Scientist, and Operations Director.

A critical Berkeley Lab contribution to the Cosmic Frontier has been the development of advanced detectors. Red-sensitive charge-coupled devices (CCDs) were invented in the MicroSystems Lab (MSL) and are the technology of choice for all Stage III and IV dark energy experiments, including BOSS, the Dark Energy Survey (DES), DESI, and the Large Synoptic Survey Telescope. With LDRD support, pioneering R&D on Germanium CCDs has been underway at MSL since 2017. The Lab also developed detectors and a multiplexed readout for cosmic microwave background (CMB) measurements, including the South Pole Telescope (SPT) and POLARBEAR/Simons Array. Located in Chile, the Simons Array has three identical telescopes with advanced multichroic polarization detectors, also invented at Berkeley Lab. With support from the Simons Foundation, the Chile site is being developed as the Simons Observatory, encompassing both the Simons Array and the ACT experiment, with the addition of several CMB telescopes. Four multi-year LDRDs have been awarded to support the development of CMB detectors, readout and polarization modulators and computing pipelines at the Lab, paving the way for the future CMB-S4 experiment, which was awarded CD-0 in July 2019. LBNL is playing critical roles in the CMB-S4 project as lead lab, including Project Director, Project Manager, Project Engineer, co-Spokesperson, Technical Baseline Development and L2 leadership roles in detectors, small aperture telescopes and data management.

On the Intensity Frontier, the Lepton Flavor group is involved in two flagship experiments at Fermilab. On Mu2e, Berkeley Lab leads the Software and Computing group which leads the simulation and reconstruction software efforts and has completed two Mock Data challenges. LBNL also played an important role in building and operating the first working prototype of the straw tube tracker and is supporting readout electronics testing. On DUNE, the Lab has made significant contributions to the conceptual design of the Near Detector, the cold electronics for the readout of the Far Detector, and the beamline and analysis of protoDUNE at CERN. A novel ASIC for low-power, cryogenic pixelated readout of the DUNE ND developed at Berkeley Lab (LArPix) led to the selection of this technology for the baseline design, multiple leadership roles in the ND, and a DOE ECRP in 2018. The Lepton Flavor group has also played leading roles in the analysis of Daya Bay, a ground-breaking reactor neutrino experiment which was conceived of and led by Berkeley Lab. Daya Bay made the first observation of the third neutrino mixing angle and has the most precise measurements to date, resulting in many awards and prizes. More recently, Daya Bay data have been used to understand the source of the so-called reactor neutrino anomaly.

Computation has become an increasingly important aspect of our program. We have taken a leading role in software, simulation and computing for ATLAS, Daya Bay, Mu2e, BOSS, DESI and CMB experiments, and leveraged resources at NERSC and the Lab's Computing Research Division for HEP. We've also incorporated ML as a tool in several of our simulation and analysis efforts. The Center for Computational Excellence has provided additional resources to take advantage of the NERSC HPC for HEP, and we have obtained other resources from ASCR. We are poised to take advantage of the latest advances in HPC and are working on cutting edge techniques that will benefit all HEP projects, including investigation of quantum computing algorithms with support from a QuantISed grant. In the past year we initiated a cross-cutting ML group that brings together scientists across the frontiers.

Berkeley Lab Theoretical Physics Group is closely integrated with the UC Berkeley Center for Theoretical Physics (BCTP) and plays a crucial role in our particle physics program, working with experimentalists to define future programs and develop strategies for data analysis.

Berkeley Lab is proud to be the host lab and provide leadership and support for the Particle Data Group, an essential resource for the field. PDG is an international collaboration that produces, on an annual cycle, the most comprehensive and trusted compendium of measurements and averages in particle physics and cosmology, together with curated reviews on many topics and techniques.

DOE's HEP is the primary sponsor of this Core Capability, with important contributions from ASCR, NNSA, NASA, NSF, and DHS. It supports DOE's missions to understand the properties of elementary particles and fundamental forces at the highest energy accelerators; the symmetries that govern the interactions of matter; and to obtain new insight on matter and energy from observations of the universe.

Nuclear Physics. Since the Lab's inception, nuclear science has been a Core Capability. Current programs provide world leadership in neutrino research, heavy-ion physics, medium energy hadronic physics, nuclear structure, and nuclear instrumentation. Machine learning techniques are being applied across the NP programs at Berkeley Lab, e.g., for pattern recognition in nuclear instrumentation, nuclear data, and heavy-ion physics, as well as in theoretical analysis of complex multi-variable information such as hadron jets and quark gluon plasma properties.

In the study of neutrinos, Berkeley Lab's critical role in the discovery of neutrino oscillations at the Sudbury Neutrino Observatory has been widely recognized. KamLAND and IceCube resulted in the first observations of geo-neutrinos and ultra-high-energy cosmic neutrinos, respectively. Experiments also search for the rare nuclear process known as neutrino-less double-beta decay, which will demonstrate if the neutrino is its own antiparticle, may provide information on the absolute neutrino mass scale, and determine if lepton number is conserved. Berkeley Lab scientists are playing important roles in the Majorana Demonstrator (MJD) SNO+, and the Cryogenic Underground Observatory for Rare Events (CUORE); CUORE has established the most stringent limit on the neutrinoless double-beta decay half-life in tellurium-130. New detector technologies are being developed at the Lab to enhance the physics sensitivities by two orders of magnitude in the next-generation experiments: the Large Enriched Germanium Experiment for Neutrinoless Double-Beta Decay (LEGEND), and the CUORE with Particle Identification (CUPID) experiments.

Berkeley Lab scientists study the structure of exotic nuclei, especially those with the largest neutron excess or the heaviest masses. Such nuclei push the boundaries of explanation by the nuclear shell model, and require modern accelerators and instrumentation to characterize. The Lab has a long and distinguished history in developing new detector systems for gamma-ray spectroscopy. These include Gammasphere and GRETINA, which run with beams of rare isotopes at NSCL at Michigan State, and also carry out experiments at ANL's CARIBU facility. This tradition continues with the next-generation Gamma-Ray Energy Tracking Array (GRETA) which received CD-1 in 2017, CD-3A in 2018, and CD-2/3 in 2020.

A core capability within Nuclear Science is our long-standing leadership in ion source development. Lab scientists pioneered VENUS, a versatile Electron Cyclotron Resonance (ECR) ion source that provides intense, highly-charged heavy-ion beams. Next generation accelerators, such as EIC, and FRIB- and ATLAS-upgrades, will require higher beam intensity than what can be delivered by current sources. A new superconducting magnet design for ECR sources – the Mixed Axial and Radial field System (MARS) – is under development, with the goal of achieving a sufficiently high magnetic field for future state-of-the-art ECR sources.

The Lab's strong nuclear theory group is building the science cases for the next-generation of advanced nuclear physics facilities to be built in the U.S. Notable is work that elucidates the nature of gluonic matter and the structure of the nucleon, which is of great relevance to the next generation Electron-Ion Collider. There is also a growing competency for HPC to study nuclear physics, especially in subfields of quantum chromodynamics on the lattice (lQCD) and nucleosynthesis in supernovae and neutron star collisions. The world-leading work on nucleosynthesis in the cosmos is being carried out with an Exascale Computing Project award to Berkeley Lab theorists. Berkeley Lab faculty scientist Daniel Kasen received one of the recent E.O. Lawrence Awards in recognition of his pioneering contributions in multi-messenger astrophysics and for his leadership in the application of high-performance computing.

With respect to quark-gluon plasma (QGP), Lab scientists made seminal measurements showing that the QGP flows with the lowest possible viscosity allowed by the laws of physics. Berkeley Lab's theoretical and experimental role in discovering the quenching of energetic "jets" was pivotal; the result indicates that the QGP has unprecedentedly high density. The Lab led construction of the ALICE EMCal and DCal, large electromagnetic calorimeters that enable the ALICE experiment to carry out unique jet measurements. We also led the construction of the STAR Heavy-Flavor Tracker (HFT), a next-generation silicon pixel tracker with unparalleled resolution and thinness, for reconstructing decays of charmed mesons amid the high particle multiplicities at RHIC. HFT results show that heavy charm quark production is quenched, similarly to jets, including charm quarks at relatively high momenta. Berkeley Lab is now leading U.S. participation in an upgrade to the Inner Tracking System of ALICE at the LHC, utilizing the next generation of silicon pixel technology pioneered in the STAR HFT. Recently, the Lab has taken on leadership roles in defining physics goals and detector components for the future Electron-Ion Collider (EIC).

We have initiated and formed a consortium to develop detectors for the EIC. Seeded by the UC Multi-campus Research Programs and Initiatives (MRPI) program, this consortium involves LBNL, UC Berkeley, UC Davis, UCLA, UC Riverside, LANL, and LLNL. The consortium will focus on its core competencies in developing tracking and calorimetry for the EIC.

In collaboration with NERSC, Lab scientists from the STAR experiment reconstructed half a petabyte of raw data in record time and resource usage efficiency. This demonstration established the feasibility of using HPC platforms to perform data crunching for future data-intensive nuclear physics experiments. This achievement has led to regular use of NERSC HPC machines for reconstruction and simulation studies for STAR, and large-scale simulation efforts for the ALICE experiment. Development of infrastructure to allow user analysis of large data sets from these experiments is underway.

The Lab's Applied Nuclear Physics program is growing, with applications ranging from international safeguards, radiological monitoring, biomedical applications, and detectors for astrophysics. This work takes advantage of the Lab's capabilities in innovative instrumentation, including the world-renowned Semiconductor Detector Laboratory (SDL), and attracts many cross-divisional collaborations at the Lab. In late 2019, Berkeley Lab scientists in this program won one of the coveted R&D 100 Awards for their portable radiation imaging, spectroscopy and mapping (PRISM) device.

The U.S. Nuclear Data Program concentrates on evaluating and organizing nuclear data for national interests. Nuclear data is used in many applications, including nuclear reactor design, nuclear safety, and many security applications. This program has embarked on a series of targeted measurements at the Lab's 88-Inch Cyclotron to address gaps in existing data, and to provide cross section and beam energy optimization information required by the U.S. Isotopes Program. This effort is joint with UC Berkeley's Nuclear Engineering Department, and attracts many young scientists. The Nuclear Data Program continues to support existing nuclear structure and reaction databases, and is embarking on the development of new gamma-ray databases for nuclear reaction modeling.

The 88-Inch Cyclotron operates to support three programs. The premier user of 88 beam time is a local research effort focused on the physics and chemistry of super-heavy nuclei. This program is unique in the U.S., and has recently achieved the first direct mass measurement of a super-heavy nucleus using the FIONA mass separator. The aforementioned Nuclear Data and Isotopes Program targeted measurements represent the second thrust for the Cyclotron. The third key area in which the 88-Inch Cyclotron contributes to the nation is in radiation hardness testing of electronics and materials destined for high altitude flights or for space.

Berkeley Lab's Nuclear Physics Core Capability includes innovative equipment and instrumentation, and commensurate handling of big data from experiments that produce multiple petabytes of data per year. The Lab leads the development of next generation ECR ion sources essential for next generation accelerator facilities, including FRIB at MSU, and the future EIC. The Majorana Demonstrator is now taking data, utilizing multiple components produced by the Lab. CUORE is also taking production data at Gran Sasso in Europe, and we have a strong lead role. CUPID-Mo was a prototype setup for CUPID, and completed its data-taking in mid-2020. GRETINA is producing data, and GRETA has commenced the purchase of detector modules and design of other systems. In heavy ion collisions, the Electromagnetic Calorimeter (EMCal) and Di-jet Calorimeter (DCAL) for ALICE, and the high precision, silicon-based STAR HFT have already taken substantial data. Construction of two Monolithic Active Pixel Sensor layers for the ALICE inner tracker upgrade was completed. This novel silicon pixel technology will be utilized for the sPHENIX experiment at RHIC, and will be further developed for the Electron Ion Collider detector. The Semiconductor Detector Lab provides world-class instrumentation for development of advanced germanium and CdZnTe detectors.

Support for this Core Capability is primarily from NP, with contributions from NNSA, ASCR, DoD, and DHS. This capability supports DOE's missions to understand how quarks and gluons assemble into various forms of matter; how protons and neutrons combine to form atomic nuclei; the fundamental properties of neutrons and neutrinos; and to advance user facilities and instrumentation that reveal the characteristics of nuclear matter.

Accelerator Science and Technology

Berkeley Lab has core expertise in synchrotron radiation sources and free-electron lasers (FELs); high performance magnetic systems; laser-plasma accelerators (LPAs); accelerator controls and instrumentation including novel laser technology; accelerator front-end systems, high brightness electron and ion sources. It is a center of excellence and community leadership in advanced accelerator modeling. AI/ML activities are incorporated in all accelerator science and technology research areas. We are also working on projects to improve QIS and on algorithms that could leverage future quantum computers for accelerator science. We support SC's mission of scientific discovery and innovation, and conceive, design, and construct scientific user facilities. We support SC's mission of scientific discovery and innovation, and conceive, design, and construct scientific user facilities.

Through a series of key upgrades, the 25-year-old ALS continues to operate as the world's brightest soft X-ray source. A major upgrade (ALS-U) now underway will provide up to three orders of magnitude brighter, fully transversely coherent soft X-ray beams. This highly cost-effective upgrade leverages the existing investment and infrastructure, and will enable premier soft X-ray source based research for decades to come.

We are a partner in construction of the LCLS-II FEL, and upgrade to LCLS-II-HE, and have delivered the injector source and hard- and soft-X-ray undulators, and contributing to linac systems, rf controls, and accelerator physics. Leveraging the development of the LCLS-II injector is the High-Resolution Electron Scattering (HiRES) beamline, developed with funds from the BES Early Career Research Program. Here we collaborate with scientists in ATAP, Material Sciences Division and the Molecular Foundry performing ultrafast structural dynamics studies in novel two-dimensional materials, and unveiling emerging transient complex phenomena. The beamline is also a platform for AS&T scientists to test new ideas related to control and diagnostic of particle accelerators, with particular emphasis to machine learning-related methods and low noise high bandwidth rf feedback systems.

After the successful delivery and commissioning the LCLS-II injector, we are currently developing the next generation normal-conducting CW RF gun – APEX2 for potential application of LCLS-II high energy upgrade (LCLS-II HE). Furthermore, as the upgrade project LCLS-II HE is now underway, we have again been asked to lead the delivery of the undulator sources, which consist of the design and procurement of new magnetic modules as well as the procurement of additional magnet structures to complement the existing FEL lines to achieve FEL saturation at the higher beam energy.

The Berkeley Center for Magnet Technology (BCMT) develops state-of-the-art superconducting high-field magnets, undulators, and specialty magnets for science and applications. We are the designated lead lab for R&D on high field accelerator magnets under the multi-institutional U.S. Magnet Development Program (MDP) and a key member of the High-Luminosity-LHC-Accelerator-Upgrade-project (HL-LHC AUP), which is contributing half of the new high-field interaction-region magnets for the LHC upgrade. The project was recently awarded CD-3, enabling full production to proceed. In 2018 the BCMT delivered the fully tested magnet system for the FRIB 28GHz ECR Source, which is slated to come online for the facility in the next years.

Berkeley Lab is the world leader in ultrahigh-gradient laser-driven plasma acceleration technology. Its BELLA Petawatt laser is used for research in support of the SC-HEP mission, including reaching 10 GeV from a sub-meter-scale accelerator. A project to add a second beamline (an independent laser arm) on the BELLA Petawatt is underway. The second beamline project will provide the capability of staging two multi-GeV laser plasma accelerator modules. BELLA Center is now operating two new 100 TW class laser systems for LPA applications. One system, funded by the Moore Foundation and BES, is used for LPA-driven FEL studies. The other system, funded by NNSA, studies LPA use for nuclear security applications. Expansion of the BELLA program includes BELLA-i, which uses the present BELLA laser for ion acceleration and high energy density physics. An FES-funded high-intensity beamline project is nearing completion and will enable the BELLA PW laser to produce very small focal spots (and corresponding very high intensities) for a variety of experiments in high energy density physics (e.g., ion acceleration). Intense ion pulses from laser plasma acceleration at BELLA-i have been used for qubit synthesis and for radiation biology studies in the FLASH regime. The kBELLA initiative would be a new 1 kHz multi-J-class laser for high-repetition-rate LPA science and applications.

The Lab is a world leader in developing simulation tools and techniques that model advanced accelerators and high-intensity laser-matter interaction physics. Our Accelerator Modeling Program (AMP) is a center of excellence and community leadership in particle accelerator modeling. AMP activities cover a broad range of accelerator technology (e.g., linacs, rings, sources, plasma-based) and beam science. In addition to providing advanced computer simulation codes - and support - in application to many accelerator projects in the U.S. and abroad, the AMP program has been pioneering many advances in algorithms that make the codes more accurate and faster. AMP scientists are also leading the U.S. DOE Exascale Computing Project application project on “Exascale Modeling of Advanced Particle Accelerators,” where a team composed of computational accelerator physicists, computer scientists and applied mathematicians, from LBNL, LLNL and SLAC, are developing the next generation tools, toward the realization of virtual particle accelerators that will run on Exascale and post-Exascale supercomputers. This program and its connections to Exascale Computing are further described in the Computational Science Core Capability.

The ATAP ALS Accelerator Physics Program is matrixed with the ALS division. Besides being responsible for the ALS operation, the program also focuses on the development of new concepts and technological improvements to enhance the performance of ring based light sources, with a particular attention to the ALS. The group skill set and areas of expertise include theoretical (both analytical and numerical) capabilities, software development, electron and photon beam diagnostics and experimental capabilities that allowed, over the almost 30 years of ALS operation, to conceive and develop upgrades to maintain the facility as the world leader soft x-ray 3rd generation synchrotron light source. A couple of notable examples of such activities are the developing and implementation of a machine learning application that allowed to dramatically improve the beam size stability of the ALS in operation and, ALS-U, the large scale upgrade of the ALS that has been approved by DOE and will provide the ALS with a brightness increase of up to 3 orders of magnitude.

The Berkeley Accelerator Controls and Instrumentation (BACI) Program brings together decades of deep expertise in electron and ion acceleration, innovative RF structure design and engineering, advanced field programmable gate array (FPGA)-based precision digital RF controls, and femtosecond synchronization including novel high average power fiber-laser technology, and qubit control.

Berkeley Lab's BACI is a world leading center in advanced FPGA-based precision digital controls for accelerators. In collaboration with several DOE national labs, BACI plays a leading role in technology development in LLRF controls for upgrades at SNS, at the PIP-II accelerator complex at Fermilab and at the Linac Coherent Light Source -II (LCLS-II) and its high energy upgrade project at SLAC (LCLS-II-HE). BACI's research programs target the most pressing problems and potential limitations impacting the scientific capabilities of accelerator-based facilities, and collaborate closely with many fellow national laboratories and institutions. BACI is also the home of Berkeley Lab's High Repetition-rate Electron Scattering (HiRES) apparatus, developed by taking advantage of the unique electron beam properties available from the Advanced Photoinjector Experiment (APEX). Based on a continuous-wave, normal-conducting, RF-driven electron beam, the HiRES beamline opens up new opportunities for structural dynamics studies using ultrafast electron diffraction (UED), it provides a unique tool for addressing unresolved fundamental questions about the dynamical behavior of interacting atoms and molecules and is a testbed for the development of ultra-precise electron beam control. BACI staff also applies its FPGA expertise to the precision control of superconducting qubits and is exploring adaptation of these techniques to other qubits, including trapped ions.

Supported by HEP and BES, with further sponsorship from FES, ASCR, NE, NNSA, DHS, DoD, ARPA-E, other federal agencies, and industrial partners, this core capability of Accelerator Science and Technology supports SC's missions to conceive, design and construct scientific user facilities; to probe the properties and dynamics of matter; to advance energy security; and to support DOE's other scientific discovery and innovation missions.

Plasma and Fusion Energy Science. Berkeley Lab has unique capabilities in Plasma and Fusion Energy Sciences that leverage our strengths in high field magnets, ultra-intense lasers, beam sources, and exascale computation. Core capabilities in superconducting magnet technology are being applied to improve future fusion reactors. Topics include development of advanced materials such as RECBO-based cable and novel quench detection methods for protection of HTS fusion magnets. The Lab has significant expertise in developing ion sources (including BELLA-i) and low-energy beam transport systems. It is developing novel accelerator architectures based on micro-electromechanical systems (MEMS) for fusion plasma heating and manufacturing applications. A series of projects funded by ARPA-E are led by Fusion Science and Ion Beam Technology (FS-IBT) staff, including the imaging of carbon in soil with neutrons, and the development of multi-beam RF linacs made using low cost MEMS techniques. Advanced plasma-based coating techniques support low temperature plasma technology applications, and at the Laboratory also the needs of ALS-U, LCLS-II. We are part of LaserNetUS via high power lasers in the BELLA Center and are hosting users to conduct experiments in discovery plasma science and high energy density science. Unique, intense lasers and particle beams are used for qubit synthesis very far from equilibrium, enabling formation of novel color center qubits with tailored properties for QIS applications (Fusion for Quantum).

Artificial Intelligence and Machine Learning. The Accelerator Technology & Applied Physics (ATAP) Division actively applies the latest techniques in AI/ML to further enhance progress in accelerator, laser, QIS, fusion and plasma science and technology. The Division's ALS Accelerator Physics Group has embarked on a study of how modern AI/ML methods can be employed to solve longstanding accelerator physics problems related to both accelerator operations and design. Using joint funding from BES (ADRP) and ASCR, an initial effort was successful in stabilizing electron beams in synchrotrons using AI/ML [*Phys. Rev. Lett.* 123, 194801 (2019)]. As a follow-up study, an exploratory effort has recently been launched in collaboration with ENG & ALS-U to employ AI/ML for rapid alignment corrections of magnets on measurement benches, as is typically required when field mapping hundreds of magnets before installation into a new storage ring as in the case of ALS-U. Finally, we have successfully employed AI/ML to accelerate multi-objective optimization algorithms such as those used to typically design magnetic lattices in storage rings. In this case AI/ML allows replacing computationally expensive physics evaluations with lightweight predictive models, and thereby accelerates a significant portion of the overall optimization cycle by orders of magnitude.

AMP is increasing its efforts in AI/ML activities, in particular on the development of (a) surrogate models as ultrafast alternative to standard beam and accelerator components modeling, and (b) tools for efficient optimization of accelerator designs. One of AMP's researchers is a leading participant in the teaching team of the upcoming USPAS course on "Optimization and ML for Accelerators," has submitted an ECRP proposal on AI/ML for accelerator simulations and is the Point of Contact on AI/ML for the ATAP Division. AMP is also exploring venues for engaging into the development of algorithms that could enable more efficient modeling of some accelerator and beam physics problems on quantum computers than on conventional supercomputers.

In the Magnet Development Program, machine learning techniques are being applied to the development of high-field superconducting accelerator magnets. Acoustic classification of mechanical quench precursors is being investigated using Deep Learning techniques, and early detection of quenching in superconducting magnets is being explored with ML-based real-time processing of multi-domain diagnostic data. In the QIS area, BCMT scientists and engineers are supporting the development of enabling cold electronics that can drastically simplify implementations of future quantum processors.

The BACI program has applied the high precision timing and RF control technology, by taking advantage of BACI's well-developed control systems for particle accelerators, to the quantum computer bit control in solving the scalability problem in the control electronics. In collaboration with the UC Berkeley Quantum Nanoelectronics Laboratory (QNL) under the support from HEP and ASCR, we have prototyped a qubit control system (QubiC) and demonstrated single and two qubits gate operation on superconducting qubits. Associated software has been developed to streamline the qubit chip characterization, gate optimization and execute circuits provided by users. The prototype system allows for further study of the parameter space of an overall control system that interacts with the qubits. In addition, we will further develop more compact modules and interconnection among them to build up a system needed for more complex quantum computers.

Within the BELLA Center, AI and ML techniques are being applied for rapid analysis of large data sets and to optimize the performance of laser-plasma accelerators. This includes, for example, the coherent combination of laser pulses from multiple fiber lasers, where machine learning techniques are used to maximize the laser efficiency and optimize the pulse characteristics. This is needed to develop the next generation of high efficiency, high repetition rate lasers that will power future laser-plasma accelerators, such as those being developed with the kBELLA initiative and the Accelerator Stewardship program of HEP. These AI and ML applications are being carried out through a collaboration between the AMP, BACI and BELLA Programs within ATAP.

Applied Science and Energy Technology

Applied Materials Science and Engineering. Our research emphasizes the design and synthesis of advanced materials for energy, information technology, structural, and other applications in a wide range of physical environments. We develop materials that improve the efficiency, economy, environmental impact, and safety for applications, including energy generation, conversion, storage, transmission, and utilization. Underlying expertise includes nanoscale phenomena, advanced microscopy, physical and mechanical behavior of materials, materials chemistry, and biomolecular materials.

Berkeley Lab's applied materials science and engineering research involves advanced materials and nanotechnology for clean energy, including electrochemical energy conversion and storage, the catalytic production and storage of fuels, and nanostructured light-emitting diodes. The Lab has world-leading expertise in the tailoring of the optical properties of window materials, including the characterization of glazing and shading systems, the chromogenics of dynamic glazing materials, and low-emittance coatings for solar performance control. Berkeley Lab has led the scientific community in the development of plasma-deposition processes to enable improved window coatings.

We have a strong development program directed toward advanced sensors and sensor materials to control industrial processes to reduce the waste of raw materials on manufacturing lines, increase the energy efficiency of manufacturing processes, and minimize waste. The Lab also studies high-temperature superconductors for electrical transmission cable that could substantially reduce losses during transmission. Capabilities include analyzing the mechanical behavior of novel materials and designing novel materials with enhanced mechanical properties. Berkeley Lab also has extensive expertise in using waste heat for electricity. In addition, the Lab conducts next-generation lithography and supports the development of tools and metrology for size reduction in the next generation of microelectronic chip manufacturing, largely sponsored by industry.

Berkeley Lab focuses software and hardware technology development on novel pathways to sense the grid at unprecedented temporal resolution, systems level integration of automated demand response, and renewables as elements of the next generation grid.

In the area of thermal materials and advanced metrology, Berkeley Lab's overall goal is to develop breakthrough solutions using thermal materials to address the fundamentally intermittent character of thermal energy supply and use in buildings and industry, an issue becoming ever more important in our renewable future. We have created a science-to-systems approach, building on fundamental advances in thermal storage and nonlinear thermal elements, that aims to impact large-scale applications in building and industrial sectors at low and moderate temperatures. Specific goals include:

- Design a new thermal storage fluid with enhanced heat capacity exceeding benchmarks like water and industry standard fluids. Similarly, design all-solid thermal storage materials surpassing paraffin benchmarks;
- Develop a new voltage controlled thermal switch with high contrast ratio;
- Leverage the new storage materials and nonlinear thermal devices to develop unprecedented thermal topologies, and model their impacts on building and industrial applications; and
- Develop advanced thermal metrologies to understand and optimize the thermal performance of these new thermal storage materials both at nano-scale and design level.

This research will establish Berkeley Lab as a leader in thermal energy storage, non-linear thermal elements, and novel thermal topologies, all aimed at building and industrial impacts.

This Core Capability is sponsored by BES, EERE, DHS, ARPA-E, and SPP programs, including DoD and industry. It is underpinned by DOE-supported basic chemistry, materials, and computational research, and contributes to DOE missions in energy, the environment, and national security. This work benefits

DOE technology programs such as water desalination, solar-energy conversion, electrical-energy storage and transmission, solid-state lighting, energy efficiency, and the study of materials in extreme energy environments.

Nuclear and Radio Chemistry. Here, the Lab's capabilities include fundamental nuclear measurements; actinide chemistry; the irradiation of electronic components for industry and the government, including post-irradiation and materials characterization; the design, development and deployment of advanced instrumentation; compact neutron and gamma-ray sources for active interrogation; nuclear data management; and substantial modeling and simulation expertise. Work for DOE's SC includes actinide chemistry with application to chelating agents; for NNSA, advanced detector materials, compact gamma and neutron sources, detection systems and algorithms development, and background data management and analysis. Our work for DOE NE through the Spent Fuel and Waste Disposition Campaign (SFWD) includes subsurface modeling and testing to evaluate and improve on the current technical bases for alternative prospective geologic environments for high-level nuclear waste disposal.

Applied Nuclear Physics. Berkeley Lab is a world leader in instrumentation to measure ionizing radiation, including scintillators and solid-state detectors that combine high density with excellent energy resolution and high-performance electronics for detector read-out. Complete detection and imaging systems are used for a variety of applications, including nuclear medical imaging, nonproliferation, and homeland security, as well as fundamental explorations of high-energy and nuclear physics. Unique materials-screening and crystal-growth capabilities in the Semiconductor Detector Laboratory enable optimized high-throughput development and design of scintillation and semiconductor detector materials. Capabilities include large-volume germanium and CdZnTe detector development emphasizing position-sensitive and low-noise systems, gamma-ray imaging using coded aperture masks, and Compton scattering telescopes.

Testing of critical space-based electronic components by the National Security Space Community (NSSC) uses heavy-ion beams at the Lab's 88-Inch Cyclotron. This facility's key national role was confirmed in an NAS study of U.S. chip testing needs and capabilities. "Cocktail beams," composed of a mixture of elements that mimic the composition of cosmic rays encountered by satellites, provide a unique national asset to greatly speed the testing of critical space-based electronic components. Other core facilities are the crystal growth facility, BELLA (where compact tunable monochromatic gamma sources are under development for NNSA and DoD), and the Semiconductor Detector Lab.

Berkeley Lab collects high-quality gamma-ray background data in urban and suburban environments with support from DHS. The Lab plans to fully characterize the gamma-ray background based on data collected from detectors in conjunction with visual imagery, light detection and ranging (LIDAR), weather, and other geospatial data that may affect distribution of incident gamma rays. The Lab also obtains and evaluates background gamma-ray data from aerial environments containing complex topographical and isotopic variations. For example, areas of elevated radiation in the contaminated Fukushima region were recently mapped by the novel High-Efficiency Multimode Imager mounted on a remotely controlled helicopter. NNSA supports a feasibility study to explore an advanced system for data storage, as well as analysis and dissemination of gamma-ray background data, including detailed annotation. Standardization and analysis frameworks developed at the Lab for the HEP and cosmology communities will vastly increase the scope of the data being analyzed in the future. This Core Capability is sponsored by SC (NP, HEP, and BES), NNSA, and NE, as well as DHS, DoD, and the NRC. It contributes to DOE missions to integrate the basic research in SC programs with research in support of NNSA and DOE technology office programs.

Systems Engineering and Integration. Berkeley Lab's demonstrated abilities to successfully engineer, construct, and integrate complex systems underpin many of the core capabilities described in this section, and those of the major user facilities described above. Within DOE's SC, the Lab is uniquely configured with a centralized organization that makes engineering, systems and project management, and technical support available to all of the Lab's scientific endeavors.

Our internationally recognized advanced instrumentation skills (e.g., accelerating structures, detectors, data acquisition and control systems, lasers, magnets, and optics) have enabled many of the scientific breakthroughs described in this Plan; these are the direct result of the holistic coordination and deployment of engineering and technical resources. Solutions and approaches developed for one application are routinely leveraged, adapted, and applied to others. This disciplined integration and systems approach is a critical part of Berkeley Lab's contribution to the LCLS-II upgrade, where we have completed the LCLS-II injector and undulators, and have major responsibilities in low-level RF systems. The Lab also responsibly leads the GRETA, US-CUORE, LUX, DESI, and LZ collaborative projects. The same approach has been used to assure that ALS-U is staffed with engineers that have prior experience from similar technically challenging projects. Other examples of successfully integrated systems and project management include: the ATLAS inner detector, US-CUORE, LUX, the GRETINA and ALICE nuclear physics detectors, and the Transmission Electron Aberration-corrected Microscope. Further illustration of this integrating, crosscutting systems approach is Berkeley Lab's world-leading expertise in integrated silicon detectors for high-energy physics detectors that has been adapted and applied to the development of massive scientific-grade CCD detectors for astronomical applications. This expertise was further adapted and improved to provide radiation-resistant high-speed X-ray and electron detectors. These direct X-ray detecting CCD systems are deployed at national and international light sources.

In addition to Berkeley Lab's demonstrated abilities to engineer and integrate complex systems for basic science, we are the recognized leader in energy efficiency in commercial and residential buildings and industrial facilities. We develop and transfer new energy-efficient building and industrial technologies from the laboratory to the industrial and commercial world, and stimulate the use of high-performance technologies through innovative deployment programs. The Lab is also a leader in developing cool surface materials for roofing, pavement, and architectural glazing, and in understanding large-scale urban heat-island effects that impact energy consumption and smog formation.

Within the national lab network, Berkeley Lab leads management of transmission reliability programs (CERTS); collaborates with DOE, independent power authorities, and states (with the Demand Response Research Center); and collaborates with other national labs on energy storage for ancillary services and renewable integration.

In addition to SC, these efforts contribute to technology research programs funded by EERE, FE, EDER, and ARPA-E, as well as the DHS Chemical and Biological Security program. Berkeley Lab leverages DOE's investment by working with state and other federal and SPP sponsors, including the Federal Energy Regulatory Commission, the California Energy Commission, the California Air Resources Board, and the California Public Utilities Commission. The Lab partners with national and international organizations to develop technical standards.

Decision Science and Analysis. Berkeley Lab performs integrated research on energy policies to mitigate carbon emissions and climate change while minimizing externalities such as health burdens, air quality impacts, economic disruptions, and water resources impacts. The Lab investigates the economic impact of energy-efficiency performance standards in industrial and commercial building equipment and systems, and for consumer products. We provide technical assistance to federal agencies to evaluate and deploy renewable, distributed energy, as well as demand-side options to reduce energy costs; manage electric power-grid stability; and assess the impact of electricity market restructuring, e.g., employing large-scale electric-energy storage systems. Research efforts integrate techno-economic analysis and lifecycle assessment with basic science and technology development to ensure sustainable scale-up.

For this core capability, Berkeley Lab's role within the national lab network is to provide analysis of energy efficiency, clean energy, and electricity market policies and standards for energy efficiency requiring complex interconnected technical, economic, and environmental analyses. This capability contributes to DOE's mission by assisting government agencies to develop long-term strategies, policies, and programs that encourage energy-efficiency in all sectors and industries. It is sponsored by EERE, OE, FE, and NE, as well as the CEC and the California Public Utilities Commission.

Mechanical Design and Engineering. Berkeley Lab's applied research addresses energy technology design and development, processes, models, networks, systems, and energy efficiency. The Lab leads the world in accelerating the transition of battery technology from lab to market, window technology and performance analysis, modeling of energy-saving technologies in building, whole-building, and component systems, and evaluating and tracking energy savings in industrial facilities. As a leader in the R&D of battery systems for automotive and stationary applications, the Lab is a lead partner in JCESR. Battery systems research encompasses the development of new materials, theoretical modeling, and systems engineering. In addition, the Lab applies its extensive experience in subsurface science to underground energy storage options involving thermal energy storage, natural gas and hydrogen storage, as well as porous medium compressed-air energy storage. The research in long term grid subsurface energy storage encompasses numerical simulations of coupled processes in the porous reservoir as well as field demonstration experiments.

The built environment is responsible for 40% of U.S. energy consumption and 70% of U.S. electrical usage; Berkeley Lab is DOE's premier lab performing research on buildings energy efficiency, energy simulation, modeling of whole building systems and components, walls, windows, heating, cooling, ventilation, plug loads, roofing systems, and refrigeration. New areas of research include analysis and development of model predictive control systems, fault diagnostics, measurement and verification, agent-based IT, energy information and management systems, and using machine learning and advanced in data science for model training and validation. The Lab is also a leader in the research of indoor environmental quality, lighting quality, ventilation and health.

Berkeley Lab researchers develop and test environmental sensing technologies for both indoor and outdoor air quality. Advanced sensing and metrology systems are also being developed to evaluate the thermal performance of advanced insulating materials and windows. New approaches are being developed to evaluate window shades and glare.

As part of DOE's grid modernization effort, the Lab advances research on electric grid storage and stationary use, electricity grid modernization through technologies for smart grid, distributed generation (microgrids), energy management and Demand Response, and improved grid reliability. This core capability is sponsored by EERE, OE, ARPA-E, EPA, other federal agencies, the State of California, and utilities. It supports DOE's mission to develop and deliver market-driven solutions for energy-saving homes, buildings, and manufacturing, as well as sustainable transportation.

Berkeley Lab has initiated a new set of research activities to support DOE's Grid Interactive Efficient Buildings Program that includes modeling the capability of building end-use loads to provide flexible loads, evaluation and development of control and automated communication technology, new technology development, and electric utility system modeling. Similarly, there is a growing research portfolio to develop and evaluate control of distributed energy resources that include EVs, demand response, electrical and thermal storage, PV, and other DERs.

FLEXLAB, or ***the Facility for Low Energy eXperiments in buildings,*** consists of testbeds and simulation platforms for research, development, testing, and demonstration of low-energy building technologies, control systems and building systems integration. FLEXLAB maintains a network of industry partners for research, demonstration, and deployment. It enables development of cost-effective integrated technology solutions to meet 50% whole-building energy savings — a feat that cannot be met solely by the use of single-component or technology upgrades alone. Our major sponsors are DOE (BTO, OE), GSA, SCE, PG&E, and CEC. With the addition of solar PV and energy storage, FLEXLAB is now fully equipped to address the cutting edge problems at the confluence of renewable integration with storage and demand response as the pathway to the next generation of energy management systems. With the addition of solar PV, smart inverters, and energy storage, FLEXLAB now supports FLEXGRID which provides cutting edge technologies to test systems related to renewable integration with storage and demand response as the pathway to the next generation of energy management systems.

Power Systems and Electrical Engineering. The Lab leads the world in advanced sensing modeling and short-term control in the distribution grid and microgrids. Berkeley Lab studies customer adoption patterns of grid technologies and distributed energy resources (DER) optimization in microgrids and buildings. We developed key analytics around grid measurement and Distributed Energy Resources Customer Adoption Model (DER-CAM) for dispatch and the control of microgrids. We also developed hierarchical control schemes and data analysis for large distributions of local power generation including solar, storage, electric vehicles to enable multi-level dispatch, and standards development of the interconnection of renewables and smart grid, all to enhance, modernize, and support the future distribution grid. The Demand Response Research Center integrates its technical expertise with electricity market analyses to identify market and policy barriers and research directions that can make the cost of market participation more consistent with added market value. This includes evaluating the capabilities of customer loads to provide various grid services and evaluating the cost requirements for technology for DR automation and program incentives.

In the National Lab network, Berkeley Lab leads and collaborates within the grid modernization activities, including program management. Collaborators include LLNL, LANL, SNL, ORNL, ANL, SLAC, and PNNL. This core capability contributes to DOE’s efforts to drive electric grid modernization and resiliency in the energy infrastructure, and the development of grid science for a high renewable penetration future. This work at Berkeley Lab is supported by EERE-OE, ARPA-E, DoD’s DARPA and ESTCP, and the CEC. The GMLC is a DOE-wide activity that is funded by EERE and OE.

Science Strategy for the Future

To sustain our ability to provide critical research to the nation requires both a strategic vision for the most promising research directions and prudent stewardship of our world-class user facilities and infrastructure, and of our outstanding corps of researchers. Berkeley Lab’s enterprise-wide priorities and initiatives are carefully chosen to provide for both this strategic vision and stewardship, thus maximizing the opportunities for scientific breakthroughs in the future. The Lab-wide **priorities** represent enduring commitments that ensure Berkeley Lab remains a world-leading research institution for the long term. The Laboratory research **initiatives** explore new directions that can leverage our unique capabilities to address the nation’s most important scientific and technological challenges.

Infrastructure

Overview of Site Facilities and Infrastructure

The Facilities and Infrastructure Strategy supports Berkeley Lab's Core Capabilities and utilizes the Campus Strategy objectives to address the Lab's strategic priorities, transforming the existing site into the Berkeley Lab of the Future. The strategy focuses on optimizing DOE mission-aligned infrastructure and space, including: the reclamation of acreage for future development and the creation of new or adaptive modernization of existing space; strengthening the continuity of critical operations through power shutdown resiliency, seismic safety improvements, deferred maintenance reduction, reliability enhancements, and improved maintenance capabilities; and implementation of COVID-19 precautions and mitigations, security and fire protection infrastructure improvements, and modernization of traffic circulation. This section provides an overview of existing infrastructure, and integrates approved, planned, and envisioned investments from the Lab, DOE, and alternative sources to comprise our 10-year infrastructure strategy. Our goal is to create a safe, secure, and sustainable research environment that supports Berkeley Lab's diverse program needs.

Berkeley Lab of the Future

Focus Areas

Strengthen Continuity of Critical Operations	Optimize Mission Aligned Space	Safety and Site Security
Power Shutdown Resilience	Bayview Redevelopment	Fire Protection
Seismic Safety	Charter Hill Redevelopment	Security and Site Access
Deferred Maintenance Reduction and Enhanced Reliability	Adaptive Modernization of Existing Space	Traffic and Parking

The main Berkeley Lab campus is adjacent to UC Berkeley, on 202 acres of (UC) land, of which 86 acres are leased to DOE. The site is located within the boundaries of Berkeley and Oakland, California; however, local land use restrictions are not applicable to Berkeley Lab. Information on Berkeley Lab land use planning is available in the Berkeley Lab Long-Range Development Plan.

The main campus structures consist of ~1.8 million gross square feet (gsf) of operating DOE-owned buildings (1.78 million gsf) and trailers/storage containers (.028 million gsf). Below, the Overall Condition - Mission Unique Facilities, and Overall Condition – Non-Mission Unique Facilities summarizes the overall asset condition, as reported in the Facilities Information Management System (FIMS) at the close of FY20.

There are 244,134 gsf of UC-owned facilities at the main site used for DOE purposes under occupancy agreements with UC, including Chu Hall (B30) and Shyh Wang Hall (B59) There is also 24,317 square footage of UC-owned space within the Advanced Light Source building. The Guest House (B23) is UC-owned and operated.

Overall Condition – Mission Unique Facilities				
Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$212.6M	57.8%	271,445	10
Substandard	$155.1M	42.2%	216,863	6
Grand Total	**$367.7M**	**100.0%**	**488,308**	**16**

Overall Condition – Non-Mission Unique Facilities				
Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$313.6M	32.4%	410,298	101
Substandard	$410.3M	42.5%	566,433	35
Inadequate	$242.6M	25.1%	3340,697	21
Grand Total	**$966.5M**	**100.0%**	**1,319428**	**157**

As of Sept. 30, 2020, Berkeley Lab leases or has licenses in place for eight off-site facilities totaling 213,599 gsf. In FY20, following completion of the Integrative Genomics Building (IGB) and program moves, Berkeley Lab terminated the Joint Genome Institute (JGI) leased space. The Lab also terminated the Oakland Scientific Facility (B943) in FY20.Additionally, the Lab extended the Potter Street (B977) and Hollis Street/ABPDU (B978-3) leases for an additional five years in FY20. The Lab expects to lease a warehouse containing 30,000 – 55,000 rentable square feet in FY21 for various storage needs. Berkeley Lab also has no-fee use of 48,211 square footage of UC space at UC Berkeley.

A summary of buildings, trailers, and other structures and facilities (OSF) that were in standby or shutdown status at the close of FY20 are summarized below.

Summary of Real Property Assets in Standby or Shutdown Status				
Asset Type	Standby		Shutdown	
	GSF	Asset Count	GSF	Asset Count
Buildings	30,298	3	1,979	3
OSFs	N/A	5	N/A	1
Trailers	1,250	2	1,160	4
Grand Total	31,548	10	3,139	8

Non-excess Building and Trailer Utilization Summary

We periodically survey the use of operational (non-excess) facilities that are also not in standby status. Our annual non-excess building and trailer utilization summary is summarized below. In any given year, the portfolio of shutdown and standby facilities is quite low, generally consisting of assets being prepared for demolition. The Lab's disposition and demolition program continues to make progress removing assets that no longer support the DOE mission.

Non-excess Building/Trailer Utilization				
Category	Building	Trailer	Total	Percent
Unutilized	1	4	6,855	3.5%
Under utilized	12	0	369,363	89.9%
Fully utilized	77	74	1,399,970	7.1%

Over utilized	90	78	1,776,188	67.4%
Grand Total	**152**	**20**	**172**	**100.00%**

The utilities infrastructure includes domestic and treated water, low conductivity water, sanitary sewer, storm drain, natural gas, compressed air, electrical, life safety and technology systems (e.g., telecommunications, optical fiber). These systems and their respective components vary greatly in age and condition, reflecting generations of alterations and improvements over Berkeley Lab's long history. Below is the summary of the overall asset condition of our utility systems:

Overall Condition – Utilities Condition as $ of RPV				
Condition	Mission Critical	Mission Dependent, Not Critical	Not Mission Dependent	Grand Total
Adequate	$483.0M	$23.3M	$.5M	$506.8M
Inadequate	$44.5M		$2.7M	$47.2M
Substandard	$67.5M	$82.3M		$149.8M
Grand Total	$595.0M	$105.6M	$3.2M	$703.8M

The Lab's Institutional General Plant Project (IGPP) is invaluable to our strategic goal to modernize core infrastructure elements, and over the past several years our investment has grown substantially. In FY18 and FY19, we invested around $9M towards IGPP, which grew to nearly $16M in FY20 costs (with $47.8M in project allocations). The Lab is currently working through a backlog of approved IGPP projects and plans to maintain annual IGPP investments on the order of $25-$35M. The average IGPP index over the planning period is 1.2%.

Overview of 10-year Campus Strategy and Summary of Investments Needed

Berkeley Lab's multiyear strategy is based on three objectives that focus on optimizing mission aligned space: strengthening the continuity of critical operations and implementation of COVID-19 precautions and mitigations, security and fire protection infrastructure improvements, and modernization of traffic circulation. Taken together, these objectives (as described in the "Berkeley Lab of the Future" at the start of this section) are intended to transform Berkeley Lab's aging facilities and infrastructure into a modern, integrated, interactive, sustainable, and fully mission-aligned environment for ground-breaking science.

Objective 1: Optimize mission aligned space

This objective includes both reclamation of acreage through the Lab's facilities D&D program and creation of new or adaptive modernization of space supporting research and operations. Much of the Objective 1-related activities are centered around the Bayview and Charter Hill (Old Town) Redevelopment areas, with several smaller projects scattered throughout the site. Redevelopment activities are central to increasing the number of buildings rated "Adequate" per the FIMS Overall Asset Condition data element.

The pandemic necessitated a new way of thinking about space and site access, based on the need for access to scientific or operational equipment and targeted collaboration. Given this new understanding, the Lab plans to adopt new space policies and standards to help drive a revised space management philosophy. For example, space could be allocated and shared based on research and/or operational need rather than employee class.

Bayview Redevelopment

Berkeley Lab's multi-year strategy includes construction of facilities to support full integration of biosciences and related programs adjacent to the recently constructed IGB in the Bayview cluster. The next building, the Biological and Environmental Program Integration Center (BioEPIC), will bring together biological and environmental research and house exciting new research capabilities that will advance interdisciplinary priorities, such as fabricated ecosystems and cryo-EM. The BioEPIC construction footprint is impacted by legacy underground site features related to the former Bevatron facility, including concrete utility tunnels, ancillary equipment, and contaminated soil. The Bayview Clean-up 1a (south tunnels), an Environmental Management (EM) funded project with completion forecast for Q3 FY21, addresses these site features. Concurrently, the IGPP-funded Site Utilities Relocation Plan (SURP) project is reconfiguring and renewing pre-1970s era utilities at the Bayview cluster, ensuring reliable utility services for decades into the future.

Redevelopment activities will continue at the northern section of the Bayview cluster throughout the planning horizon. The Bayview Phase 1b (north tunnels), another EM-funded project, addresses remaining former Bevatron facility features and contamination beyond the BioEPIC footprint. Phase 1b will be completed in Q3 2021. An envisioned EM-funded Bayview Cleanup Phase 2 will follow completion of the tunnel demolition and address the demolition of B56 and B64, including any local site contamination. Characterization of building materials and soil for Phase 2 will occur in Q4 2021. This cleanup work will free up the acreage necessary to construct the third biosciences-focused facility, the Biosciences Genome Engineering and Manufacturing (BioGEM) facility. A preliminary study in July 2020 helped scope and size this proposed building, set to house the Joint BioEnergy Institute (JBEI), the Advanced Biofuels and Bioproducts Process Development Unit (ABPDU), and the Agile BioFoundry (ABF). The BioGEM could enable those three programs to move from their leased location in Emeryville to the Lab's main site. Additional D&D efforts farther north, to remove B55, B55A, B60, and B63, will eventually follow, creating new acreage for the fourth and fifth biosciences-related buildings at Bayview.

Charter Hill (Old Town) Redevelopment

Berkeley Lab's multi-year strategy includes constructing a materials and chemical sciences building cluster at Charter Hill, adjacent to the Advanced Light Source (ALS) user facility. Charter Hill is being developed on the Lab's former "Old Town" area, which is being cleared of buildings and foundation members under the current Old Town Demolition Project. The Old Town Demolition Project's final phase address the removal and cleanup of B4 and B14 slabs, nearby utilities, B7 and B7C. Currently, substantial completion of the entire Old Town Demolition Project is planned for late FY22. Early interim uses of the newly available acreage in the Charter Hill cluster are already in place, including a new tensile structure and additional parking and laydown areas in support of projects and operations. The Linear Assets Modernization Project (LAMP) would extend some modern and adequately sized utility infrastructure into the Charter Hill area.

The new Charter Hill facilities would house research that pursues the understanding and control of materials phenomena and chemical transformations across size and time scales. Designed to enable collaboration and accelerated discovery, Charter Hill laboratories would leverage advances in ML, AI, and automation; other next-generation science concepts; and proximity to the ALS and its beamlines.

The anticipated first Charter Hill facility would be the Advanced Materials Discovery Building (AMDB), a 3-4 story, ~68,500 gsf lab/office facility with approximately 150 occupants. The AMDB would provide space to house personnel and programs from Berkeley Lab's Building 70, which has a poor seismic rating and is planned for demolition. The second would be the Interdisciplinary Chemical Sciences Building, a ~68,500 gsf lab/office facility with approximately 150 occupants. The "Chemical Observatory," is a key component of the envisioned capabilities for the site. It will be an innovative research facility designed to integrate multiple probes, such as those derived from the ALS' soft X-ray beamlines, into more traditional laboratory spaces. Site preparation would include grading, installation of modern utilities, and realignment of Segre Road. A Modular Utility Plant (MUP) would be constructed in stages nearby to efficiently distribute utilities between the buildings. One or more ALS beamlines may be extended under the Charter Hill cluster.

Laser-Plasma Acceleration Infrastructure Modernization at B71. Utility infrastructure is needed to support the installation of a future high average power laser system, kBELLA, to enable high repetition rate applications of laser plasma accelerators. This would include a new radiation shielded target area, a lab clean space for the laser and control room, and associated mechanical, electrical, and HVAC infrastructure. A design study and estimates have been prepared, and we are investigating funding sources.

Accelerator Science and Engineering Building. Accelerator science and engineering are closely integrated at Berkeley Lab, which is essential for: the efficient operation of our accelerator facilities, for world-leading R&D in advanced accelerators and superconducting magnets, for engineering of advanced scientific instruments for key stakeholders in HEP, BES, FES and NP, and for development of new applications of accelerator technology. However, accelerator and engineering staff are currently distributed across the laboratory. Many activities are housed in legacy buildings that do not encourage collaborative work, and do not meet current seismic standards. This building will bring together scientists and engineers working on activities critical to the mission of DOE across the Office of Science.

Adaptive Modernization of Existing Space

Given the high utilization rate of existing facilities and the elevated cost of new construction across the region, the Lab is renewing efforts to improve existing space and infrastructure to better align with evolving research needs. To prioritize improvements capable of increasing functionality or occupancy density, Berkeley Lab's Campus Planning Department will use a metrics-based approach.

Several years ago, B73/B73A were vacated and placed into excess status due to their very poor seismic ratings. The Lab is using IGPP funding for B73 modernization, and will seismically retrofit and renovate the building (and demolish B73A) to create safe laboratory and office space that meets current research needs. This additional space will accommodate program growth in FY22 and beyond, as well as retire the institutional liabilities related to the existing deficient structures.

At B77, two separate IGPP projects will greatly enhance the space use at the engineering complex. These improvements support programs across the Lab and several DOE complex projects, such as HL-LHC-ATLAS, HL-LHC-AUP (Accelerator upgrade), LCLS-II, ALICE, ALS-U, and eventually the EIC (Electron Ion Collider). The first of the two, the B77 Enclosure Installation, builds an enclosure over an existing mechanical yard, to accommodate reorganization of precision machinery needed to manufacture parts for experiments. This project will be completed in early FY22.

The second project, the B77 Metrology Lab, will refresh and expand specialized metrology laboratory space. This project will begin construction in FY21 and complete work in FY22. As these IGPP projects progress, the Lab will fund a non-capital project to reorganize the major pieces of equipment at B77 to better optimize the space utilization within the building. However, high bay space for large structure assemblies remains in short supply when compared to the needs of numerous programs across the Lab.

As new projects are formulated to either create new space or adapt existing infrastructure, the creation of additional high bay spaces will be a high priority. The inclusion of a notional Accelerator Science and Engineering Building in the out-years of the strategic planning horizon represents one significant step in addressing this critical space need at the Lab.

Electron Microscopy (EM). Specialized space for new types of EM will enable Berkeley Lab to remain an international powerhouse. Infrastructure that incorporates a number of synergistic characterization plans across the Lab would result in a renewed state-of-the art, world-leading electron imaging capability for a diverse set of scientific challenges in areas such as materials synthesis, catalysis, earth and environmental science, soft matter characterization, quantum materials, energy storage and structural and cellular biology. Instruments to be developed requiring state-of-the-art space include novel in situ, time-resolved and cryo and variable temperature EM instruments, and an analytical transmission electron microscopy (TEM) with high energy resolution. This proposed GPP would build an addition onto B62 – approximately 7,000 gsf of specialized laboratory space to house EMs, supporting infrastructure and systems.

Finally, as part of maintaining a minimal level of food services onsite, and to ensure that there is an outdoor temporary emergency operations center available for use throughout the duration of the pandemic, the Lab is planning the installation of a tent and related utilities in the Z parking lot (across the street from the Guest House).

Objective 2: Strengthen continuity of critical operations

This objective includes development of forced power shutdown resilience; improvements to seismic safety and reduction of landslide risks; and reducing deferred maintenance (DM), enhancing reliability, and/or increasing maintenance capabilities.

Power Shutdown Resilience

A major emerging risk to mission readiness and the continuity of Lab operations is the threat posed by regional "Public Safety Power Shutoff" (PSPS) events initiated by the Lab's local utility provider, Pacific Gas & Electric (PG&E). PSPS events are initiated to reduce the potential for wildfires caused by utility provider owned electrical infrastructure coming into contact with debris when gusty winds and dry conditions are forecasted or are present. Prior to 2019, the Lab had never been impacted in such a manner. However, in 2019, the Lab was forced to shut down operations for five business days across two separate events. Direct costs related to these events were approximately $1.7M per business day – $8.5M total. In addition to the productivity losses caused by the shutdowns, significant strain was placed on the Lab's aging infrastructure through repeated equipment de- and re-energizations. The likelihood of additional PSPS events over the next decade and beyond increases the urgency to reduce DM and modernize existing facilities and infrastructure.

The Lab receives power from PG&E at the Grizzly Peak Substation via overhead 115kV transmission lines. Power is distributed at 12.47kV from the Grizzly Peak Substation to seven switch stations throughout the site. Each switch station, in turn, serves multiple buildings. In response to the 2019 PSPS events, feasibility studies considered various options to quickly add power generation capacity in preparation for the 2020 fire season. This analysis concluded that temporary backup generation at the 12kV switch stations provided the optimal near-term solution. In partnership with PG&E, a pilot project was initiated to provide 4MW of closed transition temporary power generation at Switch A6 during the 2020 fire season, providing backup power to critical business systems. A similar temporary installation is planned for the 2021 fire season. There are also several other investments being made through GPP, IGPP, and LAMP, described in further detail throughout this subsection, that will modernize distributed utilities and increase reliability.

While the Lab is making significant investments, they unfortunately fall short of a sitewide that ensures mission critical Lab operations can be maintained during planned (PSPS) and unplanned power outages (e.g., caused by earthquakes or local wildfires), utilizing onsite power generation as well as demand side management and advanced supervisory control and data acquisition site wide control systems. This future state transitions the electrical distribution system into a flexible microgrid of interconnected loads and distributed energy resources that can operate in both a grid-connected or island mode. To meet this goal, the Lab's near term strategies include performing an independent study for the resilience posture and mission critical utility infrastructure conceptual design, providing closed transition backup generation at 12kV switch stations, replacing aging equipment (e.g., generators, automatic transfer switches), development of load shedding and demand-side management strategies, replacement and/or upgrades to legacy building automation system controllers, metering upgrades, upgrade high priority building control systems, optimization of existing generator capacity, and deployment of additional backup diesel generators at selected locations or critical buildings. Longer term strategies include implementing a microgrid strategy, incorporating alternative energy technologies such as solar photovoltaics, energy storage, fuel cells, hydrogen electrolyzers, EV charging, and dual-fuel back-up generators, and implementing new backup power strategies serving critical loads for new buildings (vs. traditional backup diesel generator approaches). Longer-term resilience strategies are being coordinated across the Facilities Division, Sustainable Berkeley Lab, and the Lab's Energy Technologies Area to foster "living lab" opportunities to advance resilience and sustainability while creating opportunities to develop and test emerging technologies.

Responding to PSPS events in real-time can be extremely challenging given the Lab's antiquated building controls systems (e.g., Barrington). Two of the four major building management systems currently in operation are legacy systems; these operate approximately 60% of the Lab's buildings. Increasingly, they do not meet the Lab's mission requirements and have capability gaps for supportability, resilience, and security. The legacy systems rely on multiple integrations in the field to remain in service, are challenging to collect field data from, and do not manage alarms and events at a level that meet our operational needs. They are hosted on obsolete operating systems, leaving them at risk for failures with excessively long lead times before functionality can be restored; our cybersecurity group have been forced to develop compensating controls. Obsolete control systems can also make it challenging to quickly and safely shutdown and restart mechanical and electrical equipment.

Another significant operational challenge, especially in the context of telework, has been the loss of IT systems during PSPS events due to the lack of back-up power capabilities for existing cooling loads at the Lab's General Purpose Data Center. Portions of the data center had to be shut down during the PSPS events, impacting ESnet systems, business systems, identity management systems, shared drive services, science division virtual machine service, and network services (e.g., VPN, firewalls, etc.). To address these critical issues, an SLI-funded sitewide HVAC Systems Improvements Project in FY21 replaced the site's most vulnerable building control systems and reconfigured cooling loads at the Lab's General Purpose Data Center, which can now be operated during PSPS events. Replacing obsolete building automation and energy management systems to meet current standards will ensure 1) they are fully supportable by the manufacturer for parts, technical support, and patching, 2) that they can integrate into the lab-wide Skyspark platform for data analytics at scale, 3) that they are resilient to utility disruptions and capable of a timely recovery with minimal intervention, 4) that they can support ventilation systems in a safe, efficient, and compliant manner, and 5) create a unified building and energy management infrastructure, meeting or exceeding established cybersecurity standards.

Modernizing the Lab's building automation and energy management systems increases the potential for harnessing the considerable in-house data analytics capabilities related to building operations, including data integration and organization, and implementation of new tools like Skyspark. In anticipation of this transition to state-of-the-art building automation and energy management systems, the Lab will be deploying algorithms that use ML or otherwise exhibit AI (i.e., able to "handle tasks on their own") to unlock advanced functionalities. Some examples include: 1) implementation of proactive maintenance capabilities through approaches such as automated control loop tuning, which uses data screening tools to identify mechanical equipment exhibiting poor control, and make adjustments to prevent energy waste and premature equipment failure, 2) occupancy/vacancy inference sensing, allowing for building services to be controlled to better match everyday conditions, as well as occasional, hazardous conditions such as those experiences during COVID or wildfire events, and 3) multi-objective model predictive control (MPC), a framework developed in collaboration by researchers in the Energy Technologies Area, NERSC, the Facilities Division, and Sustainable Berkeley Lab that can optimize comfort and energy consumption, but will also be expanded to optimize for utility cost and low marginal greenhouse gas emissions. Completion of distribution and points of connection metering across all utilities sitewide, and replacement/upgrades of obsolete building automation systems to current standards, will allow the Lab to access the full value proposition of AI/ML in operations.

The SLI-funded LAMP will significantly improve the Lab's utility resilience. The project will seek a 50-80% reduction of the $113M of high-risk linear asset-related DM backlog, and will create redundant system loops, where appropriate, to modernize system operations and increase utility service reliability. The multi-year LAMP project prioritizes essential system improvements, based on mission impacts and future programmatic needs into earliest work packages. The first phase of this project is centered around the Grizzly Substation Distribution Corridor and provides modern, state of the art sitewide power distribution, including an increase in power availability to 70MW, sitewide electrical SCADA capabilities, improved site distribution duct bank infrastructure, and delivery of 34.5KVA power to enable NERSC-10. Infrastructure collocated with this utility work, including IT and water supply, may be improved as well. The Lab will complement these investments by installing two new transformers to provide additional capacity and redundancy, allowing it to meet forecasted electricity demands and improve the safety of maintenance activities. Future phases may include natural gas and electrical distribution capabilities along the McMillan Road corridor, trunk utility installations along the Smoot and Alvarez Road corridor, and electrical and IT system improvements along the East Canyon Corridor.

Several IGPP projects are in progress to improve the Lab's PSPS posture within its existing facilities. Phase 1 of the Sitewide Electrical Safety and Maintenance Upgrades (SESMU) will address deficient and aged electrical equipment at B50A and B70A, and Switchstation A3. Construction for the switch station A3 relay replacements will be completed in FY21 and the construction phase for B70A will begin in FY21, with B50A work planned in FY22.

SESMU Phase 1 addresses several DM items that pose reliability risks and unnecessarily increase the cost of day-to-day maintenance. This project substantially completed the upgrade of boilers and controls at B62 in FY19; engineering design will begin in FY21 for upgrading controls and cooling capabilities at B2, as well as upgrades to the sitewide compressed air plant at B43, with construction planned for FY22-23. Additional phases of the SESMU and Sitewide Mechanical Plant Maintenance Upgrades are being planned for the latter half of the planning horizon. Enduring buildings that are strong candidates for IGPP investments given their large DM balances and lack of redundancy include B50A & B, B66, B70A, B71, B77, B88, and B90. For example, B71 mechanical, water, and HVAC system upgrades are needed to meet current standards. This includes providing redundancy for current single points of failure, replacing aging systems, and increasing capacity. B71 currently does not maintain temperature for work requiring equipment sensitive to minor fluctuations and air currents. This utility infrastructure will be increasingly important as multi-program activities and user operations increase, and the costs of down time or nonperformance escalates.

Improve Seismic Safety and Reduce Landslide Risks

The third Uniform California Earthquake Rupture Forecast (UCERF3) shows that there is a 98% probability that an earthquake of magnitude 6.0 or higher will occur in the next 20 years (before 2043) in the San Francisco region. The UCERF3 also predicts that a magnitude 6.7 or larger earthquake will occur on the Hayward Fault, a mere quarter of a kilometer from the main Lab site, before 2043. We must prepare for this eventuality.

After more than a decade of mitigation efforts, the Lab's number of buildings expected to perform poorly in a seismic event dropped from 34 to 19. However, national standards for seismic evaluations were revised in 2013 and 2017, and implemented into the California Building Code in 2019. Berkeley Lab is refreshing evaluations of many buildings based on the new standards, and as expected, more facilities are rated less favorably than before, up from 19 to 51. However, all currently occupied facilities met the California Building Code in effect at the time of construction, thus fulfilling DOE seismic requirements.

Recognizing the hazards presented by nearby faults, the Lab utilizes a comprehensive risk-ranked prioritization process to manage and mitigate seismic risks, and will continue to partner with DOE on implementing appropriate corrective measures (e.g., retrofit, demolition, etc.). The B6 (ALS) addition and B90 are near the top of the Lab's revised prioritized mitigation schedule, due to the mission critical nature of each facility and the number of people in each building. The Bayview plan includes demolishing several seismically poor buildings. Other facilities rated "poor" are included in the Lab's long-term redevelopment strategy. The Seismic Safety and Modernization (SSM) Project will improve the safety of Lab employees and visitors by addressing existing critical Operations facilities that are currently in an inadequate seismic condition. As indirect funding allows, other small seismically deficient buildings and trailers will be demolished. As part of the overall strategy, we are reducing staff levels in some buildings and vacating others during the multi-year seismic risk reduction efforts.

Chemical Lifecycle Management

In 2020, the Lab embarked on a substantial initiative to understand the state of chemical management, to identify programmatic and performance problems, and to provide recommendations for improvement to the level expected by Lab leadership, UCNL, and DOE Site Office management. The detailed project plan, "Chemical Lifecycle Management Corrective Action Plan" (CLM CAP), was developed from these recommendations. Significant time and effort are needed from both research and operations divisions over the next few years to improve all aspects of the chemical lifecycle, including work planning, procurement, inventory management, and disposal.

Execution of the CLM CAP began in early January 2021. Near- and long-term objectives are in progress. Radio Frequency-Identification (RFID) barcode technology is being implemented sitewide to facilitate chemical inventory reconciliation, an essential aspect of accurate chemical inventory, and improved tracking of high-risk chemicals, such as those that are time-sensitive. Central chemical receiving, which will take several years to fully implement, is in the planning stages of benchmarking and evaluation. A new chemical management system will be procured by mid-year, then configured and implemented by mid-2022. Importantly, while the CLM CAP management is being led by EHS, research divisions are closely partnered with all aspects of successful execution through participation in work groups, feedback from institutional committees and subcommittees, and additional outreach efforts.

As the CLM CAP progresses, chemical management performance will continue to improve until a high level of performance is achieved. These efforts will decrease the Lab's risk profile in both safety and security, address previous performance issues and findings, and ensure compliance with all applicable

DOE orders and regulations. Some key measures of success include implementing a centralized chemical receiving and onboarding process, transitioning to an enhanced and integrated chemical management system, and clearing R2A2s for CLM that are well communicated, understood, and enforced.

Reduce Deferred Maintenance, Enhance Reliability, and/or Increase Maintenance Capabilities

Many projects discussed previously with other strategic drivers also reduce DM and enhance reliability by increasing maintenance capabilities, but other projects do not relate directly to power shutdown resiliency or seismic safety. This subsection details these important projects needed to improve the condition and reliability of the Lab's facilities and infrastructure.

We prioritize our DM via building and utility system owners' annual review of each facility's condition assessment deficiency. They validating scope, status, and cost estimate, and assign risk based on probability and consequence of failure. Then, we use an industry-standard pairwise methodology to develop an overall ranking strategy. For FY21, the Lab adopted and incorporated *the Guidance for Categorizing DM, RN, and Modernization,* which was developed by the SC DM working group to improve accuracy. The Lab's annual review process includes identifying and categorizing repair needs. Each year, we reprioritize, categorize as DM, and address repair needs. Once addressed, these assets are retired from the DM database. Currently, DM represents approximately 45% of the entire repair needs balance. The Lab's focus is to continue prioritizing and making investments toward addressing high-risk facilities and infrastructure deficiencies with the greatest mission and operational impact. To increase the number of buildings with an "adequate" rating, we will need to raise the IGPP budget to modernize existing facilities and infrastructure, increase the maintenance budget to achieve 2% MII, remove and replace excess facilities, and partner with DOE for direct DM reduction investments.

Maintenance and repair (M&R) funding is projected at 2.69% as an average across the entire planning period. In FY30 and FY31 M&R funding dips briefly below 2% due to a combination of RPV increase from the addition of several new buildings and project priority forecasting.

The Lab recently completed the SLI-funded Supply Water (CMLC) Replacement GPP project, retiring the highest priority DM related to our domestic and fire water distribution systems. The SLI-funded Storm Drain Repair/Replacements GPP project is under construction and will be completed in FY22. The Lab has replaced several boilers that were out of compliance with local air quality standards, and this year will replace the final boiler plant with this issue at B88. The Lab has also replaced gas switches in the Strawberry Canyon cluster that were leaking SF_6 gas and at the end of their useful life. We also replaced an inoperable cooling tower at B88. The Lab will begin a program of overhauling boilers and chillers that are at highest risk of failure so that we can buy down DM related to aging building-specific mechanical equipment. Finally, we have engaged NNSA's Roof Asset Management Program to assess our portfolio of roofs with the goal of prioritizing roof repairs and replacements into the future.

Most site-wide telecommunications infrastructure used by network, telephone, mobile phone antennas, fire alarms, and EH&S related alarms is old and deteriorating, including underground conduit paths and communication vaults, copper trunks, fiber optic trunks, etc. Many infrastructure deficiencies may be reduced as a byproduct of LAMP, where economic efficiencies may be gained by replacing these system components in concert with other nearby system replacements. Telecommunications rooms in many buildings are too small and lack sufficient power or cooling to support modern resilient network and telecommunications equipment. To date, our investment has been reactive to maintain existing service levels to address leaks, corrosion, rodent damage, and ground movement. However, to address these critical technology systems the Lab is planning a series of investments over the planning horizon.

Berkeley Center for Magnet Technology (BCMT). Many Lab science programs involve experiments and facilities operating at cryogenic temperatures; these require a helium liquefier, or an upgrade to the present equipment. The HEP-funded Superconducting Magnet Program (SMP) within the BCMT is one such facility. SMP has made recent investments to improve helium gas recovery and storage, but the liquefier itself is antiquated and its performance no longer satisfies program needs. BCMT management's cryoplant upgrade plan leverages the prior He storage investments while satisfying broader LHe needs. The most critical element is the procurement of a new liquefier, which would provide liquid directly to the magnet test facility and in transportable dewars to other users. The liquefier is essential for the U.S. MDP to deliver on its goals. DOE-OHEP leadership supports this critical need and provided funding in FY19 to procure a helium liquefier. To leverage the liquefier for projects and programs beyond HEP, further procurements would be required, including LHe storage dewars and piping for gas recovery from experimental users at the ALS and Materials Science (B6 and B2), as well as associated gas purification capability. Engineering would then run the cryoplant facility and support science programs within ATAP, ALS, MSD and others.

Objective 3: Modernize Traffic Circulation, Site Access, and Safety Related Infrastructure

This objective includes implementation of COVID-19 precautions and mitigations, security and fire protection infrastructure improvements, and modernization of traffic circulation.

COVID-19 Precautions and Mitigations

In May 2020, the Lab implemented a robust COVID -19 safety plan that resulted in a highly compliant COVID-19 safety culture. The plan emphasizes learning and improving using Integrated Safety Management principles. It includes a robust work planning program, a communications plan, a COVID Info Line/Helpdesk, website, a weekly risk evaluation process, and an assurance program. High rates of employee compliance with the COVID-19 safety plan resulted in a continuously safe work environment as measured by a very low number of COVID-19 cases onsite and no COVID-19 transmission at all Lab locations (as of this writing).

In August of 2020, the Lab documented the maximum safe occupancy of each of the its buildings to determine the appropriate number of workers permitted with COVID-19 restrictions in each laboratory, office, shop, and high bay. This "Building Capacity Report" was conducted by our Space Management team, experts in EH&S, ventilation, and HVAC, with the help of an outside space management and planning consultant. Collectively, the team evaluated each space to determine the safe layout for performing work, as well as the total safe occupancy within each space. This study allowed us to determine the safe number of total workers at lab sites, and within each lab space. *(Note: these occupancy levels are equivalent to or lower than stated DOE requirements.)* Occupancy limits for each workspace are now posted on every door.

In June, we began a COVID-19 "Return to Work" Pilot series to gradually increase onsite staffing to perform mission critical work. The goal of this pilot was to implement, learn, and improve with each pilot to ensure we were continuing to keep our employees safe. The timeline below describes how we have increased and decreased our onsite workers according to the pandemic conditions in the communities surrounding the Lab.

- In late March of 2020, Berkeley Lab went into a safe and stable mode, limiting onsite workers to ~ 450. The Lab also implemented a telework policy where the majority of its 3,700 employees were working from home.
- In June 2020, the Lab safely and successfully increased onsite daily workers from 450 to 800.
- On June 26 2020, the Lab received approval to advance to what was then called "Federal Phase 1." The Lab also implemented limited shift work, with cleaning between shifts, to better utilize our facilities during non–peak hours.

- From July through August of 2020, the Lab gradually increased the number of onsite workers from 800 to 1200.
- In September 2020, we received approval to advance to what was then called "Federal Phase 2,"enabling the number of onsite workers to gradually increase to our peak number of 2,700.
- From September to mid-November 2020, according to our "Phase 2" plan, the Lab increased the number of workers from 1,200 to 1,450.
- In November 2020, our local community experienced a significant increase in COVID-19 cases, and the Lab responded by reducing the number of onsite employees to ~ 1,200.

From the last half of November 2020 until March 2021, the Lab has kept the number of onsite workers at 1,200. In January 2021 the Lab increased COVID safety measures for employees, making COVID testing available at two Lab locations to all approved onsite employees and affiliates. As of March 2020, the Lab's rate of positive tests is at 0.3%, compared to 2.4% in Alameda County, where the Lab is located.

In February of 2021, as part of the University of California (UC) system, Berkeley Lab received several allocations of vaccines and was able to implement a COVID-19 Vaccination program. To date, we have provided 1st round vaccinations to 300 employees and 2nd round vaccinations to 100 employees. We plan to continue vaccinating 200 employees a week (subject to availability).

Based on the successful implementation of the Lab's COVID-19 safety plan and current declining number of cases in the local community, the Lab will seek authority to gradually increase the onsite workforce in small increments to a previously approved cap of 2,400. This final number was determined by both a COVID-19 Building Capacity Study and an Air Ventilation Study, in which each workspace at the lab was evaluated to assess safe capacity with COVID-19 controls.

Physical Security Infrastructure Overview

Berkeley Lab's physical security infrastructure is undergoing a transformation to bring systems to present day standards, and to prepare for new Lab-wide projects that are driving system expansion. Other drivers are new DOE requirements outlined in DOE O 473.3C, *Design Basis Threat*, and DOE O 473.1A, *Physical Protection Programs*, which standardizes physical security requirements (expected to be promulgated this year).

Physical security systems service the Lab's main site and four offsite facilities: B1, B971, B977, and B978. There are both General Access Areas (GAAs) and Property Protection Areas (PPAs). As defined in DOE O 473.3A, *Protection Program Operations,* GAAs allow access for all personnel and members of the public with minimum security requirements, while PPAs are security areas that are established to protect employees and Government buildings, facilities and property through additional physical security layers. The Lab does not have Limited Areas.

Our physical security infrastructure varies by location, but in general includes (for GAAs) security fencing, doors secured by locks and keys, the Berkeley Lab security badge, and access control systems. Additional layers for PPAs include video surveillance, biometric or keypad readers, and motion-sensors. With the inception of the new Security and Emergency Services Division in 2020, and increased direct and indirect funding streams provided by DOE, we have reinvigorated our commitment to physical security improvements. We have hired a new Physical Security Supervisor, increased technical staff from two to four FTE, instituted more formal project planning with the goal of establishing a complete physical security components life cycle management, and implemented a budgetary forecasting schedule to better communicate program needs.

Access Controls Our access control system operates with Lenel program management software, V7.2 (2016). The Lab is currently upgrading to V7.6, which includes, among other enhancements, more advanced cyber security controls. The Lenel system integrates with our badge management system (HID SAFE) which was just updated this year after a nearly two-year effort to retire a separate 30-year-old system operating on an outdated and unsupported Windows platform. Updating the operating platform is the first step for our system to support the required technology to address DOE order changes. This upgrade allows us to integrate with our video surveillance platform to improve system performance and security effectiveness through new alarm monitoring capabilities. It also allows for improved performance testing and system maintenance scheduling.

Along with platform upgrades, hardware capital improvements and expansion efforts are needed to bring access control technology to current standards and meet new DOE requirements. This includes adding system controllers, card readers, and secondary authentication technology, among other projects.

The goal of our access control upgrades is a fully integrated video surveillance, visitor management, alarm monitoring, and security credential management system with the ability to upgrade software versions and system components to meet present and future requirements.

Video Surveillance (VS) The Lab's VS system operates on an outdated, analog-only platform that does not integrate with the new access control system or provide adequate video quality. Video coverage is likewise inadequate for today's environment – it does not properly cover road, fire hazard, or security areas. In response, we are phasing out two legacy VS systems while simultaneously integrating a third system (Avigilon) which will be the Lab's sole solution for VS management and integration.

The Avigilon platform is a non-proprietary system that brings improved system performance, artificial intelligence (AI) capabilities, active system health monitoring, and system integration that supports expanded coverage regardless of the brand or quantity of cameras purchased. The AI capabilities enable users to search for vehicles, cyclists, and people with basic description identifiers to locate subjects of interest. The Avigilon platform tools will enable our site operations personnel to review footage more efficiently through activity in popup windows, track and locate objects of interest, and capture video footage to attach to incident reports. It also integrates with our access control system to increase threat detection at our PPA locations.

Berkeley Lab is making significant hardware upgrades as well. Currently, we have 130 cameras installed, half of which are outdated analog units marked for digital upgrades. In response to both DOE requirements and Lab-identified needs, we have identified 80-100 new interior and exterior camera install locations that will reduce security risks and improve situational awareness and emergency response capabilities. Specific VS projects include eight multi-view cameras that will be strategically located around the main site for improved fire detection. These were acquired in response to fire-safety concerns after a recent modest and quickly contained grass fire on Lab property which, if undetected, could have caused significant damage. Additionally, we have identified new camera locations at 35 high occupancy building entrances and 16 traffic intersections.

During FY21, LBNL technicians and sub-contractors have installed a total of 19 cameras in support of these efforts (four of which for the fire safety project) and are meeting project goals. We also anticipate 49 new camera installs associated with new construction over the next decade. The table below depicts needed and anticipated access control hardware upgrades for known projects over the next ~5 to 10-year period.

The goal of the Lab's VS system is to fully integrate emerging technology, high-definition cameras, AI algorithms, and advanced system monitoring stations with the ability to upgrade software versions and system components to meet future system performance requirements.

Perimeter Protection Another cornerstone of physical security protections is the perimeter protection formed by fencing, site vehicle and pedestrian access gates. Perimeter fencing integrity is a challenge due to the varied geography of the main site. With the close proximity to the UC Berkeley campus and hiking trails, trespassing events are somewhat frequent. We are tracking similar numbers for trespassing events this year as we were last year, averaging about three events per month. While not an immediate concern, improvements to perimeter fencing will likely be necessary in the next 5-10 years – or sooner – barring new DOE requirements.

Vehicle Gates: At the main site, the Lab's three vehicle and pedestrian entry points are an area of concern and require improvement. Both the Strawberry Gate Guard House (B33A) and the Grizzly Peak Gate Guard House (33C) were constructed in 1965 and were not designed or positioned to meet today's security standards. Last year, in response to an increasing baseline security posture, the Lab implemented new security requirements, including 100% badge-in at site vehicle and pedestrian gates, and 100% ID checks for non-LBNL personnel. Geographic challenges, dated configuration and technology, and new security procedures have made these entry points marginally adequate. Further increases to the Lab's security posture in these locations will be extremely challenging, if not impossible, without technological improvements and/or repositioning. With the planned UC Berkeley-managed Centennial Bridge Replacement Project starting construction in 2022, there may be an opportunity to improve the configurations of the Strawberry Canyon and Grizzly Peak entry points. Such projects would improve vehicular safety and the Lab's security posture.

FireSAFE The average age of fire protection systems at the Lab is 26 years. Frequent equipment failures have led to costly building evacuations and operational interruptions. The Fire and Safety Alarm Future Enhancements Project will replace and upgrade our existing fire and safety alarm systems nearing their end-of-life. The new fire alarm systems will have mass notification capabilities that would replace the Lab's dated public address system. The plan is sequenced over a funding-dependent, multi-year period based on building risks, operational priorities and the condition of existing systems. The highest priority phase of this project is for B6, B15, and B80, as these fire detection and alarm systems are a critical component to the exemption that the Lab has on file with the DOE. The exemption allows the ALS complex to exceed $412M in value in a singular fire area. Without the breadth of mitigations (fire pumps, fire sprinklers, onsite Fire Department, smoke control, fire detection and alarm system), the Lab would be out of compliance with the exemption, and at risk of additional funding/value being allowed at the ALS complex (i.e., ALS-U).

Maximize Transportation and Parking Improvement Opportunities

The past year has fundamentally redefined how people across the world work and commute. The Lab is no exception, with the vast majority of our community teleworking from their homes. Recognizing that we can work differently in the future, telework will be central to the Lab's strategy to reduce commute impacts to local communities and the environment, as well as parking demand onsite. To this end, the Lab initiated the Future of Work project to assess post-pandemic opportunities and challenges (e.g., telework and flexible work), and provide recommendations to Lab management. These recommendations will play an important part of the Lab's future transportation strategy. The pandemic has also lowered local transit ridership and increased the usage of private vehicles, prompting the Lab to pause our ridesharing strategy. Ridesharing will be revisited as concerns for sharing vehicles with those outside of one's household subside. However, the Lab used the period of reduced transit demand to usher in several improvements to our shuttle service. Most significantly, the Lab is introducing an entirely new fleet of vehicles with improved technology designed to improve rider safety and service reliability. Concurrently, we have replaced all of our shuttle signage and installed monitors that display real-time Lab shuttle and local transit agency departure times on and off the Lab's campus. The goal is to drive future ridership through more reliable service supported by more robust information.

Site Sustainability Plan Summary

Berkeley Lab pursues three broad initiatives to reach sustainability goals driven by requirements of the federal government, California state law, and University of California policy. The initiatives, listed below, are described in greater detail at sbl.lbl.gov.

- Climate: Improving buildings, greening the energy grid, and low-carbon commutes
- Waste: Rethinking waste through composting, recycling, and smart purchasing
- Water: Upgrading fixtures, stopping leaks, and encouraging conservation

As of the end of FY20, the Lab has 23% of buildings by count that meet Guiding Principles, exceeding the goal of 15% by FY25. This value is up from 20% reported in FY19. The Lab's work in saving energy and water through commissioning and retrofits is funded internally using overhead funds. Berkeley Lab will continue to assess the feasibility of using energy savings performance contracts (ESPCs) or utility energy service performance contracts (UESCs) for particular projects. The Lab's next step for increasing onsite renewable energy is to add a 200kW solar photovoltaic array to the "solar-readyIGB (B91), which was completed in late 2019. In the last year, in response to new requirements identified through resilience planning, an expanded concept has been defined for the facility that integrates solar generation, battery storage, and flexible configurations of the existing standby generator.

Recent highlights include:

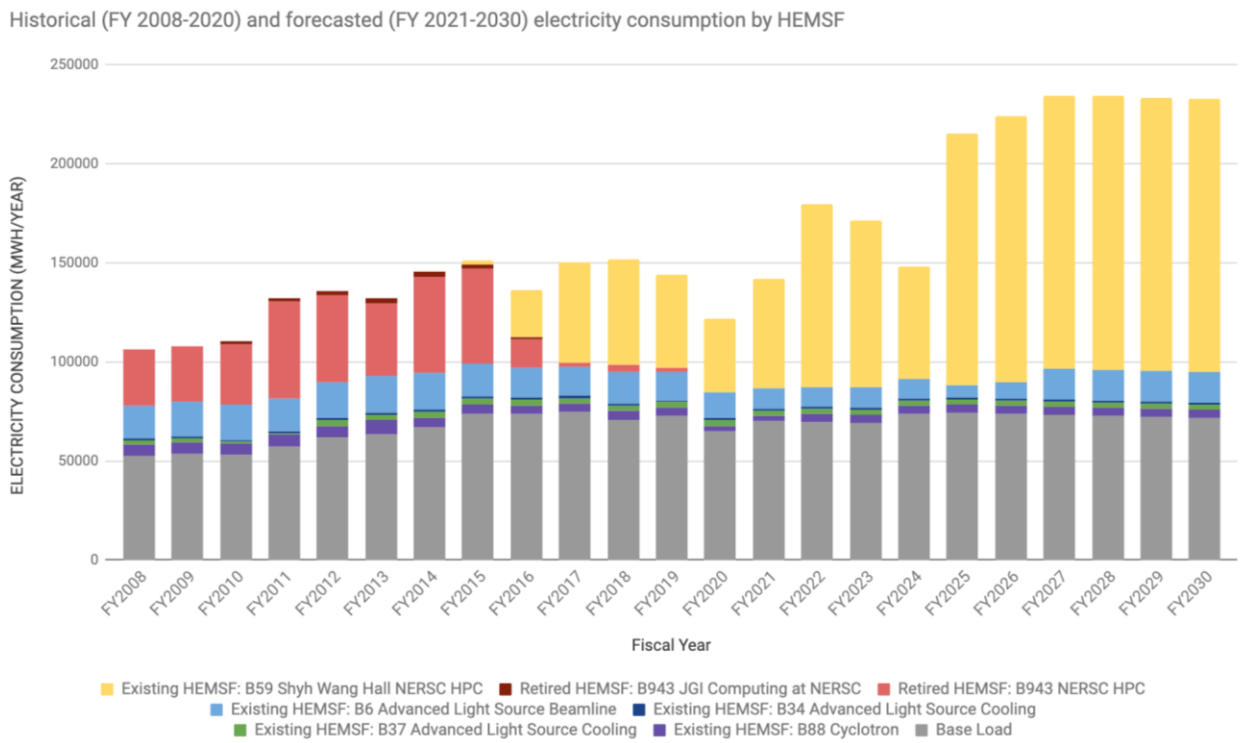
- **Maintained Energy Savings**: As of spring 2020, Berkeley Lab is maintaining annual energy savings of 12.3 million kWh and water savings of over 19 million gallons. The savings generate an annual reduction of over $900K in utility costs and are equivalent to the generation from a 7.9 MW photovoltaic array, which would occupy 24 football fields or 31 acres. These savings are being achieved primarily through improvements in facility operations, delivered by the Ongoing Commissioning Team and a focused team at NERSC. Maintained efficiency savings are updated monthly at sbl.lbl.gov/data.
- **Energy Use Intensity Reductions**: Labwide energy use intensity has decreased 25% since FY15. While energy efficiency in FY20 is lower due to the COVID shelter-in-place, the Lab was seeing a significant reduction in energy use intensity prior to COVID-related changes in operations: Lab-wide weather-corrected energy use intensity excluding major process loads as of April 1, 2020 was 19% lower than in FY15.
- **Ongoing Commissioning Team**: The Lab's Ongoing Commissioning Team, a dedicated cross-functional group from the Facilities Management division and Sustainable Berkeley Lab, has firmly established, over a period of more than three years, a process to continuously identify, prioritize, and resolve operational problems in buildings in order to improve operations and generate considerable energy and water savings. The Ongoing Commissioning approach was recognized by a 2019 DOE "Accelerating Smart Labs" Project Award given on behalf of the Better Buildings Smart Lab Accelerator. The approach is further described in a paper, "Generating Significant and Persistent Energy Savings in Building Operations Using an Ongoing Commissioning Approach," available at ocx.lbl.gov.
- **ISO 50001 Implementation**: The Lab received ISO Ready Recognition from the DOE in June 2020 and third-party certification of its energy and water management system against the ISO 50001 standard in September 2020. Aligning activities with ISO 50001 is a key approach to ensure that the Lab's energy and water management is strategic, effective, and persistent. Information

about the Lab's use of the standard and its Energy and Water Management System Manual is available at iso50001.lbl.gov.

- **New Construction**: With focused attention through the "transition to operations" period, the IGB is meeting its design intent to use only 36% of the energy used by the previous facility. The building has also validated key sustainability strategies, such as the electrification of space and water heating, that is being used in more recent designs for BioEPIC and SSM. See more details about the IGB design at sbl.lbl.gov/progress.

Historical and anticipated electricity cost and consumption data are presented below.

Figure 1. Electricity Usage & Cost Projections



OAK RIDGE NATIONAL LABORATORY

Lab-at-a-Glance

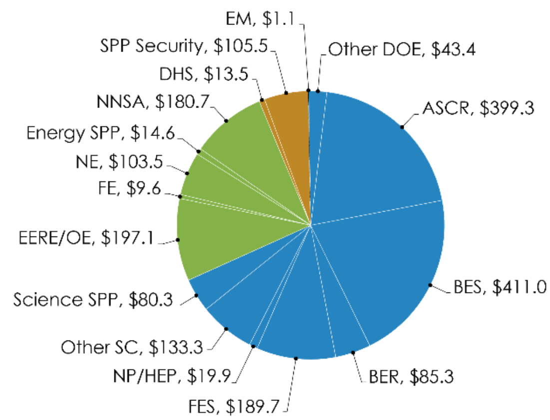
Location: Oak Ridge, TN
Type: Multi-program Laboratory
Contractor: UT-Battelle, LLC
Site Office: ORNL Site Office
Website: www.ornl.gov

- **FY 2020 Lab Operating Costs:** $1,987.7 million
- **FY 2020 DOE/NNSA Costs:** $1,773.8 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $200.4 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 10.1%
- **FY 2020 DHS Costs:** $13.5 million

Physical Assets:
- 4,421 acres and 264 buildings
- 4.5 million GSF in buildings
- Replacement Plant Value: $7.1 B
- 1.4M GSF in 62 Excess Facilities
- 0.87M GSF in Leased Facilities

Human Capital:
- 5,393 Full Time Equivalent Employees (FTEs)
- 100 Joint Faculty
- 397 Postdoctoral Researchers
- 117 Graduate Students
- 176 Undergraduate Students
- 2,844 Facility Users
- 1,096 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

The mission of Oak Ridge National Laboratory (ORNL) is to deliver scientific and technical breakthroughs needed to realize solutions in energy and national security and provide economic benefit to the nation.

Established in East Tennessee in 1943 as part of the Manhattan Project, ORNL demonstrated the production and separation of plutonium as its original mission. After World War II, ORNL led early work on nuclear energy, radioisotopes for medicine and other applications, radiation-resistant materials, and the effects of radiation on biological and environmental systems. Today, ORNL focuses an extensive set of core capabilities on the mission needs of the US Department of Energy (DOE) and other sponsors, with more than 2,600 technical staff members engaged in the execution of a diverse research and development (R&D) portfolio.

ORNL is distinguished by its close coupling of basic and applied R&D and by signature strengths in materials, neutrons, nuclear, isotopes, and computing. Oak Ridge also has a rich history in biological sciences and is addressing compelling challenges in energy and national security through the convergence of physical sciences, biological and environmental sciences, advanced manufacturing technology, and engineering.

ORNL operates the Spallation Neutron Source, the High Flux Isotope Reactor, the Center for Nanophase Materials Sciences, the Oak Ridge Leadership Computing Facility, and several other major DOE facilities for the research community to enable scientific discovery and innovation, and it applies exceptional resources in project management to manage the Second Target Station, Exascale Computing, and US ITER projects for DOE.

Building on a tradition of focusing world-leading resources on difficult problems of national scope and impact, ORNL is exploring new ways to bring its core capabilities to bear on the challenges of advancing our understanding of the natural world, enhancing our energy and national security, protecting human health and the environment, and delivering innovations that lead to new products, business, and jobs.

Core Capabilities

The 23 core capabilities assigned to Oak Ridge National Laboratory (ORNL) by the US Department of Energy (DOE) provide a broad science and technology base that catalyzes fundamental scientific advances and technology breakthroughs to support DOE's mission of addressing the nation's energy, environmental, and nuclear challenges. These capabilities, each of which has world-class or world-leading components, reflect a combination of exceptional people, equipment, and facilities. Synergies among these core capabilities accelerate the delivery of scientific discovery and technology solutions and allow ORNL to respond to changing priorities and the critical needs of the nation.

We are taking steps to recruit the highest-quality and most diverse pool of talent by establishing long-term relationships with key universities. We are emphasizing staff development, helping our people to build distinguished careers in research and development (R&D), and challenging them—individually and collectively—to reach their full potential. We also maintain and expand ORNL's research capabilities through strategic investment in facilities and equipment. With the resulting combination of highly performing and world-recognized staff and state-of-the-art facilities and equipment, ORNL seeks to be the world's premier research organization.

Accelerator Science and Technology

ORNL has world-leading expertise in the basic physics of high-intensity hadron beams and the technology to support the production, acceleration, accumulation, and utilization of such beams. The Spallation Neutron Source (SNS) accelerator complex, operating at 1.4 megawatts (MW) power on target, is the world's most powerful pulsed proton accelerator and the world's highest-power superconducting linear accelerator for hadrons. The SNS enables ORNL to lead the investigation of the dynamics of high-intensity hadron beams and the development of high-power proton targets. The Proton Power Upgrade (PPU) project will provide up to 40% more power to the First Target Station and enable novel neutron scattering experiments with thermal neutrons at high-energy resolution and is on track for completion in FY 2025.

Other ORNL leadership areas include expertise in negative hydrogen ion (H^-) sources and low-energy beam chopping and manipulation; superconducting radio-frequency (SRF) technology; high-power target systems; high-power and low-level RF systems; pulsed-power technology; sophisticated control systems for the manipulation of high-power beams; beam-tuning algorithms; high-level, real-time accelerator modeling and analysis; and instrumentation to measure properties of high-intensity, high-power hadron beams.

In addition, ORNL's strengths in computational science are used to develop beam dynamics modeling (including 6D models) and data management tools to design next-generation spallation neutron sources, high-intensity linear accelerators (linacs), storage rings, and associated radiation shielding. Expertise has been developed in artificial intelligence (AI) and machine learning (ML) with the goal of using large sets of accelerator data to predict and mitigate accelerator and target systems failures. The combination of state-of-the-art beam dynamics modeling tools and access to robust experimental data on collective, halo-formation, and instability effects in high-intensity hadron linacs and accumulator rings is unique to ORNL. These strengths underpin efforts to systematically increase the power level at which SNS operates reliably.

The comprehensive SRF and Cryogenic Test Facility supports a robust research program that has led to the development and successful deployment of a novel in situ plasma-cleaning technology that has increased the peak gradients of selected superconducting high-beta accelerator cavities by up to 25%. This project has been extended into the medium-beta cavities through a recipe modification for this configuration, and it has been successfully deployed to medium-beta cavities. Additionally, ORNL is transferring this technology to other important accelerator projects in the DOE portfolio. ORNL is also developing capabilities for laser-assisted charge exchange of energetic H^- ions to facilitate high-power beam injection into advanced rings, pursuing novel approaches to power conversion technology for klystron modulators, and developing advanced beam instrumentation systems. Continued advances in high-level real-time applications, in combination with improvements in warm accelerator structure vacuum systems, have led to a significant reduction in the time required to complete facility turn-on after planned outages.

The Beam Test Facility (BTF) is a functional duplicate of the first five meters of the SNS accelerator, the portion of the accelerator structure with the most complex beam dynamics and the most challenging reliability issues. The BTF supports continuous development and testing of critical hardware toward higher reliability, in particular new radio-frequency quadrupoles, novel beam measurement instrumentation, and ion sources. It also serves as a high-availability, easy-access research station for understanding the beam dynamics in the low energy portion of the accelerator, aimed toward improving control of the beam in the production accelerator. The research program at the BTF is an essential resource to enhance accelerator science opportunities that attract, engage, and retain staff with the expertise to drive innovation in several areas of accelerator science and technology relevant to the ORNL mission.

The impact of ORNL's research in high-intensity beam dynamics and technology spans all fields of science enabled by high-power hadron accelerators. ORNL staff members collaborate with similar international accelerator facilities as reviewers and advisors.

DOE's Office of Science (SC) is the primary source of funding.

Advanced Computer Science, Visualization, and Data

ORNL staff are deeply engaged in R&D to enable the deployment of scalable computing infrastructure to support the DOE mission, with an emphasis on the programs, facilities, and operations at ORNL. The laboratory participates in numerous Scientific Discovery through Advanced Computing (SciDAC) application teams and leads several components of RAPIDS (a SciDAC Institute for Resource and Application Productivity through Computation, Information, and Data Science). ORNL staff are prominent in the Software Technology focus area of the Exascale Computing Project (ECP), expanding ORNL capabilities in HPC including leading projects to develop an open-source algorithm and software stack that will automate the process of designing, executing, and analyzing the results of quantum algorithms, thus enabling new discovery across scientific domains.

Three interconnected areas of emphasis distinguish the ORNL computer science research program: exploring and evaluating emerging accelerated computing technologies; developing the tools and methods needed for the analysis and management of data from the computational, experimental, and observational facilities across DOE; and developing the tools and methods needed to federate facilities in support of the DOE mission. Accelerated computing technologies will be deployed throughout the resources used to federate facilities, from the edge to our large HPC systems. Exascale applications are becoming more complex in their data flows, from multiscale and multiphysics simulations that need to exchange data between separate codes to simulations that invoke data analysis and visualization services to extract information and render it to storing simulation output to the file system for later analysis. The ORNL-developed Adaptable Input/Output System (ADIOS) provides a simple way to tackle data management challenges posed by large-scale science applications running on high-performance computers. Much of the opportunity for acceleration will be related to in situ data management and analysis. Finally, support for data management and analysis spanning multiple facilities is a key foundation for federating facilities.

In addition to these research foci, the ORNL computer science program stewards two service-oriented capabilities: the engineering of research software and the engineering, curation, and visual analysis of data sets. These software and data engineering capabilities focus on ensuring quality in the software and data-related artifacts being developed across the laboratory. The overarching purpose of the computer science program is to ensure that the programs, facilities, and operations at ORNL and throughout DOE utilize the best technologies available. While the computer science program is focused on long-term impact, the service-oriented capabilities provide a critical linkage between the research program and the programs that rely on the results of the research program.

ORNL is committed to developing the tools and technologies needed to advance accelerated node computing, from extreme-scale systems deployed by the Oak Ridge Leadership Computing Facility (OLCF) to those deployed by the Experimental Computing Laboratory (ExCL). The HPC resources of the OLCF, including the 200-petaflop IBM AC922 Summit and highly anticipated Frontier (OLCF-5), which promises a peak performance over 1,500 petaflops, will be available to users to advance knowledge in areas such as designing fusion reactors, designing new materials, engineering proteins to treat diseases, efficiently releasing energy from biomass, and understanding the impact of climate change. Frontier will achieve around 50- to 100-times performance improvement in real science applications or alternatively around 5- to 10-times application performance improvement over Summit. Systems available through ExCL explore a wide range of accelerated processing technologies, from quantum and neuromorphic processors to near-memory computing systems such as an Emu Chick and systems with field-programmable gate arrays. ORNL is building capabilities in predictive performance and future-generation high-end computing architectures. Additionally, ORNL is leading one of the SC Advanced Scientific Computing Research (ASCR) program Quantum Testbed Pathfinder teams.

ORNL is equally committed to developing tools and approaches that support the evolution of applications needed to effectively utilize the computing capability enabled by computational accelerators. ORNL staff are deeply engaged in the standards activities related to directive-based programming systems, including OpenMP and OpenACC, to ensure that these standards address the needs of DOE applications. QCOR, a novel open-source software stack specific for quantum computing, enables single-source quantum computing. The high level of abstraction in the developed language is intended to accelerate the adoption of quantum computing by researchers familiar with classical HPC. ORNL staff are also developing tools aimed at supporting the transformation of scientific software. For these and other applications, ORNL researchers bring significant expertise in system software, component technologies, run-time optimization, architecture-aware algorithms, and resilient computations.

In recent years, the DOE community has begun to recognize the need for advanced computer science, visualization, and data capabilities to provide a deeper understanding of data generated at DOE user facilities, such as light sources, neutron sources, and nanoscience centers. For example, bringing OLCF resources to bear at SNS can provide a deeper understanding of materials samples. To this end, ORNL has established research programs in workflow systems (including ADIOS, BEAM, and ICE), system science (including networking), and data and information visualization (including EVAL, Eden, and Origami). The Compute and Data Environment for Science (CADES) provides focus for deploying these research capabilities. Launched internally to provide a fully integrated infrastructure offering compute and data services for researchers, CADES is now being applied to the needs of users at SNS, the High Flux Isotope Reactor (HFIR), and the Center for Nanophase Materials Sciences (CNMS). With this platform, researchers can process, manage, and analyze large amounts of data using scalable storage, data analysis, and visualization tools.

ORNL also enables scientific discovery and accelerates the deployment of technologies in energy and national security by developing, managing, and accessing scientific data repositories (e.g., the Atmospheric Radiation Measurement [ARM] Data Archive, the Distributed Active Archive Center, the Earth System Grid Federation, the National Extreme Events Data and Research Center, and A Large Ion Collider Experiment [ALICE] USA Tier 2 center). Through software and architectural advances such as quantum and neuromorphic computing for next-generation architectures, ORNL accelerates the deployment and utilization of petascale- and exascale-capable systems that will contribute to solving critical national challenges in science, energy assurance, national security, advanced manufacturing, and health care. ORNL also applies its capabilities in advanced computer science, visualization, and data in the area of geographic information system R&D. ORNL recently hired Yan Liu to provide novel expertise in high-performance geocomputation and Kelly Sims to provide expertise in open-source geographic data analysis for population modeling.

ORNL is committed to growing the nation’s capabilities in data analytics and visualization through a data science and engineering PhD program offered by the UT–ORNL Bredesen Center for Interdisciplinary Research and Graduate Education. This capability is supported by SC, the Office of Electricity (OE), the US Department of Homeland Security (DHS), and Strategic Partnership Projects (SPP) sponsors, including the US Department of Defense (DoD) and the US Department of Health and Human Services (HHS).

Applied Materials Science and Engineering

ORNL possesses exceptional expertise in the synthesis, characterization, modeling, and testing of materials for a wide variety of applications with a focus on materials under extreme environments. Expertise from leading fundamental condensed matter science and materials science and engineering programs supported by BES enables the development of new functional materials for energy and national security applications. Approaches that combine characterization and computational tools with experimental synthesis provide an opportunity to deliver highly innovative materials science solutions that can readily be translated to high-impact applications.

ORNL is also home to the Fusion Energy Sciences (FES) materials program, with an emphasis on developing and understanding structural materials relevant for fusion environments. Foundational research in plasma–material interaction is key to preparation for fusion component studies with the Material Plasma EXposure Experiment (MPEX), which is now beginning procurement and preparation for construction.

A distinguishing characteristic of materials science research at ORNL is the close coupling of basic and applied research to develop next-generation structural materials for applications in fission and fusion energy, transportation, buildings, high-efficiency steam generation, the hydrogen economy, supercritical carbon dioxide power cycles, and concentrated solar power. Research associated with this core capability is the source of the majority of ORNL's patents. For example, ORNL researchers have recently demonstrated a data analytics workflow that incorporates underlying physics in training ML models that can predict properties of high-temperature alloys. By interrogating high-fidelity models in a high-throughput manner, the team augmented the raw data set consists of simple alloy compositions with scientific features, which can serve as physical constraints in making predictions. ORNL recently published multiple papers on this topic and has leveraged ongoing DOE-funded research from the Fossil Energy (FE)[3] and Vehicle Technologies Offices.[4] These results offer insight into the future design of high-performance alloys for elevated extreme environment applications.

Specialized capabilities in applied materials science and engineering include materials joining, surface engineering and processing, corrosion studies under harsh but well-controlled conditions, mechanical testing in a variety of environments, and physical property determination. Specific materials expertise exists in the development and advanced manufacturing of alloys, ceramics, nanomaterials, carbon fiber and composites, nanostructured carbons, polymers, thermoelectrics and energy storage systems. For example, an ORNL team developed a low-cost scalable room-temperature sodium-ion based redox flow battery and enabling membranes for megawatt-scale grid scale storage.[5,6]

ORNL's applied materials science and engineering program takes advantage of state-of-the-art capabilities for materials development and testing, such as the SC user facilities CNMS, SNS, and HFIR; The Carbon Fiber Technology Facility (CFTF) and the Manufacturing Demonstration Facility (MDF) supported by the Office of Energy Efficiency and Renewable Energy (EERE); and other facilities in the Isotope and Nuclear Materials Complex (INMC), such as the Low Activation Materials Development and Analysis (LAMDA) laboratory and the Irradiated Materials Examination and Testing hot cell facility. ORNL recently uncovered foundational interactions of materials with helium plasmas relevant to fusion power. This work elucidated the complex near-surface microstructural evolutions in tungsten bombarded by low-energy helium, including the crystallographic orientation realignment. Effects of crystallographic orientation on plasma interactions of materials were known; but in this work, the effects of plasma on surface orientation were explored and found to have significant implications for plasma–materials interactions. This finding is key to implementing structures that will be in fusion reactors.[7]

ORNL is developing new materials for optimized performance, especially in extreme environments. For example, ORNL collaborated with Global Nuclear Fuel and Southern Company on the development of an advanced nuclear fuel cladding based on iron-chromium-aluminum alloys that provides superior strength with high resistance to hydriding during loss-of-coolant-accident scenarios compared with current Zircaloy-based clad materials. Overall, the core capability of the applied materials science and engineering program supports the development of materials that improve efficiency, economy, and

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[3] J. Peng, et al., npj Comput Mater 6, 141 (2020).

[4] J. Peng, et al., JOM 73, 164–173 (2021).

[5] E. C. Self, et al., *ACS Energy Lett.* **4**, 2593 (2019).

[6] M. L. Lehmann, et al. *Energy Storage Materials* **21** 85–96 (2019).

[7] C. Fan et al., *Acta Mater.* 116420 (2021).

safety in energy generation, conversion, transmission, and end-use technologies. Funding comes from EERE, OE, FE, SC, the Office of Nuclear Energy (NE), the National Nuclear Security Administration (NNSA), DHS, the Advanced Research Projects Agency–Energy (ARPA-E), DoD, and other SPP customers.

Applied Mathematics

ORNL's applied mathematics program spans four highly visible and externally recognized areas of research: (1) multiscale modeling and simulation; (2) mathematical tools for the analysis of scientific data, including AI and ML; (3) discrete mathematics, including graph theoretic methods and matrix factorizations; and (4) systems analysis and decision making, including statistics and the analysis of complex networks.

Strategic foci include (1) scalable, architecture-aware, and resilient mathematical and computational capabilities for modeling and simulation; (2) robust algorithms for ML and data analysis, including uncertainty quantification (UQ), accelerated learning, and physics-informed learning; (3) the analysis of complex, multiphysics and multiscale systems and algorithms; and (4) demonstrated impact on applications in science and engineering. Algorithms developed within the applied mathematics program are a critical component of ORNL's modeling and simulation capabilities and are widely recognized and used beyond ORNL. Examples of these capabilities include the following:

- New ML and data analytics algorithms implemented on Summit for performance (e.g., time-to-solution, reward-to-cost [flops] ratio) compared with a variety of baseline methods
- Large-scale matrix factorizations, including nonnegative matrix factorizations, that can be used in applications such as the analysis of semantic graphs
- Mathematical foundations needed to support federated facilities at ORNL, providing feature detection, image processing and reconstruction, and model calibration for large-scale experimental science using leadership computing
- New multiscale simulation tools, including novel time integrators and structure-preserving discretization schemes
- Large-scale, architecture-aware discrete event simulations with applications, e.g., in cyber-physical security and in transportation networks
- Advanced numerical methods and analysis of kinetic equations, which are used to simulate processes fundamental to energy generation, storage, and transmission, such as radiation (neutron, photon, and ion) transport, semiconductors, and fusion plasmas
- Advanced numerical methods and analysis of nonlocal models for computational mechanics and transport processes
- New optimization algorithms, including constraints reduction methods and measure-based approaches, with applications, e.g., in accelerated ML and in materials design
- The unified and massively scalable computational Toolkit for Adaptive Stochastic Modeling and Non-Intrusive Approximation (TASMANIAN), which represents an architecture-aware, predictive capability for large-scale engineering and multiphysics applications, particularly in exascale computing
- Development and maintenance of the high-level software environment Multiresolution Adaptive Numerical Environment for Scientific Simulation (MADNESS), which is designed for the solutions of integral and differential equations in many dimensions, using adaptive and fast harmonic analysis methods with guaranteed precision based on multiresolution analysis and separated representations
- Use of the discontinuous Galerkin implicit-explicit (DG-IMEX) framework to improve physical fidelity by including more neutrino–matter interactions and relativistic effects, and incorporating the solvers into the major application codes of the ECP ExaStar project

- Development and maintenance of high-quality mathematical software, including EISPACK, LINPACK, BLAS, LAPACK, ScaLAPACK, Netlib, PVM, MPI, NetSolve, ATLAS, and PAPI.

Applied mathematicians and theoretical computer scientists provided the core of the laboratory's AI initiative and have developed key results for efficient and robust learning algorithms focused on dimension reduction and stochastic optimal control using reversible networks, upper quartile, and image classification with a strong focus on scalable implementation targeting Summit. These algorithmic improvements have enhanced several applications, including medical imaging, neutron science, and materials design. In addition, the applied mathematics program develops supervised and unsupervised learning algorithms at additional experimental facilities, including CNMS, MDF, and the National Transportation Research Center (NTRC). This effort builds on strengths in upper quartile; optimal reconstruction from both sparse and extensive noisy data; optimization, control, and design of high-dimensional physical and engineered systems; and linear and nonlinear solvers. Funding comes primarily from SC, DoD, NSF, HHS, and other SPP sponsors.

Biological and Bioprocess Engineering

ORNL brings substantial strength in fundamental biology to bioprocessing and bioengineering to address DOE mission needs in bioenergy production, carbon capture and long-term storage, and environmental contaminants processing. ORNL is (1) leading the Center for Bioenergy Innovation (CBI), a nexus for research on biomass utilization for biofuels and bioproducts (e.g., higher alcohols, esters, jet/marine fuel, and lignin coproducts); (2) characterizing the largest population of *Populus* genotypes for biomass deconstruction gene discovery and expanding that analysis to switchgrass; (3) developing new microbial platforms for the conversion of biomass to products; (4) coupling fundamental and applied research in biomass production and conversion (both thermochemical and biochemical conversion) for high-value materials and chemicals, fuels, and power; and (5) making sustained contributions to assess biomass feedstock supplies at regional and national scales.

ORNL leverages its next-generation capabilities in chemical engineering, chemistry, materials science, AI, HPC, and systems engineering to accelerate the translation of research outcomes into demonstrable improvements in bioproducts and biofuels and to move research from the laboratory to the field or pilot level. ORNL uses integrated expertise in plant sciences, microbiology, molecular biology, molecular modeling, and bioinformatics—in combination with facilities such as the common gardens, high-throughput phenotyping equipment, neutron sources (SNS and HFIR), and computing resources (CADES and the OLCF)—to address the needs of the bioeconomy. ORNL continues to innovate in analytical technologies, from chemical imaging to multimodal small-angle neutron scattering.

ORNL is a recognized leader in multiple aspects and scales of bioenergy production, including biofeedstock sources and sustainability analyses, with emphasis on an integrated systems approach (e.g., landscape design) at multiple landscape scales (from hectare to nation) for applied impacts. This leadership has been leveraged to assess the potential for carbon management through bioenergy for carbon capture and long-term capture in soils. ORNL also leads in the use of a suite of biomass conversion processes: novel microbes and applied systems biology, computational chemistry and biophysics modeling for biomass conversion, and biofuels and bioproduct upgrading to advance bioenergy production.

SC and EERE are the primary sponsors of this work. ORNL also performs impact analyses for the US Environmental Protection Agency (EPA) and bioremediation design projects for DoD. Other current sponsors include the HHS National Institutes of Health (NIH), the US Department of Agriculture (USDA), and ARPA-E.

Biological Systems Science

ORNL's core capability in biological systems science directly improves understanding of complex biological systems through (1) integration of plant sciences with synthetic biology, ecology, computational biology, and microbiology; (2) discovery of gene function; (3) foundational research in plant science that enables development of sustainable plant feedstocks for bioenergy and bio-derived materials; (4) the use of neutron science and exascale computing to characterize protein structure and interaction; (5) development of imaging and chemical measurement analytics at multiple spatial and temporal scales; and (6) development and application of data analytics, AI, and simulation for biology. The fundamental understanding delivered through application of this core capability is essential to solving challenging societal problems in bioenergy, nutrient cycling, climate change, carbon management, and environmental remediation.

ORNL has strategic strengths in plant biology that have largely focused on more than 1,000 genome-sequenced *Populus* lines and is the host institution for CBI, which is in its third year. ORNL has added a state-of-the-art Advanced Plant Phenotyping Laboratory (APPL), a multispectral imaging system that enables a new level of high-throughput phenotyping of plant systems. A robotic sampling system for APPL is under development. CBI continues to lead improvements in the economics and sustainable production of biomass and its conversion to bioproducts and biomaterials. ORNL leads the shift toward a more diverse set of sustainable bioderived materials and fuels obtained through lignin valorization and biomass processing. ORNL's strengths in plant biology and microbiology support additional fundamental research in Science Focus Areas (SFAs), such as Plant-Microbe Interfaces (PMI), Secure Ecosystem Engineering and Design (Secure EED), and Biofuels. ORNL is also part of collaborative projects with other national laboratories (e.g., Ecosystems and Networks Integrated with Genes and Molecular Assemblies, National Microbiome Data Collaborative, and KBase).

ORNL has launched an effort to connect gene function with higher-order biological and ecosystem effects, and to create gold standard data sets compatible with BER resources such as the National Microbiome Data Collaborative. Integrated capabilities in biochemical sciences, neutrons, and computing benefit the Biofuels SFA and the Critical Interfaces SFA. ORNL research within the PMI SFA characterizes the soil and plant microbiome and elucidates fundamental aspects of plant–microbe signaling and symbiosis leading to chemical cycling in the terrestrial biosphere. These data-rich experimental efforts interface with bioinformatics expertise in microbial annotation and computational investigation, including AI approaches for modeling and design using complex systems biology and protein structure data.

ORNL's neutron scattering resources can be leveraged through the Center for Structural Molecular Biology, including the Biological Small-Angle Neutron Scattering (Bio-SANS) instrument at HFIR. A new BER-funded effort is prototyping a multimodal SANS instrument for the SNS Second Target Station (STS). In addition, ORNL has capabilities in both solid and solution nuclear magnetic resonance spectroscopy, optical spectroscopy, and multiple modalities of imaging.

SC and EERE are the primary sponsors of the work within this capability. Additional work is sponsored by DHS, NIH, ARPA-E, DoD, and EPA.

Chemical and Molecular Science

ORNL's core capability in chemical and molecular science is focused on understanding how local environments and functional architectures control selective chemical transformations and physical processes over multiple length and time scales in natural and synthetic systems. Research is focused in four synergistic research themes: (1) chemistry at complex interfaces, (2) reaction pathways in diverse environments, (3) chemistry in aqueous environments, and (4) charge transport and reactivity over a broad range of length and time scales. This portfolio includes research programs in catalysis, separations, geochemistry, and interfacial science and provides fundamental knowledge for the development of new chemical processes and materials for energy generation, storage, and use; for mitigation of environmental impacts of energy use; and for national security. The ORNL-led Fluid Interface Reactions, Structures and Transport (FIRST) Energy Frontier Research Center (EFRC) focuses on developing a fundamental understanding and validated predictive models of the atomic origins of electrolyte and coupled electron transport under nanoscale confinement. FIRST integrates an experimental and modeling approach, consisting of x-ray diffraction, neutron pair distribution function, scanning transmission electron microscopy (STEM), Raman spectroscopy, electrochemistry, and density functional theory modeling to gain new insights into the synthesis of metastable transition metal oxides that can be used as electrode materials for proton-based energy storage or electrochromic applications.[8]

Designing new materials for efficient chemical separations is a strength of the ORNL Chemical and Molecular Science program. For example, in a new project on separations of rare earth elements (i.e., critical materials), ligands are being designed with preorganized structures that have a high binding affinity for lanthanides. A novel release mechanism using redox processes is proposed. ORNL has recently discovered that direct air capture (DAC) of CO_2 can be dialed in by subtle structural modifications of bis-iminoguanidine crystals, resulting in major improvements in their aqueous solubilities, regeneration energies, and DAC performance.[9] High CO_2 permeance and selectivity was obtained by coating an ultrathin layer of ionic liquids on porous graphene in which the CO_2-philic anions were found to gate the molecular transport of CO_2 and N_2 molecules.[10] To guide experimental studies on optimizing gas separations with porous carbons, ML methods were used to accurately predict gas separation performances (CO_2/N_2) for porous carbons.[11]

The neutron scattering expertise in ORNL's Chemical and Molecular Science program is also enhancing our fundamental understanding of catalytic reaction mechanisms involving hydrogen. For example, in situ inelastic neutron scattering (INS) and infrared spectroscopy were used to provide the first direct evidence for the catalytic roles of cerium hydride (Ce-H) and hydroxyl group (OH) groups in acetylene hydrogenation over ceria, which provides insights into the design of active, selective, and stable ceria-based catalysts.[12] In the reduction of nitrogen under mild conditions over an electride-based catalyst, the exact nature of the reactive hydrogen species and the role of electride support remains elusive. In situ neutron diffraction, INS, density functional theory calculations, and temperature-programmed

[8] R. Wang et al., *Adv. Energy Mater.* **11**, 2003335 (2021).

[9] R. Custelcean et al., *ChemSusChem* **13**, 6381 (2020).

[10] W. Guo et al., *Nano Lett.* **20**, 7995 (2020).

[11] S. Wang et al., *Angew. Chem. Int. Ed.* **59**, 19645 (2020).

[12] J. Moon et al., A*CS Catal.* 10, 5278 (2020).

reactions were used to show for the first time the presence of encaged hydrides during ammonia synthesis on the ruthenium electride catalyst.[13]

The chemical and molecular science core capability also comprises novel characterization tools, including a comprehensive suite of surface-specific laser spectroscopy techniques developed to study reactive and dynamic interfaces over a range of time and length scales. These methods pair neutron scattering with theory and bridge the gaps in the temporal and spatial scales that can be studied, addressing problems in chemical separations, polymer science, energy storage, and biological function that are not accessible using traditional approaches. For example, the elusive chemistry at the liquid–liquid interface underlying solvent extraction has been mapped in real time using nonlinear laser spectroscopy (i.e., vibrational sum frequency generation).[14] Mass spectrometry is also being used in nuclear and radio chemistry in the quantitative characterization of stable and radioactive isotopes and for nuclear forensics, and it is the basis of the electromagnetic isotope separation capabilities established for the DOE Isotope Program.

Funding comes primarily from BES. Applied programs sponsored by DOE's Office of Environmental Management (EM), NE, NNSA, FE, and EERE benefit from this research. Research in chemical and molecular sciences also has applications to BER and Office of Nuclear Physics (NP) programs.

Chemical Engineering

ORNL's capabilities in chemical engineering leverage other core capabilities in chemical and molecular sciences, nuclear chemistry and radiochemistry, condensed matter physics and materials sciences, applied materials sciences and engineering, biological and bioprocessing science, and computational science. ORNL has leadership in chemical separations, catalysis, isotope production, high-efficiency clean combustion, and biofuel production.

Technology development through chemical engineering builds on and impacts research sponsored by (1) BES in fundamental research in materials design, synthesis, and characterization; (2) BES in chemical separations, catalysis, and computational modeling; (3) BER in bio-based fuels and chemical production; (4) the SC Office of Isotope R&D and Production–sponsored research in production of radioisotopes and stable isotopes; (5) EERE Vehicle Technologies Office and Bioenergy Technologies Office in applied chemical separations, fuels, pyrolysis, and catalysis development; and (6) FE in CO_2 separation and conversion. Stable isotope research and production depend on the utilization of specialized or potentially novel feedstock chemicals not available commercially, including the reformulation of enriched stockpiles for use in processes to further increase enrichment of the desired isotope. We are pursuing the development of synthetic processes, enrichment processes, and physical property measurement. ORNL radiochemists and radiochemical engineers developed new flow sheets for recovering plutonium-238 for the National Aeronautics and Space Administration (NASA) from irradiated targets, using a novel monoamide solvent, and completed the fifth chemical processing campaign for NASA.

ORNL advances new chemical processes and develops new materials to improve efficiency, economy, and industrial competitiveness. New environmentally friendly and economical separations methods have been developed for recovering rare earth elements such as neodymium, dysprosium, and praseodymium from scrap magnets as part of the Critical Materials Institute. Separations methods have been developed for intra-lanthanide separations protocols using preorganized phenanthroline-base

[13] J. Kammert et al., *J. Am. Chem. Soc.* **142**, 7655 (2020).

[14] A. U. Chowdhury et al., *ACS Appl. Mater. Interface* **12,** 32119 (2020).

ligands.[15] Based on our past success in incorporating lignin into a carbon fiber precursor polymer, we recently developed a new composition of a high-performance renewable polymer that (1) contains ~70% lignin from a biorefinery source, (2) demonstrates viscosity at shear rates for acceptable processability, and (3) possesses tensile strength ensured by a <100 nm dispersed lignin phase, dramatically improving on the amount of lignin incorporated while maintaining suitable physical properties. To reduce the production cost of high-strength carbon fibers, a melt-spinning process was demonstrated using an ionic liquid plasticized PAN-based carbon precursor fiber.[16]

A scalable new method was developed to produce a material that can be used as a muscular tissue-like actuator in soft robotics.[17] Under an applied electric field (through the film thickness), the material quickly and reversibly contracts at a force comparable to that of muscular tissue. The scalable synthesis and casting method involved copolymerization of an ultraviolet-sensitive monomer and rapid crosslinking of the film while stretching. The method also incorporates single-walled carbon nanotubes into a longtime candidate for morphable mechanical devices based on liquid crystal elastomers. As the national steward of uranium science and processing technology, ORNL applies expertise in chemical engineering to advance the understanding of fuel cycle operations associated with processing, purifying, and enriching uranium. Related ORNL separations expertise, in both electromagnetic and gas centrifuge techniques, is also enabling advances in stable isotope enrichment that are being applied in the design and construction of the Stable Isotope Production Facility (SIPF) and the Stable Isotope Production and Research Center (SIPRC). Innovative chemical processes being developed for the recovery and recycling of nonnuclear materials from used nuclear fuel (UNF) assemblies have great potential for simplifying secure UNF disposition pathways and for reducing the mass and volume of the waste stream. Conceptual designs of processes for converting UNF into fuel for alternative reactor concepts are being developed. Established uranium chemical processes, operated at a range of scales, support ORNL's nonproliferation mission while providing learning opportunities for the next generation of radiochemical engineers and scientists. High-speed analytical capabilities usable in two-phase systems have been developed to elucidate separations and reaction mechanisms toward the control of residence time to improve separation efficiency and reaction yields.

In light of the current national interest in nuclear reactor technologies, ORNL has developed capabilities, laboratories, and systems for producing and characterizing molten fuel and coolant salts for fast and thermal molten salt reactor (MSR) concepts, including a chemistry laboratory for measuring molten salt properties and developing models to more accurately predict the behavior of candidate fuel and coolant salts. These facilities allow us to produce and characterize beryllium- and chloride-based salts in high-temperature environments to measure and understand thermophysical and chemical (e.g., corrosion) properties with various metal alloys. Additionally, ORNL has developed a new sensor for off-gas from molten salt processing to follow the chemical reactions occurring in the MSR.

Chemical engineering research at ORNL makes use of resources that span radiological laboratories and nuclear facilities (including the INMC), biochemical laboratories for investigating environmental and biofuels technologies, and chemical and materials laboratories for synthesis and characterization resources. These include SNS, HFIR, CNMS, OLCF, and NTRC.

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[15] M. A. Healy et al., *Chem. Eur. J.* **25,** 6326–6331 (2019).

[16] H.J. Martin, et al., *ACS Appl. Mater. Interfaces* **12**, 8663−8673 (2020).

[17] T. Guin et al., *Advanced Intelligent System* **2**, 2000022 (2020).

Funding for chemical engineering originates from several sources, including SC BES, EERE, NE, EM, DHS, NNSA, and SPP sponsors.

Climate Change Science and Atmospheric Science

ORNL's core capability in climate change and atmospheric science is focused on improving understanding of the causes, impacts, and predictability of climate change by (1) conducting large-scale, long-term, complex ecosystem experiments and observations; (2) leading DOE Earth system model (ESM) development in biogeochemistry for the Energy Exascale Earth System Model (E3SM) project; (3) integrating multidisciplinary research connecting data, terrestrial and atmospheric sciences, and large-scale computing; (4) developing novel software to improve the credibility and scalability of next-generation ESMs in preparation for exascale computing; (5) developing model-data integration tools, ML methods, and synthesized data for model evaluation, diagnostics, and benchmarking; and (6) coupling ESMs to components of human systems, such as land use and land cover change, that incorporate significant feedback to the climate system. ORNL plays a major role in leveraging ASCR capabilities via the SciDAC program, with research focused on developing better strategies for model evaluation and connecting them to observational data and development of subsurface hydrology dynamical cores.

ORNL advances next-generation integrated models of the Earth system by improving the characterization of ecosystem processes and land–atmosphere exchange of carbon, nitrogen, nutrients, water, and energy, as well as human–climate-system interactions. ORNL leads in the use of knowledge derived from these long-term experiments to improve the representation of key plant and microbial traits in terrestrial biosphere models (e.g., spanning scales from genes to ecosystems) and their contributions to carbon and other biogeochemical cycles. ORNL advances a transformative watershed predictive capability through the multilaboratory ExaSheds project that leverages ML to integrate diverse data with river basin-scale simulations of unprecedented spatial resolution and mechanistic detail. This is required not only to inform model inputs but also to assist in model-data integration and to create surrogate models to support scaling of observations to river-basin scales.

ORNL is the premier data resource for the Atmospheric Radiation Measurement (ARM) Research Facility. With over 2.8 petabytes of data from 11,000 data products, the ARM data center provides key atmospheric radiation measurements from around the world to improve understanding of atmospheric dynamics and cloud processes. During FY 2020, the ARM data center was recognized as a trusted repository by the Core TrustSeal and became a regular member of the World Data System. The team successfully completed the processing and archival data from the recently concluded Multidisciplinary Drifting Observatory for the Study of Arctic Climate (MOSAiC) campaign conducted from an icebreaker near the North Pole and data from the Cold-Air Outbreaks in the Marine Boundary Layer Experiment (COMBLE) conducted in Norway. ORNL advances high-resolution modeling and value-added data product generation by continuously deploying new HPC workflow capabilities as part of the ARM Computing Environment.

ORNL infrastructure supporting climate change science and atmospheric science includes leadership-class computing through the OLCF, which supports modeling and simulation and big data applications; state-of-the-art greenhouses; field and laboratory facilities; and SNS and HFIR, which enable characterization of soil organic matter and multimodal imaging of whole plant/soil systems and plant–water interactions.

SC is the primary sponsor for these efforts; NNSA, NASA, DoD, DHS, the US Geological Survey, National Oceanic and Atmospheric Administration (NOAA), and the USDA Forest Service also sponsor or collaborate on activities that leverage and enhance DOE investments in climate change and atmospheric science to generate solutions for the nation.

Computational Science

Computational science at ORNL is focused on the development and delivery of scalable computational applications that enable researchers to combine theory, experiment, data analysis, and modeling and simulation and thereby tackle science and engineering problems of national interest. It also provides foundations and advances in quantum information sciences (QIS) to enable quantum computers, devices, and networked systems. This core capability resides within the world's most capable complex for computational science, which comprises outstanding staff, infrastructure, and computers dedicated to a research portfolio that covers the full span of ORNL's interests. Integrated teams of domain scientists, computational scientists, computer scientists, and mathematicians provide scalable computational and analytical solutions delivered through the integration of algorithms, modeling and simulation, software technologies, computer and information sciences, and HPC infrastructure.

Over the past decade, the ability to efficiently capture, analyze, and steward large volumes of highly diverse data has become increasingly important to ORNL's sponsors. In addition, data-centric discovery is one of the new frontiers of science and technology. ORNL responded to this situation by creating CADES, an integrated compute infrastructure for delivering data science solutions and workflows, which is sustained and updated by both institutional and programmatic investments. CADES is effectively creating a new environment for scientific discovery with its diverse computing and data ecosystem, enabling scientists to manage, manipulate, and process large data sets.

These solutions enable transformative science applications that span computational design and modeling of new quantum and nanomaterials; closing the carbon cycle, predictive understanding of microbial, molecular, cellular, and whole-organism systems; simulation of nuclear fission and fusion systems; simulation of energy infrastructure and energy usage; supernovae and nucleosynthesis simulations; reliable predictions of climate change at the regional scale, including biogeochemical feedbacks; and stringent model evaluation to bracket uncertainties and impacts to communities. The capability also supports early-stage research for companies of all sizes—including SmartTruck Systems, GE, Rolls-Royce, Ford, Arconic, Polyceed/Dyenamics, and Boeing—that addresses problems that are tractable only by using HPC.

Example applications under active development for current and future leadership computing platforms include LatticeQCD for chemistry and materials applications; NWChem Ex to address scientific challenges involved in the development of advanced biofuels; support for the GAMESS-US electronic structure code; QMCPACK for simulation of electron structure of atoms, molecules, and solids; E3SM-MMF to develop a cloud-resolving earth systems model for high-resolution climate simulations; and CANDLE applying the latest deep learning techniques for information extraction from COVID-19 and cancer-related literature. ORNL support for the ECP Applications Development (AD) focus area includes leading projects that are building new simulation capabilities for small modular reactors (led by Steven Hamilton), additive manufacturing (led by John Turner), and quantum materials simulation (led by Paul Kent)—as well as work with WBS L2/L3 leaders and principal investigators of 81 active WBS L4 subprojects to assess COVID-19 impacts, which are currently minor overall for ECP.

These capabilities are applied to deliver integrated, scalable solutions to complex problems of interest to DOE and other sponsors, including materials design, quantum computing and networking, advanced manufacturing, electrical energy storage (batteries and supercapacitors), smart grid, renewable energy penetration, nuclear reactor efficiencies and lifetimes, fusion plasma containment, climate change science, weather prediction modeling, health and quantitative biology, and scalable analytics to address complex problems associated with DOE missions in energy and national security.

Funding for this work comes from SC, NE, FE, the National Virtual Biotechnology Laboratory, EERE, and OE. Other offices and agencies, including the DoD, the Department of Veterans Affairs, HHS, and NSF, also sponsor or collaborate on activities that leverage DOE investments in computational science.

Condensed Matter Physics and Materials Science

The scientific themes of ORNL's condensed matter physics and materials science portfolio include (1) mastering the origin of quantum phenomena, (2) understanding and tailoring excitations and transport, (3) elucidating how functionalities emerge at interfaces, and (4) understanding and controlling defects and disorder to yield new materials and properties. These theme areas are based on ORNL's world-leading capabilities for predicting, synthesizing, characterizing, and controlling materials systems over broad temporal and spatial scales. They make it possible to ultimately design materials with specific functionalities by connecting the fundamental understanding of complex materials to applications in energy generation, storage, and use. ORNL has specialized expertise in synthesis of single crystals, thin films, artificial heterostructures, alloys, nanophase materials, polymers, and polymer composites. For example, the single crystal synthesis of a family of intrinsic magnetic topological insulators, $MnBi_2nTe_{3n+1}$, n=1,2,3, enabled the discovery that the ferromagnetism naturally possessed by the topological insulator extends right to the material's surface.[18] The successful molecular-beam epitaxy of the first two members of the intrinsic magnetic topological insulator $(MnTe)(Bi_2Te_3)_n$ was also performed, revealing that careful control of the growth parameters can be an effective means to tune the magnetic properties.[19] Thin film synthesis of oxide quantum heterostructures by pulsed laser deposition enabled the discovery of a chiral spin texture in 3*d*-5*d* transition-metal oxide heterostructures that is highly tunable by controlling the interface symmetry, yielding topological Hall effects.[20] The ability to manipulate orbital-driven interactions that direct handed-spin textures such as nanometer-scale magnetic skyrmions is important for discovering novel quantum materials that may be critical for the development of ultra-high-density information storage. Precision synthesis control by the hyperthermal implantation of clusters generated by laser ablation achieved the selective conversion of an atomically thin 2D crystal to form a Janus monolayer that offers unique quantum properties desired for future applications in sensing, computing, or catalysis.[21]

Neutron scattering experiments revealed how emergent multi-spin clusters suppress conventional magnetic ordering in a frustrated pyrochlore magnet.[22] These results showed how magnetic interactions beyond those of nearest neighbors can generate emergent magnetic clusters, and the analysis provides a blueprint for the determination of magnetic interactions in complex materials. Furthermore, neutron scattering is used to understand hybrid excitations in quantum and energy materials. For instance, it was used to reveal a giant effect of isotopic substitution on phonons in photovoltaic methylammonium lead iodide due to coupling with molecule dynamics that resulted in enhanced thermal resistivity and increased hot-carrier cooling times.[23] This route for keeping charge carriers hot longer bares new strategies for achieving record solar-to-electric conversion efficiency in novel hot carrier solar cells. Coherent x-ray scattering was also employed to reveal atomic-level correlated motion of water

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[18] B. Li et al., *Phys. Rev. Lett.* **124**, 167204 (2020); D. Nevola et al., *Phys. Rev. Lett.* **125**, 117205 (2020).

[19] J. Lapano et al., *Phys. Rev. Mater.* **4**, 111201(R) (2020).

[20] E. Skorpata et al., *Sci. Adv.* **6**, eaaz3902 (2020).

[21] Y.-C. Lin et al., *ACS Nano* **14**, 3896 (2020).

[22] G. Pokharel et al., *Phys. Rev. Lett.* **125**, 167201 (2020).

[23] M. E. Manley et al., *Sci. Adv*. **6**(31), eaaz1842 (2020).

molecules at the crucial picosecond timescale to evaluate the dynamic nature of the liquid.[24] This research approach could revolutionize the understanding and control of liquid viscosity and conductivity for novel energy technologies, from fuels and lubricants to energy storage.

QIS projects accelerate the discovery of entangled and correlated quantum states through direct control over dopants, defects, and material geometry. A new realistic strategy has recently been proposed to explore various quantum phases by strain engineering and to achieve quantum anomalous Hall insulators, potential building blocks for topological quantum electronics and quantum computers, with high thermodynamic stability.[25] Recent advancements also include the demonstration of quantum sensing with entangled light, enabling a 50% enhancement in the sensitivity of microcantilever beam displacement measurements. [26] This new approach could enable more than two orders-of-magnitude improvement in the sensitivity of scanning probe microscopes and enable the detection of more material properties at higher speeds than traditionally possible.

Leadership capabilities in materials imaging, including in situ electron microscopy and spectroscopy, scanning probe microscopy modalities, atom probe tomography, and chemical imaging, are in part made available through the CNMS user program. A scanning probe microscopy study developed a new concept for transient negative capacitance based on inverse polarization switching against the electric field in layered van der Waals ferrielectric $CuInP_2S_6$, offering a pathway toward new designs for efficient computing based on intrinsic material properties without the need for additional circuitry.[27] Developing deep learning networks from STEM is also an active research subject to advance automated image analysis and recognition of the defects in solids. A recent study demonstrated that the combination of atomic-resolution electron microscopy and statistical learning yields an approach for learning the causal structure of atomic mechanisms of ferroelectric behavior in a perovskite across ferroelectric–antiferroelectric phase transition.[28]

ORNL's experimental condensed matter and materials science efforts are deeply integrated with theory, modeling, and simulation. ORNL has strengths in the development and application of scalable computational approaches and codes (e.g., quantum Monte Carlo, or QMC, and locally self-consistent multiple scattering) that take advantage of the OLCF. For instance, powerful computers and algorithms allowed scientists to calculate the ground-state properties of challenging low-dimensional models, unveiling a spiral made in ferromagnetic islands.[29] ORNL is developing approaches to apply these codes to next-generation exascale computation as part of a BES Computational Materials Science project that was renewed in FY 2020. Recent progress in the QMCPACK code includes the development, analysis, and release of new highly efficient and accurate auxiliary field QMC methods for solids, delivering order-of-magnitude speedups, which are particularly well suited for the upcoming Perlmutter, Frontier, and

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[24] Y. Shinohara et al., *Nat. Commun.* **11***,* 6213 (2020).

[25] L. Zhang et al., *Nano Lett*. **10**, 7186 (2020).

[26] R. C. Pooser et al., *Phys. Rev. Lett.* **124**, 230504 (2020).

[27] S. M. Neumayer et al., *Adv. Energy Mater*. **10**, 2001726 (2020).

[28] M. Ziatdinov et al., *npj Comput. Mater.* **6**, 127 (2020).

[29] J. Herbrych et al., *Proc. Natl. Acad. Sci.* **117**, 16226 (2020).

Aurora machines.[30,31] A joint ASCR-BES project supported through SciDAC is developing a computational framework for controlled and unbiased studies of strongly interacting electron systems in quantum materials.[32]

The Energy Deposition Defect Evolution EFRC led by ORNL was successfully ended in FY 2020. This project provided invaluable information for designing the next generation of radiation-resistant alloys for nuclear and other applications.

This work is primarily supported by BES. Expertise in this area supports other programs, including EERE, NE, ARPA-E, DoD, the Nuclear Regulatory Commission (NRC), NASA, and other SPP programs.

Cyber and Information Sciences

ORNL's cyber and information science core capability includes expertise and resources in cybersecurity, cyber-physical security, identity sciences and biometrics, visual analytics, data analytics, AI/ML, database architectures, secure communications, signals analysis, QIS, data privacy, and information security. These resources are used to (1) securely and resiliently collect, share, intelligently store/retrieve, transmit, analyze, and classify enormous and heterogeneous collections of data; (2) create knowledge from disparate and heterogeneous data sources; and (3) understand, assess, defend against, and defeat known or unknown adversaries to protect the nation's critical infrastructure, including energy, economic, command and control systems, weapon systems, advanced manufacturing, biosecurity and essential resource management and distribution systems.

Cybersecurity is a domain in which human-centric operations drive the efficacy of network security architectures. ORNL has substantial capability in developing science and technology that optimizes and enhances the security of cyber- and cyber-physical systems and their operations. Our primary capabilities are in AI-enabled cybersecurity defense, cyber-physical security, and resilience with a focus on the power grid, manufacturing systems, transportation, and resilient/secure AI systems used in a national security context. ORNL has recently added new capabilities for the study of mathematical and ML methods applied to cybersecurity, including adversarial ML, the pragmatic evaluation of applications of ML in cybersecurity operations, and scalable vulnerability discovery for software and complex hardware/software systems. Finally, the often under-emphasized human component of cybersecurity vulnerabilities is being addressed via new technologies to identify those who interact with critical infrastructure (e.g., identity sciences) and to use physical and digital pattern-of-life data to identify and examine the intent of those who interact with cyber-physical systems.

Outcomes from the cybersecurity capability are translated from R&D to deployment through partnerships with operational cyber infrastructure and colocated expertise. ORNL is successfully transferring technologies to address cyber and information security challenges. Capabilities and tools such as scalable anomaly detection, ML-based network security, resilient AI methods, cyber-physical systems protection and resilience, and others have been licensed to multiple industry partners and/or operationally fielded within the US government. Multi-modal biometrics technologies have been licensed to global companies that intend to deploy these technologies to enhance the safety of our nation and world. Information science and data play a crucial role in both scientific discovery and mission-oriented decision making. The grand challenge is how to securely collect, organize, and structure the complex and voluminous data so they are useful and informative for end-use scenarios,

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[30] F. D. Malone et al., *J. Chem. Theory Comput*. **16**, 4286 (2020).

[31] P. R. C. Kent et al., *J. Chem. Phys*. **152**, 174105 (2020).

[32] T. A. Maier et al., *Phys. Rev. Research* **2**, 033132 (2020).

and to establish privacy-preserving methods and systems as needed for sensitive data (e.g., personally identifiable information, personal health information, and classified material) for applications such as health records data analytics and biometrics data applications in which ensuring the privacy of human subjects is paramount. Solutions to these problems require complex, sophisticated, and interdisciplinary approaches based on data science and data preparation. ORNL is among the national leaders in methods for heterogeneous big data management, open and sensitive data curation and processing, smart storage/retrieval, and feature engineering, which leverage resources such as the OLCF, Knowledge Discovery Infrastructure, and CADES. ORNL researchers apply strong mathematical rigor and computationally intensive methods to solve cybersecurity and information challenges at scale and/or in near-real time. ORNL's resources also allow for deep learning on HPC systems, providing unparalleled insights into the behavior of malicious and nefarious cyberspace actors.

Also, in the information science domain, QIS R&D is providing game-changing capabilities for secure communications and control systems, especially in protection of the electric grid. These include programs in partnership with the Cybersecurity for Energy Delivery Systems R&D program of DOE's Office of Cybersecurity, Energy Security, and Emergency Response (CESER). For example, ORNL is participating in a project to develop photonic integrated circuits of larger optical systems, such as quantum random number generators and continuous-variable key distribution systems, to dramatically reduce the technology costs and ultimately make them manufacturable. The combination of these information science and quantum communication capabilities spans areas such as sensitive data analytics/distribution, cyber-physical systems protection, trusted and secure communication architectures, and persistent threat detection and mitigation in networks. This capability extends to supercomputing, where assurances in information and data integrity can guard against adversaries who attempt to influence policy by manipulating HPC processes, data, or results.

ORNL infrastructure supporting this core capability includes the Distributed Energy Communications and Control Laboratory (DECC), the Grid Research, Integration, and Deployment Center, classified HPC systems, the Center for Trustworthy Embedded Systems, the MDF, the Vehicle Security Laboratory, the Cyber Science Research Facility, and the Cyber Operations Research Range. This infrastructure—along with multidisciplinary staff proficiencies throughout ORNL in power systems, power electronics, nuclear power systems, and transportation—enables the laboratory to tackle cyber and cyber-physical security challenges for multiple systems that include the electric grid, smart transportation systems, vehicles, and storage, and compute platforms for sensitive data and information.

Funding for this work comes from SC, OE, CESER, EERE, NNSA, the Intelligence Community, Intelligence Advanced Research Projects Activity, DHS, the Department of Veterans Affairs, the Centers for Medicare and Medicaid Services, and DoD.

Decision Science and Analysis

ORNL's decision science and analysis core capability assists a wide variety of decision makers who grapple with compelling local, regional, national, and global issues. Quantitative and qualitative social, institutional, and behavioral research is conducted on topics as diverse as technology acceptability, market transformation, societal implications of emerging technologies, linkages between science or technology and their intended users, and decision-making itself. ORNL's data-driven methods, models, analyses, and tools create knowledge and insights useful in anticipating, planning for, managing, and understanding responses to and impacts of numerous events and technologies.

In national security, ORNL's niche R&D areas in this capability are geographic information science, including human dynamics and geographic data science–driven decision support tools that aid national security sponsors in making decisions under uncertainty; data analytics for nuclear nonproliferation discovery and characterization; and data-driven cybersecurity operations research.

ORNL scientists operating at this nexus of technology and decision analysis have established critical capabilities and expertise in the practice of data-driven decision science, risk analysis, and uncertainty quantification (UQ) and uncertainty propagation. These resources are necessary to address impacts of technologies on environmental systems, market dynamics, regulation, and other social factors. Such impact assessments are complex, cross-disciplinary, data driven, and often computationally demanding. Verification and validation tools are being developed within a comprehensive UQ framework and applied across a wide breadth of modeling and simulation applications, from Earth systems to advanced nuclear energy technologies, allowing for improved predictions with reduced model uncertainties. ORNL's capabilities and expertise enable the observation, modeling, analysis, and simulation of physical, social, economic, and governance dynamics with unprecedented spatial and temporal resolution, providing an unparalleled opportunity for scenario-driven analyses and evaluation of the consequences of current and future technologies and policies. To expand and strengthen ORNL's unique expertise in geospatial science, ORNL has hired Steven Ward (Bayer Crop Science; geographic data science), Carter Christopher (Slingshot Aerospace; human dynamics), Matthew McCarthy (University of Florida; remote sensing), Chris Krapu (Duke University; Bayesian decision support systems) and Joseph Tuccillo (University of Colorado; spatial demography).

ORNL uses geographic information science for decision and risk analyses of critical infrastructure expansion and human dynamics. For critical infrastructure, ORNL supports DOE and other agencies in strategic planning and program direction, policy formulation, and implementation. ORNL is a leader in performing risk analysis of extreme events to aid in siting critical infrastructure and in understanding population dynamics for emergency response, collateral damage assessments, and urban planning. In population mapping, ORNL is now mapping and modeling the environment in which humans occupy space (i.e., both built and natural environments) at unprecedented scale and resolution. ORNL has expanded its capability in human dynamics modeling to support DoD and humanitarian organizations. This work includes endeavors such as mapping polio vaccination distribution programs and conducting rapid assessments of population dynamics in crisis and conflict areas, which support collateral damage estimates. Researchers are now leveraging and coalescing these existing investments in geospatial technologies and data to develop and deliver global building intelligence that captures information about human occupancy, materials, geometry, morphology, and function with high spatial, temporal, and attribute detail for the world. These key pieces of information are critical to address broad issues, including vulnerability and resilience; they also can be used for assessing consequences, estimating shielding protection for a variety of hazards, understanding the implications of various land use configurations and urban morphologies for future growth scenarios, and generating new insights into the impact of human activity on changing energy and transportation behaviors.

ORNL is a demonstrated leader in a number of areas within this capability, including (1) spatial demography, geographic data analytics, and technosocial analytics; (2) data-driven decision science, risk analysis, UQ, design of experiments, and probabilistic risk assessment; (3) dosimetry and development of dose coefficients and cancer risk factors for human exposure to radionuclides; (4) nuclear power plant siting, reactor operations, fuel cycle performance, and lifetime extensions; (5) climate change impacts, adaptation, and vulnerability modeling and assessment; (6) energy economics; (7) learning for heterogeneous biomedical data with UQ; and (8) development of decision-support tools for a variety of national security challenges, including support of cybersecurity, identity science, and military missions.

The Transformational Challenge Reactor (TCR) project will enable a full demonstration of the potential for combining advanced manufacturing, data science, materials science, and advanced modeling and simulation to develop advanced nuclear energy systems. Cutting-edge data science and computation may allow autonomous sensor and control systems, as well as enable ML for robust component, system, and material design and optimization. ML has been heavily used to improve reactor performance, enabling new operational regimes, improved safety, and economics. Improved sensors and controls are also being developed to enable advances toward autonomous decision-making capabilities for the nuclear power industry.

Funding for this work comes from SC, NE, EERE, DHS, DoD, the Federal Emergency Management Agency, NRC, the National Cancer Institute, and the Food and Drug Administration.

Earth Systems Science and Engineering

ORNL researchers analyze the ecological interactions of, and develop quantitative indicators for, the impacts of human activities, natural disturbances, and varying climatic conditions on spatial patterns and processes on the Earth's surface and near-surface environmental systems. Activities enabled by this core capability include (1) linking a fundamental understanding of mercury biogeochemistry to engineering applications to develop transformational solutions for DOE legacy mercury contamination; (2) developing novel, cost-effective, and time-efficient methods for measuring water quality in streams and rivers at a high spatial resolution; (3) identifying and modeling ecological functions of rivers and streams within the site selection, design, and operational decision-support systems for hydropower; and (4) developing and assessing sustainability indicators and ecosystem services for bioenergy feedstock production and hydropower development through integration of landscape and aquatic ecological science and socioeconomic analyses.

This capability supports DOE's energy and environmental missions and contributes to the technical basis for policy decisions. ORNL takes advantage of laboratory- to field-scale resources and expertise in geochemistry, hydrology, microbial ecology and genetics, aquatic ecology, and engineering to evaluate the impacts of energy production, transmission, distribution, and use on the environment.

Relevant leadership areas for ORNL include (1) novel integrated sensor and monitoring networks for long-term assessment of environmental change in response to energy production and use; (2) understanding contaminant cycling and fate in ecosystems to inform the development of innovative remediation technologies and improve risk-based decision-making; (3) assessing impacts of energy production and distribution systems, including hydropower (existing and in development), on aquatic ecosystem integrity through sensor systems, novel geospatial analyses, and modeling to identify thresholds and promote the adaptability of monitoring and management regimes; (4) modeling and assessing biomass feedstock resources and the logistical and environmental effects of supplying biomass to facilities producing biomass-based fuels, power, heat, or bioproducts; and (5) technologies, systems analysis, and decision support for sustainable hydropower and other energy production and water uses.

ORNL's Earth system science and engineering projects take advantage of world-class experimental and computational infrastructure, including neutrons at SNS and HFIR; the CADES data infrastructure; HPC at the OLCF; state-of-the-art greenhouses, field and laboratory facilities (including the Environmental Science Laboratory, Aquatic Ecology Laboratory, Mercury SFA Field Site, and Y12 National Security Complex Integrated Field Research Challenge site); the Joint Institute for Biological Sciences; and CNMS. Funding comes from SC, EM, EERE, FE, NNSA, DoD, NE, and NRC.

Environmental Subsurface Science

ORNL's core capability in environmental subsurface science is foundational to advancing the fundamental understanding of processes that control the biogeochemical transformation and fate of metals, carbon, and nutrients in complex, heterogeneous, multiscale environmental systems. Examples of activities supported by this core capability include (1) watershed- to molecular-scale hydrology, geochemistry, and microbiology to elucidate the coupled physical and biogeochemical processes that govern the formation of hotspots for mercury and nutrient transformations in headwater streams and their surrounding watersheds; (2) state-of-the-art subsurface hydrology and reactive transport model development; (3) delivery of a deeper understanding of how hydrogeochemistry drives the day-to-day population shifts of subsurface microbial communities (via the ENIGMA consortium); and (4) integration of neutron scattering, neutron imaging, and exascale computing to understand enzymatic mechanisms for metal transformation in subsurface systems, the distribution of pore sizes in heterogeneous solid matrices (e.g., soils and rocks), and estimates of fluid uptake rates by plant roots. ORNL's strengths in predicting the states, fluxes, and residence times of metals, nutrients, and contaminants in environmental systems contribute to basic and applied R&D programs focused on extraction of fossil fuels, disposal of nuclear waste, cleanup of DOE legacy contamination, and delivery of freshwater by watersheds for human consumption and energy production. ORNL leads one of the world's largest ongoing efforts in mercury research. The Critical Interfaces SFA is a multi-institutional, interdisciplinary program that integrates ORNL's leadership expertise in molecular- to field-scale hydrology, geochemistry, microbial ecology and genetics, biochemistry, and computational modeling to determine the fundamental mechanisms and environmental controls on mercury biogeochemical transformations in metabolically active transient storage zones in low-order stream systems.

This core capability comprises a wide range of state-of-the-art facilities, including the Critical Interfaces SFA Field Site, the Y12 Integrated Field Research Challenge site, SNS, HFIR, OLCF, and CNMS. DOE user facilities at other national laboratories (e.g., Stanford Synchrotron Radiation Lightsource, Advanced Photon Source, National Synchrotron Light Source–II, and Environmental Molecular Sciences Laboratory) are also used. Funding comes from SC, EM, FE, NNSA, DoD, and NRC.

Large Scale User Facilities and Advanced Instrumentation

ORNL has a distinguished record in developing and operating major facilities for DOE and in designing and deploying instrumentation. ORNL is noted for the breadth of the facilities and instrumentation it develops and deploys for DOE and for its integration of these assets to deliver mission outcomes. The user facilities at ORNL attract thousands of researchers each year and support the development of the next generation of advanced techniques and capabilities and skilled, scientific researchers.

The SNS and HFIR together provide the world's foremost neutron-based capabilities for studying the structure and dynamics of materials, biological systems, and basic neutron physics. SNS is currently the world's most powerful pulsed spallation neutron source. For neutron scattering experiments that require a steady-state source, HFIR offers thermal and cold neutron beams that are unsurpassed worldwide. Thirty neutron scattering instruments are available to scientists at SNS and HFIR, and the Fundamental Neutron Physics Beamline is available at SNS. Significant investments in instrument improvements, sample environment, remote access, and data reduction and analysis capabilities make ORNL's neutron scattering instruments world leading. Construction of the Versatile Neutron Imaging Instrument (VENUS) at SNS, in progress, will provide wholly new and unique capabilities for neutron tomography.

As part of a three-source strategy for ORNL, construction of a high-brightness, long-wavelength Second Target Station (STS) at SNS is planned. The PPU and STS projects leverage DOE's investment in neutron sciences.

The PPU will increase the neutron peak brightness and flux at the SNS FTS), thereby increasing scientific capacity and capability on currently oversubscribed instruments. The PPU Project also provides the platform for the STS. PPU construction activities and fabrications are under way, with buildout of the klystron gallery progressing and key components such as superconducting cavities and cryomodules, high-power RF equipment (including modulators and klystrons), and target system upgrades on schedule for delivery. Critical Decision 2 (CD-2) and Critical Decision 3 (CD-3) have been approved for PPU.

The STS, which received Critical Decision 1 (CD-1) approval in November 2020 and is therefore in the preliminary design and R&D phase, will provide researchers from a wide range of disciplines with new experimental capabilities that can be used to probe the structure and dynamics of materials over extended length, time, and energy scales. The project leverages the capacity of the existing SNS accelerator, accumulator ring, and infrastructure and takes full advantage of the performance gains that will be delivered by the PPU Project.

HFIR's capabilities for radioisotope production, materials irradiation, neutron activation analysis, and neutrino research make it an asset for isotope R&D and production, materials and fuels testing, high-energy physics, and nuclear security science programs. HFIR also plays a critical role in the neutron scattering program, providing opportunities for studies for which the SNS (including the STS) is poorly suited. The capabilities in spectroscopy, diffraction, imaging, and small-angle scattering, find applications in quantum materials, soft matter, and energy and engineering materials. In response to a BES Advisory Committee report issued in September 2020, DOE SC approved a CD-0 Mission Need Statement in December for replacement of the reactor pressure vessel and other major components to sustain HFIR operation through the end of this century. Plans are being developed to proceed with these replacements and to evaluate the potential enhancements the upgrades would enable for HFIR's multiple scientific capabilities. Reactor outage scenarios, including the planned installation of a new beryllium reflector, are being evaluated to minimize impacts to all missions.

The HPC resources of OLCF, including the IBM AC922 Summit, are available to users to solve computationally intensive scientific problems and to accelerate innovation for industry partners. Summit is now in full user operation. This pre-exascale, hybrid platform provides 200 petaflops of computing power for modeling and simulation and more than 3 exaops of computational power for AI applications and research. The OLCF-5/CORAL-2 system, Frontier, has received CD-2/3 approvals, and a build contract was awarded in 2019 for delivery in 2021. ORNL also operates high-performance computers to support multi-agency cooperation and R&D partnerships that include the Gaea computer, operated for NOAA, and the Miller and Fawbush computers, operated for the US Air Force.

CNMS provides world-leading expertise in synthesis, characterization, nanofabrication, theory, and modeling and simulation to the greater user community. Synthesis capabilities at CNMS have been expanded as part of the BES Quantum Information Science and Research Infrastructure project, including recent deployment of (1) rapid synthesis and characterization via a pulsed laser deposition synthesis platform that will support ML approaches, rapid in situ diagnostics, high-throughput characterization using x-ray photoelectron spectroscopy and diffraction, and optical spectroscopies and (2) a cathodoluminescence scanning electron microscope (CL-SEM) that offers angle, polarization, temperature, wavelength, spatial, and time-resolved CL microscopy. Photon correlation measurements with superconducting nanowire single photon detectors and time-resolved experiments are possible with up to 30 ps timing resolution. Femtosecond pump-probe experiments that combine pulsed electron and laser beams are in development. In situ patterning of quantum emitters and plasmonic cavities is possible with environmental electron beam patterning and electron beam–induced deposition. As part of the CNMS QIS infrastructure project, CNMS recently ordered a vector field, ultralow-temperature, spin-polarized scanning tunneling microscope. Injecting electrons with the controllable angular momentum necessary for probing spatially resolved spin entanglements with atomic resolution at ultralow temperature and in a variable vector magnetic field is beyond the capabilities of currently available instruments. This unique platform for nanoscale probing of magnetic structures and entangled spin states will provide critically needed information for QIS, such as the spin manifold of exciton dynamics, the true nature of the quantum spin liquid ground state, and the detection of Majorana zero modes. CNMS is now conducting experiments using the Raith VELION nanofabrication system, combining focused ion beam (FIB) and SEM, that operates a variety of isotopically controlled ion sources for imaging, milling, and deposition and builds on ORNL's demonstrated strengths in nanofabrication, electron/ion beam–induced deposition, HPC, and AI algorithms for materials processing.

The CNMS user community will benefit immensely from the Nanoscale Science Research Center (NSRC) Major Item of Equipment (MIE) project, which will recapitalize the five NSRCs and deliver new capabilities for the next decade of nanoscience. CNMS has prioritized a cryo-plasma FIB and a liquid-helium–cooled monochromated aberration-corrected STEM (MAC-STEM).

CNMS and SNS are working together to develop coordinated research efforts in polymer science, biomaterials, AI/ML, and novel technique and capability development. For example, CNMS supports neutron studies of nanoscale structure in soft matter by providing site-specific deuteration capabilities; these efforts will be advanced by the recent hire of a dedicated CNMS staff chemist to develop and improve deuteration methods for small molecules critical for neutron experiments on biomaterials and polymers. In addition, CNMS hired a new staff member to lead the combined CNMS/SNS focus on building a user base for the liquids neutron reflectometer.

ORNL is home to three EERE-sponsored R&D facilities: MDF, which includes the pilot-scale CFTF; the Buildings Technology Research and Integration Center (BTRIC), which includes the Maximum Building Energy Efficiency Laboratory (MAXLAB); and NTRC. These facilities enable R&D and demonstration of innovations in renewable electricity generation; energy-efficient homes, buildings, and manufacturing; and sustainable transportation, respectively. This cluster of industry-facing facilities enhances engagement with industry and provides a linkage to SC user facilities with complementary capabilities.

Large-scale user facilities and instrumentation are fundamental to ORNL's ability to deliver on its mission assignments for DOE, especially supporting the broader science and technology user community and increasing American competitiveness through industry engagement. Work in this area is supported primarily by SC and EERE.

Mechanical Design and Engineering

ORNL deploys extensive expertise in mechanical design and engineering to support the development of a wide range of projects (e.g., reactors, accelerators, fusion experimental devices, enrichment technology) and instruments. For example, this core capability supports the US ITER project, the PPU and STS projects at SNS, the MAJORANA Demonstrator project, the MPEX project, and the neutron electric dipole moment (nEDM) experiment. In many cases, mechanical design and engineering efforts have drawn upon expertise across ORNL. For example, ORNL mechanical engineering staff used their expertise to design a new target for irradiation of Np-237 to produce Pu-238 at the Advanced Test Reactor at the Idaho National Laboratory. Expertise in the analysis of stress, strain, and thermal effects in composite materials, fluid dynamics, and dynamic analysis of rapidly rotating devices have been key to the development of advanced isotope separation devices. Further, ORNL capabilities in basic science and associated characterization tools have been exploited to provide innovative solutions in support of mechanical engineering applications. For example, HFIR's neutron scattering capabilities have been applied to map residual stress in manufactured components, helping to improve material reliability in various devices, including additively manufactured heat exchangers and fuel injectors. Further, ORNL's mechanical design and engineering capabilities provide breakthroughs in energy-efficient manufacturing; in the energy efficiency and durability of building envelopes, equipment, and appliances; and in transportation (including multicylinder combustion R&D and exhaust aftertreatment development).

Mechanical engineering capabilities at ORNL have been used to developed remote systems for SNS and INMC, as well as production-level separation processes based on electromagnetic and gas centrifuge separation techniques that are being advanced for both radioisotopes and stable isotopes. The Centrifuge Manufacturing Capability, completed in FY 2021, supports the fabrication of Gaseous Centrifuge Isotope Separation machines for the SIPF and SIPRC. Also, ORNL combines its expertise in mechanical design and engineering with other disciplines to support a range of nuclear capabilities, including the thermal/hydraulic design of HFIR irradiation experiments, the HFIR closed-loop supercritical-hydrogen cold neutron source, a novel molten salt experimental loop facility, the SNS mercury target systems, and the high-heat-flux divertor components for the Wendelstein 7-X superconducting stellarator.[33] Foundational capabilities for remote operations have also been translated into the development of big-area additive manufacturing devices for the 3D fabrication of very large builds.

ORNL's applied research facilities (MDF, CFTF, BTRIC, NTRC, and the remote systems development high-bay facility) support work by staff with expertise in robotics and remote systems design, thermal hydraulics, energy-efficient manufacturing, transportation, and residential and commercial buildings. Funding in this area originates from several sources, including SC, NE, EERE, NNSA, and SPP sponsors.

Nuclear and Radio Chemistry

Major focus areas for ORNL's nuclear and radiochemistry research are the nuclear engineering design of advanced targets for efficient production of isotopes and the development of highly selective separation techniques for the harvesting of isotopes after target irradiation for a broad range of applications, including cancer treatment, commercial uses, and research.

ORNL's nuclear chemistry and enrichment expertise is also critical in preserving and advancing US uranium enrichment capabilities. Production-level separation processes based on electromagnetic and gas centrifuge separation techniques are being advanced for both radioisotopes and stable isotopes. ORNL maintains and distributes the US inventory of enriched stable isotopes and radioisotopes for DOE's National Isotope Development Center.

HFIR, which provides the world's highest neutron flux, is used to irradiate target materials for the production of various radioisotopes through the DOE Isotope Program and other sponsors. Separations are conducted in INMC facilities, including the Radiochemical Engineering Development Center, laboratories and hot cells in Buildings 4501 and 3047, and other radiological laboratories. As part of the DOE Isotope Program, ORNL examined long-term needs for radiochemistry facilities to support increasing demand for radioisotopes for use in medical, industrial, and research applications. ORNL has provided technical input to the Isotope Program to support a mission needs statement for the proposed new radioisotope processing facility. It has since been communicated to ORNL that the RPF CD-0 was

[33] M. Shafer et. al., *Nuclear Materials and Energy* **19**, 487–492 (2019).

approved on April 29, 2021. ORNL has established production capability for delivery of Ac-227 for medical applications and has launched an effort to identify the resources needed to meet the increasing demand for this radioisotope. A new chemical purification strategy for Ac-227 was implemented and was shown to simplify operations and reduce waste. Funding provided by NASA supports the production of Pu-238 for use in radioisotope power supplies and heat sources for planetary science missions. ORNL shipped plutonium-238 to the Los Alamos National Laboratory which was subsequently used on the Perseverance Rover. A newly designed second automated pellet pressing system for the Pu-238 Supply Program enables the scale-up of plutonium oxide production from about 400 to 1500 g/year. ORNL leveraged radiochemistry knowledge and removed Pm-147 from a waste stream created during Pu-238 processing. This new source of Pm-147 was shipped to a customer.

ORNL's nuclear and radiochemistry expertise, extensive radioanalytical capabilities (especially mass spectrometry), and neutron activation analysis capability at HFIR provide world-leading resources for ultra-trace analysis with applications that include environmental analysis, forensics, and security. For example, the Neutron Activation Analysis Laboratory, located within the HFIR complex, is the sole provider of routine analysis of International Atomic Energy Agency pre-inspection samples. Expertise in radiochemical separations, analyses, and nuclear material examinations is being applied to the management of nuclear material such as UNF; the detection of materials important to the management and security of the nuclear fuel cycle; the development of safer, more efficient nuclear fuels; and improvements in nuclear waste treatment. Funding in this area comes from several sources, including SC, NE, NNSA, DHS, DoD, NASA, NRC, and other government agencies.

Nuclear Engineering

Early work at ORNL demanded expertise in handling and processing unirradiated and irradiated nuclear materials and fuels, developing and operating nuclear reactors, and detecting radiation. These are the very foundations of the discipline of nuclear engineering. Today, ORNL leads nuclear engineering in many subfields, all oriented towards acceleration of deployment of advanced nuclear technologies from concept to industry. This includes the addressing engineering needs for the entire nuclear fuel cycle, development of new materials and systems for fission and fusion, taking advantage of specialized facilities and core capabilities in materials science, chemistry, advanced manufacturing, chemical engineering, computing, artificial intelligence, and other areas. ORNL is also a leader in modeling and simulation for reactor physics and radiation transport, computational thermal hydraulics, reactor systems, nuclear criticality safety, and reactor safety; radiation detection and imaging; and radioisotope production.

Supporting all of these activities is the ability to develop, benchmark, and distribute validated modeling and simulation tools. ORNL has a wide range of specialized facilities for nuclear materials development and characterization. Capabilities include a complete "cradle to grave" suite, spanning materials irradiation capabilities at HFIR and post-irradiation characterization facilities at LAMDA, as well as hot cells within INMC. Instrumentation and controls are another area of strength, with ORNL developing improved sensors and measurement techniques, which, when coupled with modern data science, enable advances toward autonomous decision-making capabilities for the nuclear power industry.

A leading example of applying modern, multidisciplinary science to nuclear energy is the TCR program (referenced in Section A.13). TCR leverages advances in manufacturing and computational science to deliver advanced nuclear technology at a reduced cost. To achieve this goal, TCR brings together advanced manufacturing with computational design and artificial intelligence. In addition, the program takes advantage of unique ORNL research facilities, including the Spallation Neutron Source, Oak Ridge Leadership Computing Facility, the High Flux Isotope Reactor (HFIR), and the Manufacturing

Demonstration Facility. The TCR program has already demonstrated a number of significant achievements, including transfer of additively manufactured components to industry. Recently, ORNL partnered with Tennessee Valley Authority and Framatome Inc., a TVA nuclear fuel supplier based in Richland, Washington, to introduce parts produced using additive manufacturing, or 3D printing, techniques into existing nuclear reactors. The current focus of the TCR program is to further mature and demonstrate industry-ready technology informed by artificial intelligence, advanced manufacturing, integrated sensing, and deployment of a digital platform for design iteration.

ORNL's nuclear engineering expertise is critical to the continued viability of the nuclear power industry, including improved operations and extended operations of the existing fleet.[34,35] ORNL's expertise in the design and post-irradiation examination of HFIR irradiation capsules is used to study reactor materials and accident-tolerant fuels.[36] ORNL applies modern tools to carry out optical, scanning electron, and transmission electron microscopy as well as chemical, physical, and mechanical property measurements on irradiated fuel and structural materials in support of reactor and UNF systems R&D. ORNL contributes to next-generation reactor technology through the development and testing of new fuels,4 materials, and salts; improved instrumentation and controls; regulatory research; thermal-hydraulic experiments; and innovative system concepts. ORNL is the world leader in Molten Salt Reactor technology, collaborating domestically and internationally, and leading NE's MSR R&D program to advance the concept's maturation through modeling and simulation, development, and operation of liquid salt flow loops for component and materials testing, and system studies to ensure safe and efficient operations.

ORNL is engaged through the Gateway for Accelerated Innovation in Nuclear (GAIN) and with industry on the development of MSRs, gas-cooled reactors, and other advanced reactor concepts. The development of an energy portfolio climate impact tool is in development for GAIN by ORNL to support policy decisions related to short and long-term emissions goals.

ORNL nuclear engineers provide critical experiment design, validation and nuclear data testing activities, working with nuclear data and the NRC for licensee support. ORNL also performs burnup credit and used nuclear fuel analysis for the DOE-NE and NRC. Nuclear engineers also support the execution of the DOE/NNSA Nuclear Criticality Safety Program (NCSP) and provides project management support for all subcritical and critical experiments at Sandia National Laboratories and the National Criticality Experiments Research Center at the Nevada National Security Site. Nuclear Engineers also organize and conduct all DOE NCS 1- and 2-week hands-on training courses to support DOE-wide NCS engineer training and qualifications. Radiation transport experts at ORNL develop, apply, and deploy state-of-the-art modeling and simulation capabilities to solve radiation transport problems across a range of applications, including shielding for ITER and other facilities, as well as spent nuclear fuel.

Through the development and application of computational analysis tools and nuclear data to advance the scientific understanding of observed phenomena, ORNL is solving complex problems that improve the efficiency and safe utilization of nuclear systems. The ORNL-developed SCALE code system is applied worldwide to perform design and safety analysis for reactor and nuclear facilities. ORNL's hybrid deterministic Monte Carlo methods have transformed computational radiation transport and have

[34] A. Abd-Elssamd et al., *ACI Mater. J.* **117** (1), 265–277 (2020).

[35] R. Montgomery et al., *Nucl. Sci. Eng.* **193,** 884–902 (2019).

[36] N. M. George et al., *Ann. Nucl. Energy* **132,** 486–503 (2019).

enabled reliable, high-fidelity solutions for large-scale, complex problems. The conclusion of the ORNL-led Consortium for Advanced Simulation of Light Water Reactors (CASL) resulted in deployed tools that combine nuclear engineering and HPC to develop a high-fidelity virtual reactor capability that has been validated using more than 200 operating cycles representing more than 60% of the nuclear fleet. Achievements include the blind prediction of the startup and power ascension of the Tennessee Valley Authority's Watts Bar 2 pressurized water reactor (PWR), the first US nuclear reactor to enter service in the twenty-first century. The Virtual Environment for Reactor Applications (VERA), developed by the CASL program, delivers the cutting edge in light water reactor modeling and simulation to industry via an active Users Group. VERA integrates physics components based on science-based models, state-of-the-art numerical methods, and modern computational science, and is verified and validated using data from operating reactors, single-effect experiments, and integral tests.

ORNL expertise is being leveraged to provide scientific understanding and solutions for new industry operation and safety challenge problems, including currently operating PWR and BWR reactors, introduction of accident tolerant fuels, and the next generation of small modular reactors. In support of ITER, ORNL has developed innovative neutronics-modeling tools such as ADVANTG, making it possible to calculate neutron fluxes faster and more accurately for very large facilities and structures.

ORNL nuclear engineering efforts employ HFIR, the hot cells of the Irradiated Fuels Examination Laboratory, the Irradiated Materials Examination and Testing Laboratory, the LAMDA laboratory, various hot cells and other radiological facilities within INMC, and OLCF. Funding in this area comes from diverse sources, including NE, SC, NNSA, DHS, DoD, NASA, NRC, and other government agencies, plus partners in private industry.

To preserve the expertise that is vital to this core capability, ORNL is incorporating knowledge transfer and succession planning into its hiring, recruiting, and retention practices as it continues its efforts to attract and retain staff in key leadership positions. In addition, the 2020 organization change to bring fusion and fission expertise together in one directorate is expected to enable impactful synergies across the nuclear spectrum. A recent GAMOW award to an ORNL team from ARPA-E for a fusion energy reactor model simulator is one example of bringing together fission experience and tools to fusion challenges.

Nuclear Physics

ORNL's nuclear physics researchers lead a world-class fundamental symmetries program, enable experimentation at the DOE NP user facilities and make crucial contributions to the ORNL research portfolio in both discovery science and applied science. Their work spans theoretical and experimental research that is relevant to DOE's mission of developing an understanding of nuclear matter and fundamental interactions that will help unlock the secrets of how the universe is formed.

ORNL carries out an ambitious multi-pronged research program in fundamental symmetries addressing the matter-antimatter asymmetry in the universe and completing the standard model of interactions. It is the lead laboratory for the MAJORANA Demonstrator and leads research supporting the ton-scale Large Enriched Germanium Experiment for Neutrinoless Double Beta Decay (LEGEND) experiment to search for the hypothesized neutrinoless double-beta decay mode of nuclei. It also operates the Fundamental Nuclear Physics Beamline at the SNS, which is home to the ORNL-led search for the electric dipole moment of the neutron and the Nab experiment that will make precision measurement of the beta decay of the neutron. The analysis of the data from the n-^{3}He experiment, combined with the NPDGamma results, have provided the most precise measurement of parity violation in hadronic weak interactions.

Low-energy nuclear experimental research at ORNL focuses on understanding properties of nuclei far from the “valley of stability” through beta-decay spectroscopy, low-energy nuclear reactions, and gamma-ray spectroscopy. Experiments at RIKEN in Japan have studied the beta and beta-delayed neutron decays of very neutron-rich nuclei beyond doubly magic nickel-78 in unprecedented detail. ORNL has developed, in collaboration with Japanese laboratories, a novel experimental method for fast determination of the optimum heavy-ion beam energy for the synthesis of superheavy elements. A search for the superheavy element 119 is under way at RIKEN using ORNL-provided curium-248 targets and digital electronics for an anticipated increase in overall efficiency of nearly an order of magnitude.

ORNL leads gas jet target development for nuclear astrophysics experiments using secondary beams at FRIB and helps lead aspects of the Separator for Capture Reactions, which is being commissioned. ORNL has assumed leadership roles for the FRIB Decay Station Initiator project to design and construct instrumentation for radioactive decay studies at FRIB on day one.

In nuclear theory, OLCF is used to investigate the structure and reactions of neutron-rich rare isotopes and nuclear astrophysical processes. ORNL develops world-leading approaches to relevant nuclei based on ab initio methods, HPC, and effective field theory. The highest-fidelity core-collapse supernova and neutron-star merger simulations are provided with cell-by-cell adaptive mesh refinement, coupled hydrodynamics, radiation transport, thermonuclear kinetics, and nuclear microphysics. These simulations will provide the capability to predict multi-messenger signatures of core-collapse phenomena.

ORNL leads in the analysis of jet physics in the relativistic heavy ion program at the Large Hadron Collider (LHC) at European Organization for Nuclear Research (CERN). It has unique expertise in the design and development of specialized electronics and detectors relevant to research at the LHC and led the deployment of a new measurement paradigm by providing new technology readout chambers for the central tracking detector, the world’s largest time projection chamber. ORNL will lead physics analyses of aspects of the ALICE data, including jet shapes, jet substructure, photon-jet and jet-hadron correlations, and direct photons. ORNL is also contributing to the development of detectors for the future Electron Ion Collider.

ORNL has made breakthrough advances in resolving the computing problem for the detailed simulation of detector response for collider experiments in particle and nuclear physics using the ORNL HPC systems. This initiative aims to achieve an order-of-magnitude speedup of the simulation process.

ORNL’s nuclear data program includes cross-section measurements, the development of evaluation and data analysis methods, and data processing. These activities provide nuclear data libraries for radiation transport analysis. Further, ORNL leads the ENDF/B Formats Committee to standardize all nuclear data formatting.

Leveraging the broad range of expertise across ORNL, advanced detector technologies will enable precision nuclear physics measurements and application to safeguards and nuclear material security. Novel germanium detector designs have been invented at ORNL and developed with NP support. 3D-printing methods are being developed to produce novel, background-free scintillator to support low-background measurements and interaction-resolving detectors for prevision neutron measurements and imaging.

Funding in this area originates from SC, DHS, DoD, and NNSA programs.

Plasma and Fusion Energy Sciences

ORNL has a long history as a key player in the development of the knowledge base for plasma and fusion energy sciences essential for fusion energy deployment. With activities ranging from developing and testing innovative confinement concepts to delivery of large-scale fusion components, ORNL is the US leader, and in many cases the world leader, in several key areas of fusion development. ORNL's expertise coupled with its demonstrated abilities in large-scale project management, international collaboration, and computational simulation, is applied to support the mission of the SC Fusion Energy Sciences (FES) program.

ORNL is DOE's lead laboratory for fusion nuclear science and fusion materials, which are required to fully enable fusion energy. Materials scientists at ORNL conduct experiments to support development of alloys and silicon carbide composites, that have been leveraged to develop a suite of economical high-strength, radiation-resistant steels that derive their properties from a fine dispersion of engineered precipitate nanoclusters.[37] The development of radiation-tolerant low-activation materials will be required to make a fusion pilot plant reliable and economical. Recent experiments have leveraged the capabilities on HFIR to expose candidate materials to high-energy neutrons to better characterize the response of these materials to fusion-like conditions. This capability is unparalleled in the world program with numerous international labs partnering with ORNL to develop data of interest for specific materials they are contemplating using in future fusion systems. Recent recommendations for the Fusion Energy Sciences Advisory Committee (FESAC) indicate that ORNL's aforementioned positioning in fusion nuclear science and materials will be a key capability in the FES program in the coming years.[38]

ORNL is the world leader in pellet fueling and blanket systems for fusion applications. This is evidenced by the recent development of the design basis for a steady-state pellet injector to be deployed on the W7-X stellarator in Germany.[39] In addition, ORNL has delivered multiple shattered pellet injection (SPI) systems to devices around the world to support development of the technical basis of using SPI for disruption mitigation in ITER and future fusion devices.[40] ORNL recently delivered a Blanket and Fuel Cycle Strategic Framework document to FES that outlines the potential activities of such a program in the future.[41] In addition, ORNL is developing the technical expertise and capabilities to be a world leader in blanket technology. Combining a newly developed Helium Flow Loop to better understand helium flow in complex structures with ORNL core strengths in advanced manufacturing of complex structures and advanced computational tools, ORNL is well positioned to develop the foundational basis for optimizing the use of helium as a coolant of fusion blankets of the future.

ITER remains a key investment for US fusion goals, as noted in multiple reports from the National Academies of Science, Engineering and Medicine[42] and in the recently published DOE Fusion Energy

[37] B. Kim et al., *Journal of Nuclear Materials* **545,** 152634 (2020).

[38] Fusion Energy Sciences Advisory Committee Report, *Powering the Future: Fusion and Plasmas* (2020).

[39] S. Meitner et al., IEEE Transactions on Plasma Science **48,** 1585 (2020).

[40] T. Gebhart et al., "Shear Strength and Release of Large Cryogenic Pellets from the Barrel of a Shattered Pellet Injector for Disruption Mitigation," submitted to *Fusion Sci. Technol.* (2020).

[41] C. Kessel and M. Wade, "A Strategic Framework for the U.S. Blanket and Fuel Cycle Program 2020," submitted to Fusion Energy Sciences (2020).

[42] National Research Council, *Burning Plasma: Bringing a Star to Earth* (2004); National Academies of Sciences, Engineering, and Mathematics (NASEM), *A Strategic Plan for U.S. Burning Plasma Research* (2019); NASEM, *Bringing Fusion to the U.S. Grid* (2021).

Sciences Advisory Committee long-range plan for fusion energy and plasma science.[43] For a path to fusion energy—not just fusion science—US fusion leaders emphasize that it is essential to master both the science and the technology required for producing and controlling a reactor-scale burning plasma. ORNL is well positioned to support the recommendations of these reports.

As directed by DOE, ORNL leads the US ITER project and executes the program in conjunction with its partner laboratories, Princeton Plasma Physics Laboratory and Savannah River National Laboratory. The project draws on ORNL's breadth of experience in fusion technology, radiation transport, high-power plasma heating systems, and advanced electronics for extreme environments. US ITER fabrication activities and participation in the project will lead to the capability for creating, sustaining, and studying burning plasmas, the next step toward fusion energy. US hardware contributions include the world's highest-stored-energy pulsed superconducting magnet; superconductor for ITER toroidal field coils; a 1-GW cooling water system; high-power, long-pulse plasma heating systems; plasma diagnostics; parts of the tritium exhaust system; plasma instrumentation; and plasma disruption mitigation systems. The US ITER Project Office also works with the ITER Organization and other ITER domestic agencies to achieve the required integration of management, design, and procurement activities. Much of the R&D is also executed at ORNL.

In parallel with US ITER efforts, ORNL continues to provide key capabilities in the understanding and demonstration of sustained magnetically confined plasma with the properties needed for a compact fusion pilot plant. ORNL scientists are world leaders in the application of state-of-the-art simulation tools towards the understanding of present-day facilities and design of future fusion facilities. Recently, an ORNL team of experts from applied math, computer science, HPC engineering, and fusion theory developed a new Adaptive Sparse Grid framework that enables solutions of high-dimensional PDEs typical to fusion. Initial applications of this tool delivered about a 100-times reduction in the number of elements required for Maxwell's equations in 3D compared with traditional methods.[44] ORNL scientists are also the world leaders in boundary modeling of present-day devices and the use of core modeling tools to simulate future devices. Of the multiple studies conducted along this line in the United States in recent years, ORNL scientists have played a key role in a large fraction of them.[45]

ORNL scientists and engineers are building MPEX to address the challenges associated with exposing materials to high-energy, high-density plasmas. As a testament to ORNL's capabilities in this area, both CD-1 and CD-3/a were successfully achieved in 2020 and significant progress has been made towards CD-2. This engineering and design activity is exposing ORNL staff to the rigors required in operating a steady-state facility with MW-level heat sources and sinks. This experience will be invaluable in designing future fusion systems. Once operating, MPEX will provide world-leading capability for experiments in which power plant–level fluxes and fluences of particles will be incident on neutron-irradiated materials in prototypic geometries.[46]

Additional facilities supporting this core capability include HFIR for materials irradiation; INMC (including hot cells for materials handling and testing and the Irradiated Materials Examination and Testing

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[43] FESAC Committee Report, *Powering the Future: Fusion and Plasmas* (2020).

[44] E. D'Azevedo, et al., *Comput. Phys. Commun.* **256**, 107412 (2020).

[45] J.M. Park et al., *Phys. Plasmas* **25**, 012506 (2018).

[46] J. Rapp et al., *Fusion Science and Technology*, **75**:7 (2019); J. Rapp et al., *Fusion Engineering and Design* **156**, 1115863 (2020).

Laboratory and the LAMDA laboratory for materials characterization); the Fusion Pellet Laboratory for commissioning systems for use on fusion experiments around the world; and Proto-MPEX for necessary R&D and testing for MPEX.

ORNL continues to hire leading experts in nuclear fusion and fusion engineering, including Kathy McCarthy, Associate Laboratory Director of the Fusion and Fission Energy Science Directorate, and Mickey Wade, Fusion Energy Division director.

SC funds the work in this area, including the US ITER project. Additional funding is received via SPP sponsors.

Power Systems and Electrical Engineering

ORNL researchers deliver innovations in power flow, electric grid modernization, energy-efficient buildings and transportation, and smart manufacturing. For example, ORNL developed high-performance inverters and converters for electric vehicles (EVs) and demonstrated the first wireless bidirectional charging and energy management system for a building and a vehicle operating as an integrated energy system. This core capability (1) delivers advances in high-temperature, high-power-density applications; (2) enables high-efficiency transportation and electrification systems to reduce US reliance on foreign oil; (3) develops technologies for power flow control, grid monitoring (e.g., FNET/GridEye), and grid protection that support the development of a secure and reliable 21st century electricity delivery system; and (4) creates advanced building sensors, communications, and controls for power management systems to maximize energy efficiency.

Through DOE's Grid Modernization Laboratory Consortium (GMLC), ORNL addresses the challenges of integrating conventional and renewable electric generating sources with energy storage and smart buildings while ensuring that the grid is sufficiently resilient and secure to withstand growing cybersecurity concerns. ORNL tests controllers in multiple environments, including both simulation and full hardware environments on different scales of power and voltage levels (24 to 480 V), as well as different grid configurations and communications protocols. A strong partnership with the Chattanooga Electric Power Board reinforces this core capability by providing real-world understanding and commercial-scale implementation of emerging technologies. ORNL's Grid Research, Integration, and Deployment Center combines and integrates electrification research activities across the utility, buildings, energy storage, and vehicle missions.

ORNL leads in the creation of alternating-current power flow control systems for grid control and increased resilience. An advanced grid requires new materials for power electronics and energy storage devices. ORNL is a leader in power electronics R&D (serving as the Vehicle Technologies Office lead laboratory for power electronics) and is taking advantage of resources at NTRC to develop high-power devices to improve reliability and reduce costs. ORNL is leading the way in innovative wireless charging of EVs. In addition to providing an autonomous, safe, and convenient option for charging EVs, wireless charging, when applied to dynamic or quasi-dynamic scenarios, can provide virtually unlimited range to EVs. It can do away with "range anxiety" and long charging times because vehicles can be charged continuously while they are in motion. Recent achievements include the demonstration of bidirectional wireless charging on a medium-duty plug-in hybrid electric delivery truck.

ORNL designs, develops, and tests new materials capable of supporting cost-effective and higher-performing electricity control devices and systems. ORNL collaborates in developing power electronics from concept to prototype and applies its expertise in materials to develop innovative electronics and sensors.

Enhanced cybersecurity measures are required to prevent malicious attacks on energy infrastructure. ORNL's Acceleration Project for the Smart Grid is improving the efforts for securing smart grid systems.

Expertise gained in supporting a stable energy infrastructure for ORNL operations has been leveraged to facilitate large science experiments at other sites, such as LHC and FRIB. Current activities leverage broad expertise in electronics for extreme environments; compact high-voltage power supplies; pulsed power conversion; the Internet of Things, including connected sensor and internet frameworks; radio frequency; and communications capabilities for intelligent systems support.

ORNL supports DOE's energy mission by providing resources that can be used to catalyze the timely, material, and efficient transformation of the nation's energy system. Work in this area is conducted using the NTRC Power Electronics and Electrical Machinery Laboratory, the DECC microgrid, and the Powerline Conductor Accelerated Testing Facility; resources for thin-film deposition (i.e., inkjet printing, ultrasonic spray, sputtering, evaporation, low-temperature photonic curing); and tools for characterization of materials, devices, and communications. EERE, OE, and DOE's Office of Policy are the primary sponsors. SC also benefits from ORNL expertise in this area.

Systems Engineering and Integration

ORNL's core capability in systems engineering and integration takes advantage of the full range of capabilities across the laboratory. Solutions to pressing scientific and technical challenges are developed by integrating expertise in fundamental science, technology, and project management in multidisciplinary and multi-institutional teams. This approach allows us to accelerate research innovation in managing scientific projects of various sizes through partnerships across ORNL and with universities, other national laboratories, and private industry. Examples of recent accomplishments in working with private industry include modeling combustion processes, understanding materials properties for advanced manufacturing, improving technology to advance fusion energy systems, and modeling the energy use of buildings at the community scale.

ORNL's strength in pursuing solutions from concept to implementation and in spanning fundamental to applied research ensures the success of national and international projects, such as SNS, OLCF, MPEX, the Pu-238 process development project, the MAJORANA Demonstrator project, the nEDM experiment, ALICE at CERN, and ITER. ORNL also relies on deep systems engineering capabilities to deliver innovative solutions for manufacturing, transportation, and buildings by applying broad capabilities in materials science and engineering, computational science, decision science and analysis, mechanical design and engineering, nuclear engineering, chemical engineering, and power systems and electrical engineering. In addition, ORNL has a successful track record of delivering innovative tools and technologies as a lead and partner on Energy Innovation Hubs (CASL and the Critical Materials Institute), the Institute for Advanced Composite Materials Innovation, and other multi-institutional collaborations (Fuels/Engine Co-Optima, GMLC, Lightweight Innovations for Tomorrow, Clean Energy Smart Manufacturing Innovation Institute).

Additionally, ORNL's EERE R&D facilities (NTRC; BTRIC, including MAXLAB and DECC; MDF; and CFTF) build on ORNL scientific systems infrastructure to develop and deliver market-driven solutions for energy-saving homes, buildings, and manufacturing; sustainable transportation; and power generation. Capabilities and scientific expertise available within these facilities are highly sought after by industry and other sponsors. Recent achievements include combining materials and advanced manufacturing to fabricate 72 turbine blades for a 5 MW Solar Turbines engine.

The primary sponsors for these efforts include SC, EERE, OE, FES, NE, and NNSA. Some support is also provided by DHS, NRC, DoD, and other SPP sponsors.

Science and Technology Strategy for the Future

With the same sense of urgency and purpose that drove the laboratory's original mission, ORNL will deliver scientific advances to support DOE's mission in energy, environment, and security, catalyzing new technologies to support the nation's future economic development. With a vision to be among the world's premier research institutions, ORNL is distinguished within the DOE system of national laboratories by excelling at the translation of fundamental discovery science into applied use to solve important problems that face the nation. In the areas of neutron sciences, computational science, materials science, nuclear technologies, isotopes R&D and production, and advanced manufacturing, we intend to sustain world-leading capabilities that enable our staff—and those who partner with us—the opportunity to impact the world. Our broad scientific and facility capabilities enable pursuit of synergistic activities to advance DOE missions.

ORNL are stewarding and advancing world-leading capabilities at a set of DOE user facilities in neutron scattering, nanoscience, high-performance computing (HPC), advanced manufacturing, building technologies, and clean transportation for researchers in academia, government, and industry. Advances at the Spallation Neutron Source (SNS) connect strongly with synthesis and characterization capabilities at the Center for Nanophase Materials Sciences (CNMS) and with exascale computing and artificial intelligence (AI) capabilities at the Oak Ridge Leadership Computing Facility (OLCF). ORNL is leading the exascale computing revolution by delivering the Frontier system at the OLCF in FY 2021 and by examining approaches to realize next-generation, scalable computing ecosystems. ORNL is enhancing capabilities at our applied energy facilities to deliver technical breakthroughs that address decarbonization, electrification, and integrated energy systems challenges. An ongoing LDRD initiative is assessing potential upgrades for extending the life of the High Flux Isotope Reactor (HFIR) through the end of this century while adding new capabilities for its primary missions in neutron scattering, isotope production, and materials irradiation.

Currently, both the rate and output of traditional materials synthesis and discovery are simply too slow and too small to efficiently provide needed advances. To accelerate discovery across ORNL's signature strengths in neutrons, computing, materials, nuclear, and advanced manufacturing, we aim to develop and implement a scalable lab-wide ecosystem, known as the Interconnected Science Ecosystem (INTERSECT), to connect edge computing, artificial intelligence (AI), exascale systems such as Frontier, and scientific instruments to enable a steerable, smart, high-throughput "lab of the future" environment through an LDRD initiative.

ORNL has a long history in translating discoveries in materials science to practical uses and deployment. The key challenges in the deployment of carbon capture and conversion are to reduce the cost and make it scalable. ORNL's carbon R&D LDRD initiative will address this challenge by developing the foundational knowledge to demonstrate scalable, reactive electrochemical membranes for CO_2 separation and conversion in a device-scale system. Together, the INTERSECT and carbon R&D LDRD initiatives will establish an autonomous chemistry lab and integrate ORNL's strengths in computational chemistry, in situ neutron characterizations, and advanced manufacturing to codesign the permeability, selectivity, reactivity, and chemical/electrochemical stability of carbon capture and conversion materials. These capabilities could be further extended to accelerate development of novel catalysts and electrochemical pathways for nitrogen reduction and hydrogen production.

As another element of ORNL's efforts towards carbon reduction, the Climate Change Science Institute (CCSI) facilitates innovation and interdisciplinary approaches for development of climate models and weather forecasting. We are integrating AI-driven synthesis of multimodal data (e.g., remote sensing, weather data) with HPC-enabled Earth system models (ESMs) to determine pathways to net-zero carbon emissions and to inform appropriate mitigation strategies, opening new areas of research at the intersection of climate change and adaptation, biology, and clean energy.

The Quantum Science Center (QSC) at ORNL harnesses the facilities and expertise of the laboratory and its partner organizations to overcome key roadblocks in quantum state resilience, controllability, and ultimately the scalability of quantum technologies. ORNL's core capabilities and world-leading user facilities provide unparalleled scientific instruments to support the quantum community in the discovery and development of quantum science and technology, advancing quantum devices and ensuring US scientific leadership and national security. We will advance heterogenous quantum/classical computing through the development and benchmarking of scalable fault-tolerant algorithms and provide access to a variety of qubits through the Quantum Computing User Program at the OLCF.

The Manufacturing Demonstration Facility (MDF) is an open innovation center where subject matter experts work with industry and academia to advance materials and manufacturing. The Carbon Fiber Technology Facility (CFTF) is an export-controlled facility enabling production of carbon fiber as well as development of new materials and manufacturing processes for some defense programs. ORNL is building off the successes of MDF and CFTF to enable national security missions.

As ORNL expands and enhances its scientific capabilities and diverse workforce talent and strengthens partnerships with its core universities and regional Historically Black Colleges and Universities (HBCUs) and Minority-Serving Institutions (MSIs), we will leverage the strategies described in this section to solve scientific challenges, to promote equitable regional energy transitions, and to continue to position the nation as the world's leader of innovation.

Infrastructure

Overview of Site Facilities and Infrastructure

Located 10 miles southwest of the city of Oak Ridge, Tennessee, ORNL occupies about 4,421 acres of the federal Oak Ridge Reservation (ORR; 34,000 acres). Annually, ORNL hosts approximately 35,000 people, comprising UT-Battelle's roughly 5,400 employees, other prime contractors' staff, subcontractors, and guests. To support its R&D missions, ORNL provides a wide variety of on-site services, including operation and maintenance of all supporting utilities and infrastructure, 24/7 security, dedicated fire and emergency response, medical facilities, fabrication and assembly services, a guest house, and other support functions. Work is performed in 182 operational buildings (4.4 million gross sq. ft. [GSF]) owned by the DOE Office of Science (SC) and 75 operational buildings (0.37 million GSF) owned by DOE's Office of Environmental Management (EM). Seventy-two buildings in shutdown status, owned by SC and EM, represent 1.2 million GSF of ORNL's building inventory. A total of 37 SC-owned buildings (1.03 million GSF) are awaiting disposition, having been excessed to DOE, and 11 SC-owned buildings, 1 NE-owned building, and 1 EM-owned building (1.08 million GSF) are in a standby status, awaiting repurpose or reuse. All SC mission-unique facilities (1.0 million GSF) have an adequate condition rating. Of SC's nonmission unique facilities, 93% are rated adequate, with the balance rated substandard. Building 4500N (363,758 sq. ft.) is the largest substandard building on campus, with $2.6 million in operating costs and repair needs of $15 million. This facility and aging plantwide utility systems (i.e., substandard Other Structures and Facilities [OSFs]) are important focus areas for modernization.

Research requiring ready access for industrial partners is conducted in 10 off-site leased facilities totaling 0.32M GSF. ORNL's Hardin Valley Campus, about 7 miles from the main campus, hosts the Manufacturing Demonstration Facility (MDF); the Battery Manufacturing Facility; and the National

Transportation Research Center. The Carbon Fiber Technology Facility is located at a separate site in Oak Ridge about 5 miles from the main campus. In pursuit of optimal support for mission needs, ORNL's leased space portfolio is evaluated frequently to identify consolidation and reduction opportunities. The 2020 evaluation indicated there were no opportunities to consolidate therefore no change was made to the leased space portfolio. ORR land use is governed by the current ORR Land Use Plan (*Oak Ridge Reservation Planning: Integrating Multiple Land Use Needs. FY 2012 Update*, DOE/ORO/2411, ORNL, Oak Ridge, Tennessee), and ORNL's *Site Wide Master Plan* which can be found at https://services.ornl.gov/ronweb/Media/ORNLswmp.pdf.

Campus Strategy

ORNL's campus strategy is to develop new assets, revitalize existing assets, and sustain facilities and infrastructure to advance scientific missions. Success of this strategy relies on achieving three primary objectives:

1. Support science missions, initiatives, and critical programs.
2. Establish a modern, adaptable support infrastructure.
3. Reduce excess facility liabilities and footprint.

These objectives will be accomplished, in part, by successfully addressing critical infrastructure needs identified through ORNL's Mission Readiness process, culminating in the planned investments shown in Fig. 6.1. At ORNL, space is an institutional resource and a strategic asset. Space is managed to underpin the delivery of ORNL's campus strategy. Clear understanding of design, limitations, and utilization is leveraged to provide efficient solutions. Space utilization in support of scientific initiatives is maximized by co-locating and consolidating scientific disciplines, thus creating synergies in support of ORNL's vision to become the world's premiere R&D laboratory. ORNL is continuing to evaluate the impact of teleworking on office space needs and has paused new office building and campus parking additions until the evaluation is complete.

ORNL is implementing a Net-Zero Carbon Campus initiative to demonstrate a variety of technologies that eliminate carbon emissions. The strategy will require the deployment of new nuclear generation, electrical storage, carbon capture, integration of renewables, and other technologies, such as use of an electrical vehicle fleet. The Oak Ridge Reservation (which includes ORNL and Y-12) is a small city and an ideal site for demonstrating and deploying carbon neutral approaches. The Tennessee Valley Authority is evaluating options for deployment of a small modular reactor at its Nuclear Regulatory Commission (NRC)-licensed site, which would provide carbon-free electricity to the reservation and the region. ORNL's work in areas such as energy storage, carbon capture, and dynamic electric vehicle charging enables the demonstration of these technologies at scale. Additionally, investments in the deployment of an all-electric vehicle fleet and the electrical infrastructure on the site will reduce emissions and increase efficiency. These and other approaches are envisioned to achieve ORNL's goal of achieving net-zero emissions.

Figure 6.1 illustrates ORNL's vision that combines DOE and institutional investments needed to advance the laboratory's scientific and technical capabilities and continue transforming the ORNL campus into modern research space.

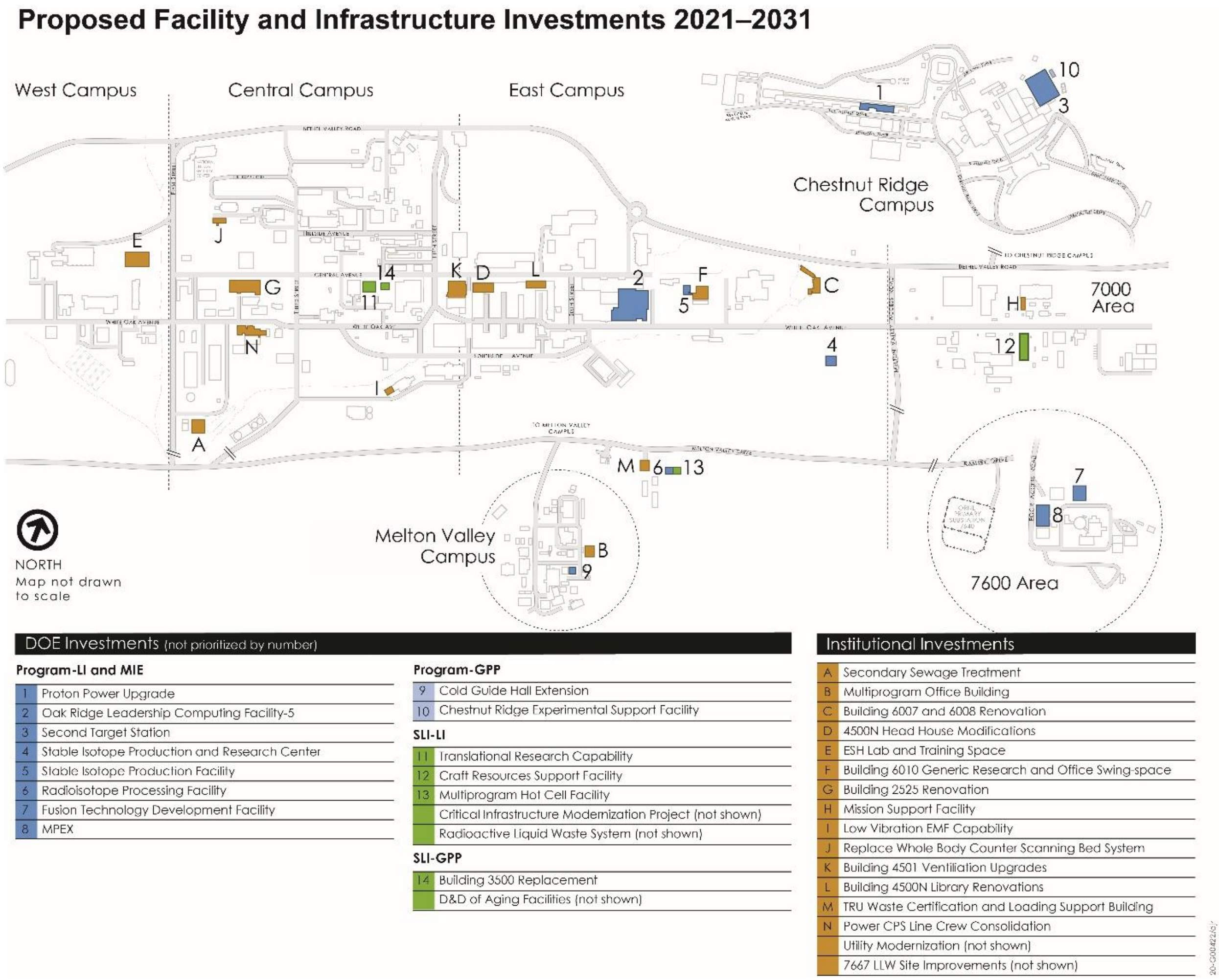


Figure: Proposed facility and infrastructure investments 2021-2031

Key facilities and infrastructure investments are crucial for successful delivery of ORNL's science strategies. These key investments shown in Figure 6.1 are summarized below.

Six programmatic line item construction projects:

- Spallation Neutron Source (SNS) Proton Power Upgrade (PPU) project, supported by DOE SC Basic Energy Sciences (BES) (CD-2/3 approved)
- SNS Second Target Station (STS), supported by BES (CD-1 approved)
- Stable Isotope Production and Research Center (SIPRC), supported by the Office of Isotope R&D and Production (IP) (CD-0 approved, CD-1 in process)
- Radioisotope Processing Facility, supported by the IP (CD-0 was approved on April 29, 2021)
- Fusion Technology Development Facility, supported by DOE SC Fusion Energy Sciences (FES) (proposed for FY 2025)

One lease-to-own leadership-class computing systems:

- Oak Ridge Leadership Computing Facility (OLCF)-5 (Frontier), supported by DOE SC Advanced Scientific Computing Research (CD-3 approved)

Two Major Item of Equipment (MIE) projects:

- Stable Isotope Production Facility (SIPF), supported by IP (PD-2/3 approved, progressing to PD-4 Q3 FY 2025)
- Material Plasma Exposure Experiment (MPEX), supported by FES (CD-3a approved)

Five Science Laboratories Infrastructure (SLI) line item (LI) construction projects:

- Translational Research Capability (TRC) (CD-2/3 approved)
- Craft Resources Support Facility (CRSF), (CD-1 approved, status delegated)
- Radioactive Liquid Waste System (CD-0 approved)
- Critical Infrastructure Modernization Project (CD-0 approved, CD-1in process)
- Multiprogram Hot Cell Facility (proposed)

Two programmatic General Plant Projects (GPPs):

- High Flux Isotope Reactor (HFIR) Cold Guide Hall, supported by BES (proposed for FY 2022)
- Chestnut Ridge Experiment Support Facility, supported by BES (proposed for FY 2022)

Two SLI GPPs:

- Building 3500 Replacement (proposed for FY 2023–FY 2024)
- Decontamination and Decommissioning (D&D) of Aging Facilities (proposed for FY 2023–FY 2024)

These projects, as well as numerous smaller projects supported through Institutional GPP (IGPP) funding, are discussed in detail below.

Objective 1: Advance Science and Energy Leadership

Our campus strategy focuses on five areas of infrastructure investment to advance ORNL's science and energy leadership and enable accomplishment of major initiatives described in Section 4.

Maintain and strengthen global leadership in neutron sciences

Continued operation of SNS and HFIR as world-leading neutron scattering user facilities requires two major programmatic investments. The PPU project at SNS will increase power delivered to the First Target Station to 2 MW, increase neutron flux on available beamlines, and provide additional proton pulses to support operation of the STS. The addition of the STS will provide ORNL with three complementary neutron sources, ensuring US leadership in neutron sciences into the foreseeable future. HFIR has operated for 55 years and is a key scientific asset. In response to the September 2020 Basic Energy Sciences Advisory Committee (BESAC) report, DOE-SC has approved the mission need statement for the replacement of the reactor pressure vessel and other major components for long-term sustainment of HFIR capabilities. Upgrading HFIR with a new pressure vessel and making strategic facility improvements will improve and extend the reactor's capabilities for at least another half-century at a fraction of the cost of new construction.

Growth in the use of ORNL's neutron scattering facilities will increase demands on research support functions, requiring an infrastructure investment of $9 million for the GPP-funded HFIR Cold Guide Hall Extension. The extension will allow us to optimize neutron instrumentation, expand capabilities, and properly store samples. GPP funding is also requested for an experimental support facility at Chestnut Ridge to accommodate increasing demand for interdisciplinary research.

Deliver exascale computing from system to ecosystem

Leadership-class computing underpins nearly all scientific disciplines. Thus, continued development of ORNL's HPC infrastructure as part of the OLCF is a high priority. DOE's well-defined path to maintain leadership in HPC includes continued operation of the pre-exascale Summit machine (OLCF-4) in 2021 and acquisition, installation, and operation of an initial exascale system, Frontier (OLCF-5), in 2021–2022 located in the former Titan location in Building 5600. To leverage significant prior investments in power and cooling systems, a new mechanical plant is located in Building 5800, and new power feeders from the 7640 substation will increase power and cooling for the computing complex. Construction of the TRC facility will provide additional resources for housing novel capabilities in quantum and neuromorphic computing. To support SC's goal of delivering exascale computing and data curation for scientific instruments and sensors, ORNL has created the Scalable Data Infrastructure (SDI) initiative to capture, store, and curate data and metadata from various sources in scalable fashion, for which institutional investments are planned for high-bandwidth network capability.

The ESNET 400G upgrade will require campus redundant border routers, new fiber optic cables and upgraded border routers. ORNL has initiated the replacement of older router technology and core fiber technology to be installed in FY 2022. Beyond this, the INTERSECT initiative will be supported by targeted investment in building connectivity to meet scientific mission demands and 400G requirements. High bandwidth, low latency connectivity between supercomputer (e.g., Summit and Frontier) and the edge (e.g., edge devices at SNS, CNMS, MDF, etc.) will be driven by the need to use the supercomputer to build AI models from data generated from many edges. Additional upgrades to WANs and LANs will be required to address connectivity between Central campus and Chestnut Ridge campus, Hardin Valley campus and other parts of ORNL where edge deployments are desired.

5G technology is permeating communications networks and represents the next step in wireless high bandwidth applications. ORNL continues to lead in studying emerging technologies with a long-running working group focused on next generation wireless communication. We are establishing a 5G test bed and expect to make other 5G investments in FY 2022 to evaluate use cases in operations as well as scientific applications.

Discover and design next-generation materials and chemical processes for energy

Accelerating design, discovery, and deployment of new materials and manufacturing processes requires specialized instrumentation and facilities. Over the past 5 years, ORNL has made discretionary investments to secure new, world-class tools for materials science, including a secondary ion time-of-flight mass spectrometer, a MAC-STEM, an x-ray tomography system, and a low-temperature four-probe scanning tunneling microscope. Further investments are planned to support the Quantum Science Center (QSC) for the quantum materials and QIS initiative. To support increasingly sensitive imaging equipment, institutional funds have been allocated to provide a low-vibration, low-electromagnetic field space. In preparation for the TRC facility, a $93 million investment, ORNL has successfully completed CD-2/3 approval.

Advanced manufacturing is an important component of our materials portfolio. The MDF houses integrated capabilities to assist industry in adopting new manufacturing technologies and provides a gateway to expertise in materials synthesis, characterization, and process technology. SC-funded Nuclear Facility operations within the Isotopes and Nuclear Materials Complex (INMC) also support these investments.

Advance the fundamental science, engineering, and integrated technologies to accelerate the deployment of fusion and advanced fission energy

ORNL's nuclear capabilities support a broad range of efforts: several SC programs (NP, FES, and BES), other DOE programs (NE and NNSA), and other sponsors in areas that span fission energy technologies, fusion R&D for plasma-facing materials and fuel cycle, radioisotope production and R&D, and nuclear security. These capabilities are dependent on the following:

- *HFIR operation as a high-flux irradiation source.* Continued success in this area depends on sustained programmatic operations support, new fuel fabrication, spent fuel shipment, and annual funding to perform necessary planned maintenance and life extension projects. Investments above fixed operating costs will be required to address fuel fabrication and inspection process improvements as production activities resume by BWX Technologies. In addition, a new permanent beryllium reflector and four, new beam tubes are being fabricated in preparation for the beryllium reflector replacement outage schedule to start in FY 2024 with an anticipated completed in FY 2025.
- *INMC operation for radioisotope production and for processing and handling of irradiated and nuclear materials*. INMC comprises five nonreactor nuclear facilities, including the Radiochemical Engineering Development Center (REDC), four primary radiological facilities, and various research and support facilities in Bethel and Melton valleys. Significant program growth, particularly in isotope production, is challenging the capacity of the INMC. A mission-oriented steward that consistently funded INMC operation would ensure long-term sustainability and compliance with DOE's nuclear safety standards.
- *The Material Plasma Exposure Experiment (MPEX) project*. MPEX, which has received CD-1 and CD-3A approval, will be a key tool in understanding plasma-surface interactions, and ultimately, the performance of divertor and plasma-facing materials. ORNL continues to place high priority on the execution of the MPEX project leading to the successful construction and commissioning. Resources are being prioritized to assist project execution as needed. Institutional investments, including replacement of the cooling water tower, are planned to support MPEX and other experimental facilities in the immediate area.
- *Fusion Prototypic Neutron Source.* A fusion prototypic neutron source has been identified by the American Physical Society Division of Plasma Physics Community Planning Process as a high-priority facility for fusion energy and has also been endorsed by the recent Fusion Energy Sciences Advisory Committee (FESAC) report. Options to repurpose existing ORNL facilities are being evaluated, but utilities would be required. ORNL is ready to support a mission need statement and identification of potential approaches when the sponsor is ready to move forward.
- *Fusion Technology Development Facility.* ORNL is developing plans for the Fusion Technology Development Facility (proposed for 2025), enabling advancement in several key fusion technology areas. This plan will require investment in a facility with multiple flexible laboratories, high bay space, and sufficient utilities to support a diverse R&D program.
- *Multiprogram Hot Cell Facility (MHCF).* ORNL is proposing a new Hazard Category 2 R&D facility to replace nuclear and radiological facilities in the Central Campus scheduled for deactivation and decommissioning by DOE-EM between 2030 and 2035. R&D in the areas of radioisotope applications, radioisotope processing methods, fusion materials, and nonproliferation science are currently enabled by 3025E, and radiological facilities such as 4501/4505 will be curtailed once they are transferred to DOE-EM.

Providing strategic capabilities in isotope R&D and production

The DOE Isotope Program makes extensive use of ORNL's research and production facilities: HFIR, the Enriched Stable Isotope Prototype Plant (ESIPP), and INMC (including REDC).

- *Stable isotope portfolio.* To meet demand for critical isotope production and to eliminate national dependence on foreign suppliers, ORNL proposes to complete the SIPF MIE by 2025 and to continue to expand stable isotope research and production capabilities through several major initiatives. SIPRC, which received CD-0 approval in FY 2019 with CD-1 in process, will greatly expand research and production capabilities for stable isotopes using several different enrichment technologies. In close association with SIPRC, ORNL proposes to optimize all aspects of the stable isotope portfolio, including electromagnetic, gas centrifuge, and other isotope enrichment technologies; R&D and other supporting laboratories; stable isotope storage and dispensing operations; and technical services for preparing special isotope forms through physical and chemical conversions.
- *Radioisotopes.* Continued growth in demand for ORNL radioisotope production is anticipated to meet multiple needs in areas such as basic science, applied R&D, and medical applications. The proposed Radioisotope Processing Facility (CD-0 was approved on April 29, 2021) will eliminate the capacity gap introduced with increased demand and will provide wider availability and improved quality assurance for multiple emerging reactor-produced radioisotopes. Eliminating this capacity gap allows for increased radioisotope production in support of the entire DOE complex and other needs.

Objective 2: Establish a Modern Adaptable Infrastructure to Support Research

The cornerstone of this objective consists of strategic investments that optimize, modernize, and sustain facilities and utility systems to best accomplish current and future ORNL missions. ORNL fosters safe, efficient, reliable, and environmentally responsible operations through targeted investments.

Modernization of ORNL's utility systems: Reliable, efficient, and maintainable utility infrastructure provides the foundation for successful scientific achievement. Uninterrupted reliable operation of ORNL utilities underpins modern scientific tools used to support cutting-edge research that drives technological breakthroughs. ORNL has consistently provided a high level of service through routine preventive maintenance and continued institutional investments. However, many of ORNL's core utilities were installed as part of the Manhattan Project and are becoming increasingly inefficient and difficult to maintain. Aged infrastructure requires more frequent emergency repairs, which are complicated by the need to secure obsolescent parts. These factors ultimately culminate in decreased reliability, increasing inefficiency, and escalating costs. To correct the highest risk utility system deficiencies identified by utility system stewards through condition assessments and inspection, an SLI-LI is proposed for FY 2023 (CD-1 in process). ORNL will implement both enabling structures and technologies to drive adoption of ML/AI capabilities in the CIMP project. The IGPP-funded secondary sewage system, slated for completion in FY 2024, will provide much needed increased capacity and improve operational efficiency by reducing costs associated with outdated and deteriorated equipment. Additional institutional investments are being made in the 7600 area and Central Campus to support research activities and improve utility distribution systems, thus providing interconnections for redundancy.

Revitalization of mission support campus: ORNL's 7000 area is a centralized craft asset supporting research and laboratory operations. This campus area hosts multiple craft shops and services, centralized and colocated security and fire response personnel, and 600 craft personnel. Institutional investments are funding the construction of a new Mission Support Facility that will provide an environmentally controlled, conditioned workspace. Additional infrastructure modernization funded by IGPP to address roads, parking, and sidewalks will be completed in FY 2022.

The Craft Resources Support Facility, which received CD-1 approval (status delegated) in April 2020, will provide modern facilities to include vehicle garage and shops for sheet metal workers, carpenters, mechanics, and electricians. This new facility will eliminate current infrastructure capability gaps such as inadequately designed aging infrastructure, insufficient storage capacity, and poor environmental controls needed to maintain high value equipment and materials. The CRSF will also enable the D&D of 10 or more 1950s vintage facilities, eliminating the high cost required to maintain and operate aging buildings.

Repurposing space to maximize utilization: ORNL continues to maximize utilization by repurposing and modernizing existing facilities. Institutional investments have repurposed an old data center in Building 4500N to modern swing office space. Warehouse facilities in the 7000 area have been converted to much needed conditioned storage space, while work is underway to continue Building 6010 modernization. Additional institutional investments planned to modernize and maximize space utilization in Building 4500N include: headhouse modernization, library renovation, and renovation of Wings 1 and 2.

Management of radioactive waste: Historically, ORNL has relied on EM infrastructure for management of gaseous, liquid, and transuranic waste from nuclear and radiological facilities. EM infrastructure is 30–60 years old, oversized, and not designed for the waste generated by today's isotope production and nuclear R&D missions. EM plans to shut down portions of existing infrastructure once legacy waste missions are completed. With this in mind, ORNL is developing independent waste management capabilities to achieve self-sufficiency. IGPP investments have created a remote-handled waste loading station at REDC. Building 3525 investments to construct a local high-efficiency particulate air filtration system and exhaust ventilation stack will enable independence from the EM-operated central stack in early FY 2022. As EM completes its transuranic mission in Oak Ridge in 2022–2023, ORNL SC needs to acquire storage facilities from EM and adapt this space for packaging transuranic waste. Future infrastructure investments will be needed, most notably a liquid waste treatment capability for high-activity radioactive liquids, which will require an SLI LI in the FY 2026–FY 2028 timeframe and is dependent on the EM schedule. The mission need (CD-0) for this capability has already been approved. Effort over the past few years has been devoted to waste minimization to reduce the capital investment for this capability. Institutional investments are also planned for FY 2022 to construct a TRU waste Certification and Loading Support Building to support WIPP campaigns and to: provide loading capabilities, dose-to-curie measurements, and flammable gas analysis. To improve efficiency, institutional investments are planned for site improvements at the 7667 liquid low-level waste (LLW) area to consolidate waste handling operations.

Objective 3: Reduce Excess Facility Liabilities and Footprint

ORNL currently expends approximately $2.5 million annually to address environmental and safety risks associated with excess SC facilities. ORNL's rationale in prioritizing facilities for demolition is based on:

- removing significant risks and liabilities;
- enabling future development by clearing aging facilities from prime locations; and
- eliminating assets which are unlikely candidates for renovation due to age, condition, and deferred maintenance (DM).

Working with DOE's Excess Contaminated Facilities Working Group, ORNL has prioritized excess facilities into four groups: (1) ORNL-managed SC and NE facilities at Y-12, (2) SC facilities in ORNL's Central Campus, (3) 7000-area facilities, and (4) balance of buildings for demolition.

SC and NE facilities at Y-12: Due to deteriorated condition and size, ORNL facilities at Y-12 represent the highest ORNL cost risk. EM has demolished 9207A and 9210 and is preparing to complete the Biology

Complex demolition with Building 9207, followed by preparation of Buildings 9201-2, 9204-1, 9401-1, 9422, and 9732-2 for demolition.

SC facilities in ORNL's Central Campus: A prime location for future development, the Central Campus houses several excess facilities awaiting demolition. The presence of these aging facilities hinders mission delivery and modernization while increasing liabilities and risks. Modernization of this campus area will be most quickly enabled when facility demolition is accompanied by associated contaminated soil removal, allowing for immediate redevelopment. Continuation of a strong EM funding profile is key to ensuring ORNL's ability to deliver on its mission. EM actions to complete the cleanup of the Central Campus, in parallel with investments in modernization by SC and ORNL, are enabling future mission assignments. ORNL has transferred operational responsibility of several SC-owned buildings to EM in preparation for demolition (Buildings 3003, 3010A, and 3080 in 2019; Buildings 3034 and 3036 in 2020). EM is currently removing the 3026 C&D hot cells and is planning for the removal of Isotope Row facilities, and the research reactors (Buildings 3005, 3010, and 3042) in Central Campus. ORNL actively coordinates with EM contractors to remove barriers. ORNL's plan for this campus is the construction of a series of modern facilities built upon a revitalized utility infrastructure. Planned actions include (1) construct TRC, (2) replace aging facilities, and (3) vacate and demolish 1940s-era facilities.

1. *Construct TRC:* The TRC facility will be constructed in the 3000 area of the ORNL campus, providing world-class, highly flexible, and collaborative laboratory facilities to support advances in computing, materials science, and multidisciplinary research areas. TRC construction will also enable deployment of exascale computing by freeing up space in Building 5800. ORNL has received CD-2/3b approval.

2. *Replace aging facilities:* A proposed FY 2023 SLI GPP investment will provide modern space for staff currently housed in Building 3500, a 1950s-era facility in the Central Campus area. Demolition of Building 3500 will also eliminate $2 million in DM.

3. *Vacate and demolish aging mission support facilities:* Upon completion of the Research Operations Support Center (ROSC), ORNL has vacated the fire station (Building 2500) and the Protective Force station (Building 3037). Three other Central Campus buildings (Buildings 2518, 2523, and 2621) are all more than 55 years old.

7000 area facilities: Demolition preparation work continues to take place in FY 2021 to make way for construction of the CRSF. Facilities slated for demolition in FY 2021 to clear space for construction of the CRSF include Buildings 7033, 7035, 7035A, 7035B, 7035C, 7035E, 7035F, 7062, 7070, and 7082. Extensive underground utilities will also be removed for utility upgrades.

Balance of buildings for demolition: SC transferred operational responsibility of Buildings 7600, 7609, 7610, and 7014 to EM to prepare for demolition. Buildings 7914, 7914A, and 7915 have also been demolished at the Melton Valley campus. ORNL continues to clean up and dispose of abandoned facilities and experiments throughout its campus. For example, Building 2644 is being prepared for demolition to support the construction of the new Sewage Treatment Facility.

Future Infrastructure Gaps within a 10-Year Window

Anticipated future infrastructure gaps include:

- New greenhouse space to support secure biosystems design, biodesign goals, robotics systems for automated sampling, mass spectrometry, and advanced, high-throughput imaging equipment.

- Additional space to optimize all aspects of the stable isotope portfolio by consolidation of existing small-scale enrichment science, engineering, and technical services activities across the ORNL campus into the 6000 area to enable more efficient enrichment research and production.
- New INMC engineering, maintenance, and support capabilities will be required to replace current capabilities in Central Campus buildings 3025E, 3104, and 3502 that are to be turned over to DOE-EM in 2030. Addition of the RPF will require expanded manipulator capabilities as the existing building 7935 manipulator shop will be fully utilized by REDC. A mix of conventional and radiological space will be required. A proposed study to define the need for facility and infrastructure to house classified computing, labs, and additive manufacturing.

Infrastructure Investment Summary

A detailed investment profile by year is provided as a separate enclosure ("Infrastructure Investment Table"), including all ongoing and planned capital investments by funding type and source. Over the last 18 years, institutional investments have been the predominant funding mechanism for continued site modernization. Since FY 2002, when ORNL began using IGPP for core infrastructure improvements, 103 projects have been completed at a total cost of $258 million. Over the next decade, we expect to continue investing $25–$30 million per year in infrastructure to recapitalize and sustain aging assets, some of which are 75 years old. Funding priorities for disposing of excess facilities are identified in Section 6.2.

Maintenance and repair investments are between 2% and 4% of the replacement plant value. Forty-two percent of ORNL's operational nonmission-unique facilities, representing approximately 51% of the total GSF, are more than 50 years old and carry nearly 93% of DM. ORNL will continue to demolish shutdown assets that carry a high DM.

Site Sustainability Plan Summary

The ORNL Site Sustainability Plan (SSP), submitted in December 2020, fulfills ORNL's commitment to deliver a complete and accurate SSP and quality performance data for entry into the DOE Sustainability Dashboard. Major efforts include the following:

- Greenhouse gas (GHG) emissions have been reduced by 29% from the FY 2008 baseline.
- Energy use intensity (EUI) has decreased by 34.9% since FY 2003 and by 1.4% since FY 2019, exceeding the 1.0% year-over-year reduction target.
- Water use intensity (WUI) has decreased by 24.9% from FY 2007, yet increased by 20.9% from FY 2019, missing the 0.5% year-over-year target. In FY 2020, HFIR returned to service from an extended outage in FY 2019, contributing to the year-over-year increase from FY 2019 consumption. Changes in HPC and associated mission-specific growth also contributed to FY 2020 increases. ORNL will continue to aggressively identify and repair leaks and seek creative solutions to reduce consumption.

High Performance Sustainable Buildings (HPSBs)

ORNL's on-site HPSB inventory included a total of 22 buildings that are certified by either being grandfathered through LEED certification or having attained 100% of the HPSB Guiding Principles.

Energy Savings Performance Contracts (ESPCs)

The ESPC with Johnson Controls is in its ninth performance period. DOE, Johnson Controls, and ORNL regularly meet to review performance. The Year Eight Performance Period identified annual savings of 324,423 million Btus of electricity, natural gas, and fuel oil and 187 million gallons of water, all of which contribute to lower EUI and WUI.

High Energy Mission-Specific Facilities (HEMSFs) Electrical Use with Projections

The current and projected electrical energy consumption by ORNL's Base Facilities and HEMSFs are shown below. HEMSF energy consumption accounted for 66% of ORNL's total energy use in FY 2020. It is expected to grow to 81% of total electrical energy use by FY 2032 based on projections for HPC expansion and STS. The FY 2020 HEMSF reductions are due to the retirement of the Titan supercomputer yet offset by the increase in operations for the SNS Process and HFIR as these systems returned to a normal operating schedule. Research in general continued at ORNL with limited on-site personnel despite COVID-19 impacts.

The power usage increases in FY 2026 and FY 2031 are based on the assumption that multiple HPC systems will be running concurrently as one system is decommissioned and a new system is installed. The forecast assumes no large increase in power due to SPP projects.

Renewable Energy Credit (REC) cost projections

In FY 2020, ORNL purchased 47,400 MWh of renewable energy credits or certificates to supplement on-site renewable energy generation, representing 9.2% of the laboratory's electrical energy consumption, exceeding the current DOE target of 7.5% renewable energy as identified in the Energy Policy Act of 2005. As ORNL's mission grows, specifically in HPC and neutron scattering (PPU and STS), the quantity of RECs purchased will increase to meet or exceed the DOE/EPA targets unless ORNL develops significant on-site renewable energy generation capabilities. ORNL continues to look for renewable energy projects and research opportunities.

PACIFIC NORTHWEST NATIONAL LABORATORY

Lab-at-a-Glance

Location: Richland, Washington
Type: Multi-program Laboratory
Contractor: Battelle Memorial Institute
Site Office: Pacific Northwest Site Office
Website: www.pnnl.gov

- **FY 2020 Lab Operating Costs:** $1,058.2 million
- **FY 2020 DOE/NNSA Costs:** $766.7 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $222 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 27.5%
- **FY 2020 DHS Costs:** $69.5 million

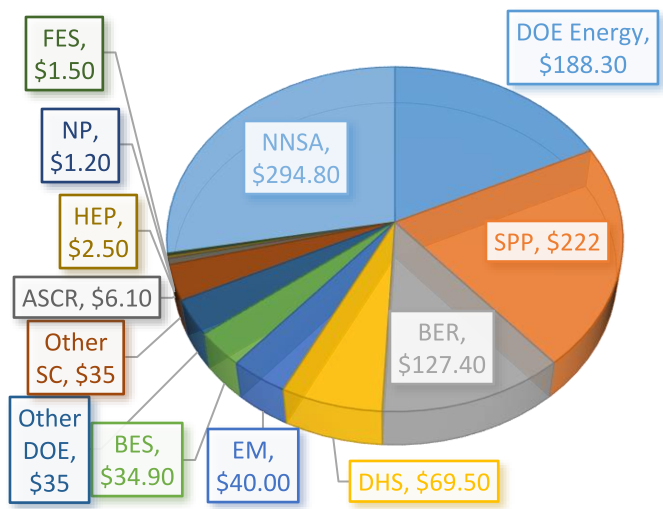
Physical Assets:

- 549 acres and 86 buildings (DOE & Battelle Facilities)
- 1,188,747 GSF in buildings
- Replacement Plant Value: $1.153B
- 983,731 GSF in 30 Leased Facilities
- 168,050 GSF in 16 Battelle Buildings

Human Capital:

- 4,623 Full Time Equivalent Employees (FTEs)
- 83 Joint Appointments
- 313 Postdoctoral Researchers
- 435 Graduate Student
- 338 Undergraduate Students
- 1,767 Facility Users
- 136 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

Pacific Northwest National Laboratory (PNNL) draws on signature capabilities in chemistry, Earth sciences, biology, and data science to advance scientific discovery and create solutions to the nation's toughest challenges in energy resiliency and national security.

As a Department of Energy (DOE) Office of Science (SC) laboratory, PNNL focuses on discovery science. In chemistry, we design catalysts and chemical pathways for new fuels, feedstocks, and energy storage materials. In Earth sciences, we work to improve the predictive power of DOE's Earth system models, emphasizing Earth systems in transition. In biology, we seek to understand, predict, and control the phenotypes of biological systems to produce desired functions and products. In data science, we combine machine learning (ML), data visualization, and modeling to create new knowledge from "Big Data." PNNL also operates two DOE user facilities—the Environmental Molecular Sciences Laboratory (EMSL) and the Atmospheric Radiation Measurement (ARM) user facility.

PNNL research enhances energy resiliency by applying our knowledge of North American grid situational awareness and high-performance contingency analysis to design, test, and evaluate technologies for security and optimization. We apply our chemistry and materials science capabilities to develop advanced energy storage solutions for grid resiliency.

We integrate our expertise in data sciences, chemistry, biology, and nuclear science to address the national security challenges of detecting weapons of mass effect, accelerate nuclear materials characterization, advance non- proliferation and nuclear forensics, automate threat analysis for greater intelligence, secure our borders, and protect critical infrastructures from cyberattacks.

PNNL is on track to meet a 10-year goal of investing more than $250M in internally funded facilities recapitalization by 2025 and has committed itself to becoming a net-zero (NZERO) emissions DOE laboratory.

Core Capabilities

PNNL's ability to meet changing DOE needs relies on the strength of 19 core S&T capabilities resident at the Laboratory. Eighteen of these core capabilities are discipline-based and are grouped into four categories—Biological and Earth Sciences, Chemical and Materials Sciences, Engineering, and Computational and Mathematical Sciences. The nineteenth capability, User Facilities and Advanced Instrumentation, supports two DOE-SC BER user facilities managed by PNNL—EMSL and ARM.

PNNL's *Integrated Capability Management (ICM) Program Description Document – April 2021* provides a complete description of our capability health assessment process and the underlying data sources. Wherever possible, PNNL has chosen indicators that are quantifiable and comparable across laboratories. A brief summary of relevant highlights of this assessment is included as the last paragraph discussion of each core capability below.

One of the most important functions served by a DOE national laboratory within the U.S research ecosystem is that of integrating a diverse set of scientific disciplines, sponsor needs and funding streams, and practical problems requiring S&T solutions. It is at the intersection of these that the most significant breakthroughs occur, and from which discoveries with the most far-reaching impact originate. One way to illustrate the vibrancy of this interaction of ideas, capabilities, and research at PNNL is through the lens of sponsor support for our core capabilities.

Chemical and Materials Sciences

Chemical and Molecular Sciences

Chemical and molecular sciences advance the understanding, prediction, and control of chemical and physical processes in complex, multiphase environments. PNNL has significant domain expertise in condensed phase and interfacial molecular science, chemical physics, catalysis science, chemical separations, geochemistry, theoretical and computational chemistry, physical biosciences, and heavy element chemistry. This core capability has strong ties to the Condensed Matter Physics and Materials Science, Computational Science, and Applied Mathematics core capabilities, leveraging expertise in those areas to advance our understanding of complex phenomena at interfaces and produce high-fidelity simulations of molecular processes controlling macroscopic phenomena. A key strength of our chemical and molecular sciences capability is the close and purposeful integration of experiments and theory, achieving rapid feedback for understanding and control of interactions, transport, and reactivity in multiphase, multicomponent systems. Connections to data science are growing as well, to increase our rate of predictive learning.

The Laboratory has the largest fundamental research effort within the national laboratory system in catalysis science and condensed phase and interfacial molecular science, which provided the foundation for establishing the Institute for Integrated Catalysis. These capabilities were essential for the second renewal of an EFRC (the Center for Molecular Electrocatalysis) from DOE's BES program and an award from DOE-SC's Early Career Research Program for the Combined Capture and Conversion of CO_2 project, selected by BES. Further, a new program in direct air capture that builds on these strengths was awarded by BES. The Laboratory also has significant strength in geochemical sciences, which contributed to the successful renewal of the iDREAM EFRC. Contributing to PNNL's strength in this area is EMSL's computational chemistry software suite (NWChem), which is used worldwide to efficiently address large molecular science problems on computing architectures ranging from workstation clusters to high-performance leadership class computer architectures. A major redesign of the architecture of NWChem is under way (in the NWChemEx project, funded by ASCR) to dramatically improve its scalability, performance, extensibility, and portability to take full advantage of exascale computing technologies.

NWChemEx will target the development of high-performance computational models for the ground states of complex systems that will be used for the production of advanced biofuels and other bioproducts. Further computational capabilities targeting excited states are being designed in the Scalable Predictive Methods for Excitations and Correlated Phenomena (SPEC) project, funded by BES, which will deliver scalable, open-source electronic structure software libraries required to address challenges in excited-state and correlated phenomena in complex chemical systems, and are appropriate to interpret the signals obtained at DOE's light source facilities. Novel computational chemistry tools for catalysis, photo-induced charge transfer, and actinide chemistry studies are also utilizing emerging QIS technologies, which enables optimal design of accurate many-body frameworks that will take advantage of the evolving quantum and classical resources to describe complex electron correlation effects in molecular systems. Capability stewardship efforts, such as those proposed in the ESC project, will accelerate scientific discovery in chemical transformations by enabling close integration of synthesis with dynamic characterization capabilities and real-time computational capabilities.

This capability receives support from programs in BES, BER, ASCR, DHS, EERE (geothermal, biomass, and hydrogen; fuel cells; and infrastructure technology), the Office of Fossil Energy (FE; carbon- and co-sequestration), OE (battery chemistries), the Office of Environmental Management (EM; environmental remediation), NNSA (nonproliferation), the Department of Health and Human Services (DHHS), and DoD. In addition to our primary DOE-SC sponsor (programs in BES Chemical Sciences, Geosciences, and Biosciences), a number of applied programs rely on our chemical and molecular sciences capabilities for improvements in sustainable energy technologies, catalysis and reaction engineering, hydrogen storage, biomass conversions, environmental remediation, and carbon capture/sequestration. BER's support of EMSL capabilities also greatly enhances this core capability through the continued focus on molecular transformations that occur in complex systems (including biocatalysts), as well as at complex interfaces.

Health: The predominant sponsor is BES, with very long-term stable programs. This core capability is benefiting from strong partnerships (joint appointments and three joint institutes). A majority of the staff have been at the Lab less than five years, bringing new vitality to this important area. Some existing space shortfalls will be addressed with the construction of the ESC. ESC related equipment will significantly enhance this capability. Issues remain with respect to replacing aging workhorse research equipment.

Condensed Matter Physics and Materials Science

PNNL is an emerging leader in Condensed Matter Physics and Materials Science, a core capability that provides the knowledge base for discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for development of new materials for energy generation, storage, and conversion, as well as manipulating electronic and quantum effects and mitigating materials degradation due to environmental factors. The Laboratory has domain expertise in the synthesis of inorganic and biomolecular nanostructures and heterointerfaces, interfacial dynamics of solid-solid and solid-solution liquid interfaces, electrical energy storage, in situ electron and scanning probe microscopy, radiation effects and degradation in materials, and computational materials science. This core capability has strong ties to the Chemical and Molecular Sciences, Applied Materials Science and Engineering, Computational Science, and Applied Mathematics core capabilities. In combination, these capabilities advance our ability to understand and manipulate complex phenomena at solution-solid and solid-solid interfaces, design and direct synthesis of hierarchical matter, and develop computational tools that elucidate the mesoscale principles linking atomistic details of structure and interactions to outcomes of synthesis and function. Capability stewardship efforts enabled by the ESC project will strengthen the strategic link with our world-class efforts in the predictive design and understanding of chemical transformation processes.

The ESC project will provide close integration with the chemical and molecular sciences capabilities through emphasis on predictive synthesis of hierarchical and atomically precise materials, enabling a strategic link to this core capability through the need to translate an understanding of catalytic processes into multifunctional catalytic materials.

PNNL has a distinctive strength in the emerging science of materials synthesis, to which it brings synthesis of hierarchical and atomically precise materials, both inorganic and organic; the most advanced imaging, tomography, and spectroscopy tools, many of which are applied in situ and operando; and computational approaches that draw on PNNL's long-standing leadership in computational chemical physics, as well as new capabilities in condensed matter theory and computation. PNNL's capability is particularly strong in understanding the complexity at interfaces, specifically their role in synthesis and their control of electronic, magnetic, and quantum properties, as well as transfer of matter and energy. These strengths have advanced PNNL's research in the JCESR, an Energy Innovation Hub led by Argonne National Laboratory that was renewed at the end of FY 2018, and in CSSAS, an EFRC led by UW that was awarded in late FY 2018. The latter includes a thrust that brings together deep learning approaches for data analytics and modeling machine learning for molecular design. Most recently, this core capability has enabled PNNL to play a significant role in the Co-Design Center for Quantum Advantage, a new Quantum Information Science Research Center led by Brookhaven National Laboratory.

This capability forms the basis for PNNL's sponsor-funded, fundamental science programs in synthesis and processing, biomolecular materials, quantum information science, electron and scanning probe microscopy, mechanical behavior, and radiation effects. Applied programs to which this core capability contributes include radiation effects in materials, multiscale behavior of structural materials, design and scalable synthesis of materials and chemicals that bridge the mesoscale fuel cells and energy storage, electric and lightweight vehicle technology, nuclear reactor safety assessment, regulatory criteria and life extension, and legacy waste forms. This capability receives support from programs in BES, BER, OE, DOE Office of Nuclear Energy (NE), EERE, and NIH. BER's support of EMSL capabilities (e.g., Quiet Wing and the high-resolution mass accuracy capability) greatly enhances this core capability. Staff members are housed primarily in the Physical Sciences Laboratory, EMSL, and LSL2.

Health: This core capability is stable; however, the condensed matter physics portion is smaller than optimal and this is being addressed. Some existing space shortfalls will be addressed with the construction of the ESC.

Applied Materials Science and Engineering

PNNL's capability in Applied Materials Science and Engineering emphasizes the development and validation of materials synthesis, manufacturing, and component fabrication concepts that are relevant to DOE mission needs and readily scalable for industry adoption. PNNL has made significant contributions over the years to the commercialization of automobile catalysts, organic light-emitting devices, redox flow batteries, tailor-welded blanks, and many other zero-carbon emission energy technologies. PNNL holds domain expertise in materials characterization, and especially in situ characterization; solid phase processing approaches for the production of alloys and composites as well as the fabrication of semi-finished products; the scalable synthesis and validation of electrodes and electrolytes for emerging battery systems; materials theory and simulation, including machine learning approaches to accelerate the materials development cycle; solid oxide reactors for fuel cells and/or electrolysis; advanced polymers and composites for hydrogen infrastructure; and materials performance in hostile environments, including the effects of radiation. This capability includes the ability to engineer enabling nanostructured and self-assembled materials, as well as tailored thin films, ceramics, glasses, cements, polymers, metal alloys, and composites.

The Laboratory leverages its Applied Materials Science and Engineering capability to develop new materials and strategies to enable a variety of technology areas, including grid- and transportation-scale energy storage, renewable hydrogen production via solid oxide water electrolysis, solid-state lighting, absorption cooling, lighter-weight vehicles, next-generation reactors, magnetics, separations, and nuclear waste management. PNNL also leverages this capability to develop advanced waste forms (e.g., glass, glass-ceramic, ceramic, metallic, and cementitious), key process control models, and tactical processing strategies to assure safe and successful immobilization and processing of nuclear wastes around the DOE complex. To support these R&D efforts, PNNL has built a number of unique laboratory facilities, including high- and low-dose radiological facilities, laboratories for material synthesis and deposition, the Solid Phase Processing Demonstration Facility, the Advanced Battery Facility, and the Solid-State Lighting Test and Analysis Facility. PNNL is currently in the early construction stage for a new DOE-OE funded battery development facility. Working in collaboration with academia, industry, and other national laboratories, PNNL plays a critical role in high-impact national programs, such as BES's JCESR; FE's XMAT; HFTO's Hydrogen Materials Compatibility, H2NEW, Hydrogen Materials Advanced Research, and Million Mile Fuel Cell Truck consortia; and VTO's Battery500, Lightweight Metals, and LightMat consortia.

The Applied Materials Science and Engineering capability forms the basis of PNNL's sponsor-funded research programs in metals manufacturing; electrochemical energy storage; radiation effects in materials; multiscale behavior of structural materials; integrated computational materials engineering; gas and liquid separations; electric and lightweight vehicle technology; nuclear reactor safety assessment, regulatory criteria, and life extension; and legacy waste forms. These efforts are funded by a variety of DOE programs, including the DOE-SC (BES and FES), many of the DOE Applied Energy Offices (EERE, OE, NE, FE, EM), ARPA-E, NNSA, and the Nuclear Regulatory Commission (NRC). This capability is also leveraged in support of research programs for DoD and for the private sector through SPPs.

Health: This capability continues to be strong with multiple publications in high-impact journals and multiple national awards. Staff continue to be recognized for their technical impact by sponsors and by the professional community. However, realizing full business growth potential is hampered by difficulties in hiring at the early-career level, for added capacity, and at the senior level, for added leadership. There is a shortage of office and lab space, though these will ease as ESC and GSL are completed and brought online. A dedicated high bay space that can accommodate growing capabilities in manufacturing remains a need.

Nuclear and Radiochemistry

PNNL possesses expertise in interfacial chemistry, radiochemical separations, analytical measurement techniques, actinides, separations, irradiated materials characterization, spectroscopy, and microscopy. The Laboratory processes and measures plutonium and its fission products across a wide range of highly radioactive samples that require the use of hot cells to tiny samples that undergo ultratrace measurements in clean rooms. PNNL possesses a unique combination of in-depth knowledge of sample analysis combined with instrumentation, including a FIB and state-of-the-art measurement systems such as the Aberration-Corrected Nuclear Scanning Transmission Electron Microscope. Mission-ready instrumentation includes suites of microscopy, mass spectroscopy detection, magnetic resonance, and specialized ultra-low-background radiation detectors; numerous specialized wet chemistry laboratories; and ultratrace radio analytical and radiometric facilities, including a shallow underground lab, providing one of the largest collections of instrumentation and expertise at any single institution in the world.

At the core of PNNL's nuclear and radiochemistry capability is leadership in plutonium production and waste processing knowledge (specifically in Hanford's legacy waste), forensic signatures of plutonium production, post-irradiation examination of materials, and tritium target fabrication. This includes the development and deployment of the world's most sensitive radionuclide detection systems. A system called Xenon International won awards for its engineering accomplishments and international impact. Through mitigation of the nation's nuclear waste legacy, PNNL researchers are developing new real-time sensors and radiochemical insights to enable EM to expand waste processing operational windows, enable new treatment alternatives, and accelerate the waste processing timelines at Hanford waste treatment facilities. PNNL is also leading two international teams, one on glass corrosion and another on ancient analogs, to predict the long-term performance of glass waste forms, which are the basis for high-level waste disposal.

PNNL stewards a set of facilities unique to the DOE complex. These facilities include Hazard Category II and III nuclear assets, such as 325RPL. 325RPL has the capability to perform an extraordinary range of S&T in a fast and flexible fashion, process materials adjacent to world-class assay technology, and perform testbed scale operation with a wide operational envelope. At 325RPL, PNNL can work with micrograms to kilograms of fissionable materials and megacurie activities of other radionuclides. Programmatic support for nuclear and radiochemistry includes scientific discovery (HEP, NP, and BES) in the search for dark matter and neutrino mass. EM depends on PNNL for rapid understanding of legacy waste behaviors, pilot-scale testing and validations, and the development of new processing options. The NNSA Office of Defense Nuclear Nonproliferation R&D relies heavily on these capabilities for next-generation nuclear detection systems, along with DTRA.

Health: Aggressive hiring over the last 12 months has resulted in new, high-quality staff at all levels. This portfolio is strong in applied research and operational projects; leadership emphasis now is on growing the more fundamental aspects of the research portfolio. PNNL will be upgrading the infrastructure in 325RPL to support operations with special nuclear materials. Some short-term facility gaps exist (insufficient ventilation and glove boxes to support research). Options to address shortfalls in high bay and limited purpose space are being considered as part of the new federally owned facility in the higher hazard zone of the PNNL Richland Campus.

Biological and Earth Sciences

Climate Change Science and Atmospheric Science

PNNL has extensive experience and strengths in measuring, modeling, and understanding atmospheric and climate system processes from molecular to global scales, as well as the interactions between human activities and Earth system processes. This core capability includes activities ranging from laboratory and field measurements to multiscale numerical simulations to integrated analyses of climate impacts and response options. PNNL has domain expertise in atmospheric aerosol chemistry, cloud physics, boundary layer meteorology, land-atmosphere interactions, extreme weather, hydrology, biogeochemistry, ecosystem science, coastal system science, energy-water-land interactions, multisector dynamics, and adaptation and resilience. We leverage expertise from related core capabilities, including Chemical and Molecular Sciences; Biological Systems Science; Earth Systems Sciences and Engineering; Decision Science and Analysis; Power Systems and Electrical Engineering; Advanced Computer Science, Visualization, and Data; and User Facilities and Advanced Instrumentation.

PNNL's climate change and atmospheric science research focuses on improving our basic understanding of and ability to project changes in the Earth system and related human systems, and on developing the measurements and data-driven modeling frameworks needed to do so. Key facilities include the ARM user facilities, AAF, Atmospheric Measurements Laboratory, EMSL, MCRL, and the JGCRI (a partnership between PNNL and the University of Maryland focused on understanding the interactions among climate, natural resources, energy production and use, economic activity, and the environment). These facilities house a wide range of world-class equipment, such as a flow-through environmental chamber, cutting-edge radar systems, and manned and unmanned aerial observational systems. PNNL is also a leading developer of atmospheric, climate, land surface, coastal, and integrated human-Earth system models, including the Global Change Analysis Model, the Weather Research and Forecasting model, and the Energy Exascale Earth System Model, as well as in integrating modeling and observational systems to yield new insights into the evolution of the coupled human-environment system.

PNNL's capability includes programs in atmospheric process research, regional and global Earth system modeling, multisector dynamics, coastal and Arctic systems research, and atmospheric wind energy, along with advanced computation and data management techniques. Our observational and modeling capabilities are deployed to develop a more robust understanding of how extreme events and long-term stresses influence the Earth system and human systems, especially the energy sector and national security. This core capability is funded by programs in BER, ASCR, EERE, NASA, EPA, NOAA, and other sponsors.

Health: Key leadership gaps and staffing needs (e.g., Land Systems Modeling Team Lead, and Senior Atmospheric Scientist), as well as 20+ other open positions need to be filled. The portfolio is very strong, and equipment is good. Office space shortages are being addressed and reviewed in light of Future of Work efforts.

Earth Systems Sciences and Engineering

PNNL's Earth systems science and engineering capability researches the impacts of energy production, storage, and use on valued environmental resources and functions; develops and deploys technologies to mitigate the impacts of past, current, and future energy production systems; and develops and deploys technologies that improve the performance of energy generation and minerals extraction. This capability spans terrestrial, aquatic, and coastal ocean systems, both biological and abiotic. Applications of our expertise include Arctic and deep-ocean oil and gas, hydropower, wind power, marine and hydrokinetic generation, algal biomass production, nuclear energy, and legacy waste.

PNNL has scientists and engineers in a variety of fields, including aquatic and terrestrial ecosystems science, oceanography, biogeochemistry, hydrology, environmental engineering, and microbiology, with domain expertise in molecular-to-field-scale biogeochemistry, laboratory-to-field-scale hydrology, multiphase flow modeling, integrated (e.g., biogeochemical, physical, and ecological) aquatic modeling, aquatic acoustics and tracking technologies, ecosystem-level adaptive management, biofouling/bio-corrosion, climate-simulating culturing of algae and higher plants, minerals extraction, ecosystems modeling and restoration, human health and environmental risk assessment, and environmental systems technology development and deployment.

PNNL's marine research laboratory in Sequim, Washington, provides coastal locations and facilities that enable studies of anthropogenic impacts on marine species and systems; a controlled study area for development and testing of marine energy systems; biogeochemical, ecotoxicological, and biotechnology investigations with ambient seawater; and a platform for development and testing of autonomous and in situ marine technologies. In addition, PNNL's distinctive Aquatics Research Laboratory supports fisheries research focused on sustainable hydropower operations and development. Advanced environmental monitors and ecological sensors for conventional hydropower, wind, marine, and hydrokinetic renewable energy systems are developed and tested at PNNL's Bio-Acoustics and Flow Laboratory (LSL2). The advanced experimental and instrument capabilities of EMSL are also used to advance research in this area, with a focus in molecular-scale biogeochemistry and proteomics.

PNNL conducts research at the bench, pilot, and field-scale, integrated with advanced modeling and simulation, to provide the technical underpinnings, scientific approaches, and technological advancements to support breakthrough solutions, improve system knowledge, and champion new protocols that are protective of human health and the environment. The Earth systems science and engineering capability is funded through DOE programs in BER, BES, EM, NE, EERE, as well as NRC, EPA, DHS, BPA, Department of Interior, NOAA, and the U.S. Army Corps of Engineers.

Health: Scholarly output trend is increasing. The majority of staff have been at the Lab for less than 10 years. Leadership in this core capability benefits from strong partnerships, but attention is needed on leadership recruitment and development. The portfolio is moderately diverse, but risks exist, and diversification should be pursued. Significant infrastructure needs, including renovations and new laboratory spaces at Richland and MCRL, have been identified.

Environmental Subsurface Science

PNNL's environmental subsurface science capability focuses on developing and applying knowledge of fundamental biogeochemical reactions, thermodynamics, and mass transfer processes to the prediction and assessment of natural processes and engineered systems. PNNL provides DOE with domain expertise in molecular through-field-scale biogeochemistry, reactive transport modeling, lab-to-field-scale geohydrology, multiphase flow and geomechanical modeling, computational geochemistry, subsurface technology development and deployment, advanced geophysical monitoring, isotopic analytical capabilities, and high temperature and pressure geochemistry. Potential applications include enhanced oil recovery systems, the design and operation of carbon sequestration reservoirs and enhanced geothermal systems, technology development for nuclear waste repositories, and remediation of contaminant plumes.

For DOE-EM, PNNL applies an integrated experimental and modeling approach to resolve technical issues necessary to inform decisions for environmental remediation, waste management, adaptive site management, and long-term stewardship. PNNL leads the Deep Vadose Zone-Applied Field Research initiative, providing the technical basis to quantify, mitigate, and monitor natural processes and contaminants in the vadose zone and groundwater. Outcomes include advanced predictive, characterization, remediation, and monitoring approaches for environmental contamination and protecting human and ecological health.

This capability is also applied to numerous energy and water challenges, including sustainable energy generation, production, and use. PNNL led one of the world's first carbon storage projects into basalt formations, completing a 1,000-ton injection into the Grande Ronde basalt formation, and is exploring potential carbon storage in the sub-seafloor Cascadia basin basalt offshore of Washington State. PNNL has key roles in DOE-FE's National Risk Assessment Partnership and in the new Enhanced Geothermal Stimulation project funded by the Geothermal Technologies Office (GTO). Through its BER-funded SFA, PNNL is leading research in molecular and microscopic electron transfer processes, pore-scale reactive transport and upscaling, and field-scale microbial ecology and biogeochemistry. Staff members support programs funded by BER, BES, EM, FE, EERE (GTO), NRC, NNSA, DHS, EPA, NASA, and DoD, and have numerous active collaborations with other national laboratories and universities nationwide. Staff and capabilities are located across the PNNL campus in Richland and Sequim facilities, including EMSL, LSL1, LSL2, ISB2, Environmental Technology Building (ETB), and MCRL.

Health: The scholarly output trend is improving. Over one-half of the staff have either been at the Lab more than 10 years or are early career. Retirement of critical capability leaders is increasing, and management is actively recruiting and growing new leaders as a consequence. Portfolio diversification is increasing. Significant infrastructure needs, including renovations and new laboratory spaces at Richland, have been identified and new equipment is needed.

Biological Systems Science

Through PNNL's Biological Systems Science core capability, the Laboratory is developing a predictive understanding of complex multicellular systems and their response to perturbation to enable improved predictions of the impacts of environmental change, energy production, and emerging technologies and biothreats on ecosystem sustainability and human health.

PNNL has made significant contributions in deciphering mechanisms of microbial community metabolic interactions and dynamics, understanding multiscale terrestrial biogeochemistry, predicting contaminant behavior and microbial ecology of the subsurface, quantifying the effects of renewable energy devices on aquatic ecosystems, and applying a systems biology approach to plant, microbial, and algal systems relevant to DOE's missions in science, energy, and environment. PNNL's Soil Microbiome SFA aims to achieve a systems- level and predictive understanding of the soil microbiome's phenotypic response to changing moisture through spatially explicit examination of the molecular and ecological interactions occurring within and between members of microbial consortia. Capabilities in microbiome science, multi-omics measurement, and computational biology are used to understand functional interactions across biological kingdoms, as well as how metagenomic information is translated to the function of microbial communities to influence the resilience and sustainability of ecosystems, bioenergy crops, and human health. Investments in synthetic biology have expanded into programmatically supported capabilities to identify novel functions of gene products within soil microbe and plant rhizosphere environments and develop strategies for the secure biodesign of engineered functions in these systems to advance BER bioenergy missions. PNNL's expertise in fungal biology has generated an in-depth understanding of the biological processes underlying efficient fungal bioprocesses that produce fuels and other chemicals. In addition, PNNL is providing insight into the development of medical countermeasures and early diagnostics, characterizing emerging pathogens, and advancing human exposure assessment to improve health and biodefense. This is particularly true for toxins with a growing capability to assess the threat from bacterial and viral pathogens.

In combination with other core capabilities—including Chemical and Molecular Sciences; Environmental Subsurface Science; Advanced Computer Science, Visualization, and Data; and User Facilities and Advanced Instrumentation—this core capability delivers expertise in microbial ecology, microbiome science, fungal biology and biotechnology, pathogen biology and biological threat prediction, systems toxicology, plant science, biochemistry and structural biology, trace chemical analysis, biomolecular separations, advanced in situ and dynamic imaging, computational biology and biophysics, and signature discovery through data analytics. PNNL's role in BER's National Microbiome Data Collaborative program is also accelerating data analytics expertise for multi-omics data integration and workflows, which also enhances the EMSL user facility capabilities. PNNL's integrative 'omics capabilities, widely used by the BER programs (e.g., the phenotypic response of the soil microbiome to environmental perturbations), leverage this broad suite of expertise to provide unprecedented molecular to mesoscale resolution of the function of biological systems. BER investments in advanced bioimaging capabilities at PNNL (e.g., cryo-EM, nanospectroscopy), including a new program to develop a first-of-kind quantum bioimaging capability, further strengthen PNNL's effort to elucidate the structure and functions of proteins and other gene products needed to advance predictive modeling of biological systems.

This capability is funded through programs in BER, ASCR, BES, EERE, EM, DHS's Science and Technology, DoD, NIH, NASA, and the EPA. Key facilities supporting this capability include BSF; the Computational Sciences Facility (CSF); the Bioproducts, Sciences, and Engineering Laboratory (WSU-BSEL); MCRL; the Aquatic Research Laboratory; Life Sciences Laboratory 1 (Gnotobiotic Animal Facility); the Microbial Cell Dynamics Laboratory; EMSL; and Building 331. PNNL partners with the JGI to provide large-scale genome sequencing and analysis for DOE missions. EMSL and JGI now issue an annual joint call for user projects focused on synergistic use of capabilities at both facilities, targeting collaborative science projects in biogeochemistry, carbon cycling, and biofuels.

Health: Scholarly output grew significantly. The capability has grown by 20 staff; seniority and pipeline have a good distribution. The portfolio is growing through increased programmatic support by both BER and NIH, as well as new funding from the Defense Advanced Research Projects Agency (DARPA) and DTRA. Capital equipment through internal and programmatic investments (x-ray nanotomography, Cryo-EM, quantum imaging) is expanding the bioimaging capability. Workhorse equipment that support multiple sponsors (e.g., mass spectrometers and NMRs) is aging, and the path for replacement is unclear. Modern laboratory space in Building 331 will be required for growth; in particular, a cell tissue suite is needed to maintain quality experiments and the supporting ventilation for biosafety cabinets.

Computational and Mathematical Sciences

Advanced Computer Science, Visualization, and Data

PNNL has depth and breadth of expertise in advanced data analytics and artificial intelligence; energy-efficient computing; performance, power, and reliability modeling; exploration and design of novel computing architectures; and runtime and system software. Specific domain areas include machine learning and artificial intelligence, predictive modeling and simulation of complex architectures, programming models, resiliency, architectural testbeds, fault tolerance, image processing, information visualization, data analytics, and data management. Our work is recognized internationally by scientific peers in areas of performance, power and reliability modeling for co-design of systems and applications, design space exploration and optimization, visual analytics, and deep learning. PNNL is also advancing the state-of-the-art in QIS and its application to address problems in various domains, including computational chemistry, energy resiliency, and materials science. Research that supports quantum computing, simulation, communication, and sensing is at the core of PNNL's QIS capability.

PNNL has advanced the state-of-the-art in machine learning algorithms and in their application to DOE missions such as biology, the power grid, and cybersecurity, and has developed new approaches for domain-aware machine learning to accelerate training and interpretability of classifiers as well as few-shot learning to accelerate scientific discovery. PNNL also develops new methods to characterize the robustness and security of artificial intelligence algorithms. Through the Center for ARtificial Intelligence-focused Architectures and Algorithms (ARIAA), PNNL is collaborating with other research institutions to co-design core technologies to apply artificial intelligence to DOE mission priorities, such as cybersecurity and electric grid resilience. PNNL is making investments in artificial intelligence to increase interpretability and automated reasoning, and is advancing research in DMC to integrate the historically distinct computing platforms for HPC (particularly for its use in physical simulation), data analytics, and machine learning. Our expertise in programming models for extreme-scale computing is demonstrated through toolkits such as Global Arrays, which powers NWChem and other important scientific applications, including subsurface flow modeling code Subsurface Transport Over Multiple Phases (STOMP) and power grid modeling code GridPACK™. PNNL data scientists lead research in data exploitation, workflow, and provenance at extreme scales for science, energy, and security domains (i.e., ARM, Livewire, A2e, Project 8, and Cooperative Protection Program efforts). In the field of visualization, PNNL has developed new techniques to improve human interfaces to artificial intelligence systems, enhance situational awareness and discovery in high-throughput streaming data analytics, and interactively train and evaluate machine learning algorithms. PNNL is also making significant advances in graph analytics, including hybrid architectures for exploiting large graph datasets and algorithms for scalable graph query on multithreaded systems. Finally, PNNL has deep expertise in scientific data management, including workflow, system architecture, and database architecture; PNNL's DataHub provides secure, timely, efficient, and open access to all laboratory, field, and benchmark model data produced in the course of research, while the Data Stewardship Board and Living Laboratory provide controlled access to risk-sensitive data sets (including internal PNNL data) for use in PNNL research.

Special facilities in support of this core capability include the CENATE, an advanced architecture testbed capability for measuring performance, power, thermal effects, and cyber vulnerabilities to assess their overall potential and guide their designs; computing resources, such as the 3.4 petaflop Cascade and Tahoma supercomputers, the Constance institutional computing cluster, the Marianas cluster (including Tonga, an NVIDIA DGX-2 system, and Deception, a state-of-the-art NVIDIA A100 system) optimized for machine learning workloads, and Newell, an experimental IBM Power9 testbed for on-ramping codes to ORNL's Summit; private research cloud and public cloud access through Amazon's AWS, Microsoft's Azure and Google's Cloud Platform; testbeds for IoT and industrial internet of things (IIoT) devices and new FPGA and ARM processor-based hybrid architectures; laboratory-scale scientific data management platforms and services; and human-computer interaction research laboratories for visual interfaces, including emerging virtual reality environments. These resources are housed primarily in CSF and EMSL. This capability receives support through programs from ASCR, BES, BER, HEP, EERE, FE, NNSA, DHS, and other sponsors, including DHHS and DoD.

Health: Recruiting and retention is strong with good gender diversity; however, market competitiveness for computing talent, particularly in artificial intelligence, continues to be a challenge. Demand remains extremely high, thus hiring and retention are anticipated to remain among leadership priorities. Infrastructure and equipment are good, and recent investments in machine learning hardware have provided up-to-date capabilities.

Computational Science

Computing permeates all research domains at PNNL. The Laboratory actively employs HPC to solve compelling, extreme-scale scientific problems, and has a long history of developing computational tools and application codes built collaboratively by multidisciplinary teams composed of domain scientists, computer scientists, data scientists, and applied mathematicians. PNNL maintains strong capabilities across many computational science domains, including computational chemistry, computational materials science, high energy physics, computational engineering, computational biology, computational geochemistry with subsurface flow, and computational fluid dynamics, as well as climate, including participation in developing community climate codes and management of the ARM user facilities. This capability uses the state-of-the-art computing infrastructure and services provided by PNNL's Research Computing, which includes CPU/GPU supercomputers (Cascade and Tahoma), AI/ML clusters (Marianas), and on-ramp systems to optimize computational codes for DOE Leadership Computing Facilities (LCFs). PNNL also has cloud access to advanced quantum systems through IBM's Quantum Network.

Multidisciplinary teams of domain and computer scientists and applied mathematicians have long been a key part of the research and innovation process at the Lab. In the area of computational chemistry, PNNL has developed NWChem, a unique molecular modeling capability that dramatically advances the state-of-the-art through the development of scalable predictive methods for excitation and correlated phenomena and directly ties to experiments at DOE light sources. The software is continuously updated to incorporate new theoretical approaches and to adapt to the changing computing landscape through efforts such as the Exascale Computing Project, which includes developing NWChemEx. The exceptional scalability of PNNL's chemistry codes has resulted in DOE grants providing significant computing time and resources on Leadership Computing Facility systems and at the National Energy Research Scientific Computing Center. This computational science capability will be a key component of the nascent Institute for Computational Chemistry, a multidisciplinary effort aimed at positioning PNNL as a world-leader in computational chemistry. The Northwest Quantum Nexus partnership and PNNL's participation in three of the new DOE Quantum Information Science Centers also provide new leadership opportunities at the intersection of quantum computing with quantum chemistry with the goal of applying quantum computing in computational chemistry and materials science.

The same integrative, co-design-based approach is now being employed to develop advanced computational models at multiple length and time scales for the power grid, high energy physics, materials science, health, and climate, to name only a few. Internal LDRD investments have focused on bringing together interdisciplinary teams of data scientists, computer scientists, applied mathematicians, applied statisticians, and domain scientists to work on a wide range of DOE-relevant problems in microbiology, soil science, climate sciences, materials, renewable energy, and nonproliferation. Recently, these investments have focused on the development of novel software and hardware architectures to support scalable scientific machine learning methods that can be applied to a wide range of DOE problems.

This capability leverages PNNL's Applied Mathematics and Advanced Computer Science, Visualization, and Data core capabilities. The core capability supports sponsor-funded research by DOE-SC, including BES, BER, ASCR, HEP, FE, and NP. In addition, internal LDRD support across multiple initiatives and Agile investments has also contributed to further develop this core capability.

Health: Solid project portfolios exist for all DOE-SC sponsors. The focus is now on expanding the project portfolio to include sponsors outside of DOE-SC. Workforce development efforts should focus on mid-senior hires and on continuing to improve diversity metrics. Research computing provides adequate infrastructure; however, hardware requires continuous update/upgrade plans to ensure state-of-the-art resources. Office space needs to be reorganized to improve collaboration, absorb planned growth, and to accommodate new modes of work resulting from the new "Future of Work" model.

Applied Mathematics

PNNL is a leader in applied mathematics and statistics, using mathematical models to predict the behavior of dynamic, complex systems and quantify associated uncertainty to accelerate scientific discovery. Our researchers develop novel mathematical methods for predictive modeling, uncertainty quantification, risk and decision analysis, physics-informed AI/ML, complex information modeling, data analytics, and control of complex systems. A strength at PNNL is the seamless integration of applied mathematics with computer science, data science, and domain expertise to make major impacts in national problems, such as the reliability and security of critical infrastructures.

PNNL has broad expertise in multiscale mathematics, including dimension reduction, mesoscale Lagrangian particle methods, and hybrid methods for coupling multi-physics models operating at different scales. Building on our strength in multiscale modeling, we develop capabilities in domain-aware machine learning, as well as physics-informed methods for parameter estimation and uncertainty quantification. These techniques focus on solutions for nonlinear and high-dimensional systems and include surrogate and multifidelity modeling for both forward prediction and inverse models. In addition, PNNL develops strategies to generate scientifically interpretable mathematical models that are capable of reasoning over numerous complex scenarios defined by partial information and partial model understanding. The integrated use of mathematical or statistical techniques—such as uncertainty quantification, machine learning, signature discovery, causal reasoning, and game theory—enables domain scientists to generate novel hypotheses in both static and streaming applications.

PNNL develops operational models focused on resource utilization and risk assessment via simulation, optimization, and mathematical programming. In addition, PNNL is growing capabilities in distributed and hierarchical decision systems, reinforcement learning, verifiable machine learning based control, and concurrent system and control design for safety-critical systems.

PNNL pursues innovative research in the analysis and integration of complex, high-dimensional data. Our mathematicians advance methods in computational topology, hypergraph theory, and applied category theory. We use these methods to build novel representations of tabular, relational, and time-series data, aimed at synthesizing quantitative and qualitative information with complex, multi-way dependencies. Applications include sensor fusion, anomaly detection, and visualization of complex data for critical problems in cybersecurity, computational biology, geolocation, and open-source data analysis. PNNL also has an emerging capability in the applications of discrete mathematical techniques to a range of problems in the DOE mission space to solve crosscutting problems of national interest. PNNL is heavily invested in solving issues related to large-scale graph analysis, time evolution of discrete structures, and the development of network invariants and their applications. PNNL researchers leverage emerging capabilities in quantum information sciences to develop algorithms for combinatorial optimization.

The core capability supports sponsor-funded research by DOE-SC, including BER and ASCR, as well as government funded innovation and technology transfer programs such as Small Business Innovation Research/Small Business Technology Transfer. Most of the research in our data sciences and machine learning portfolio is currently funded by internal LDRD investments, such as DMC and Mathematics for Artificial Reasoning in Science (MARS), as well as from external sponsors, such as DOE-ASCR, DoD, and NNSA.

Health: A solid project portfolio, which is focused on DOE-SC with an emerging presence of other sponsors such as DoD and NNSA. There are well-established national partnerships; the focus is now on expanding collaborations to include international partners to increase visibility and leadership. Research computing provides adequate infrastructure to support computational mathematics research; however, hardware requires continuous update/upgrade plans to ensure access to state-of-the-art resources. Office space needs to be reorganized to improve collaboration, absorb planned growth, and to accommodate new modes of work resulting from the new “Future of Work” model.

Cyber and Information Sciences

The Laboratory conducts research and develops technology that brings scientific approaches to cyber operations and defense, giving the United States a strategic advantage in the cyber domain. PNNL's work enables cyber resilience for U.S. critical infrastructures, based on expertise in the development and implementation of advanced sensing techniques, analytic techniques to extract value from data, and the design of resilient control systems. Research, engineering, and analysis staff are nationally and internationally recognized in cybersecurity, the development of secure design principles for control systems, cyber analytics, graph theory, machine learning, text and multimedia analytics, statistics, and emerging techniques for human-machine teaming.

PNNL's cybersecurity expertise spans IT, industrial controls systems, operational technology, and the IoT. The Laboratory's cybersecurity portfolio is based on decades of expertise in developing and deploying novel cybersecurity sensors for wide-scale enterprise network intrusion monitoring and situational awareness, including operation of the Cooperative Protection Program (CPP) for DOE complex cyber defense and CRISP, a voluntary information sharing and threat intelligence program for the energy sector. PNNL has developed unique expertise in the scientific and mathematical foundations of cybersecurity, including leadership in biologically inspired cybersecurity, multiscale graph methods for active cyber defense, critical infrastructure resiliency analysis and modeling, supply chain security, vulnerability assessment, and integrated cyber and physical security. An emerging area of focus is in autonomous resilience in cyber systems, including predicting and mitigating the consequences of failures across linked cyber and physical systems. PNNL's expertise focuses on applications for critical infrastructures and industrial control systems, with emphasis on the power grid. PNNL has also developed a research-to-operations model for cybersecurity in which its cybersecurity research staff and internal cybersecurity operations staff partner closely to use PNNL-developed analytic and security solutions to defend PNNL from cyber threats, as well as use PNNL's operational expertise to inspire the next generation of cybersecurity technologies.

PNNL's information science expertise is in areas of data acquisition and management (e.g., experimental design, data workflow, provenance, and quality assurance); analytics and algorithms (e.g., streaming and graph analytics and scalable machine learning); and decision support (e.g., user experience, real-time analysis, and model/algorithm steering in response to user input). PNNL places special emphasis on developing next-generation techniques for analysis and visualization of unstructured data from streaming heterogeneous sources, including new approaches for human-machine teaming to improve analytic quality and efficiency. PNNL maintains a world-class capability in text and image processing and in the development and application of machine learning to text and image understanding. PNNL has significant expertise in applying deep learning to accelerate discovery across all of PNNL's missions.

Major computing resources that support this capability include Research Computing resources, including the Constance cluster; real-time operating system and scalability testbeds; multiple systems optimized to support scalable AI/ML research; and the CyberNET and PowerNET virtual enterprise testbeds to simulate real-world cyber activity and improve cybersecurity for industrial control systems. In addition, facilities such as the Cyber Security Operations Center, the EIOC, the Visualization and Interaction Studio, the Machine Learning Studio, and the Electricity Infrastructure Cyber Security/Resilience Center support this capability. External collaborations include industry, academic, and governmental partners from across the nation and around the world. Primary sponsors for PNNL's cyber and information sciences research include ASCR, OE, DoD, DHS, and Strategic Intelligence Partnership Program (SIPP) sponsors.

Health: Demand for this core capability remains very strong. Aggressive hiring among early-career cyber and data scientists has improved the staffing situation; however, additional attention is still required for mid/senior hires. The demand, coupled with continued strong competition for talent with relevant hot skills and the associated high compensation levels, makes this core capability one of several being addressed through intensive recruiting and cross-training. Currently, there is insufficient federally owned office and laboratory space for research in data science and cybersecurity; however, PNNL plans to renovate space on the PNNL Richland Campus to support this need.

Decision Science and Analysis

PNNL maintains strong capabilities in modeling, analyzing, communicating, and mitigating crosscutting impacts at the interface between science, technology, policy, and society. Working collaboratively with scientists and engineers across the Laboratory and with external partner organizations, our experts continue to develop and implement innovative, resilient, and holistic solutions to complex decision problems on the front lines of the nation's energy, environment, and national security challenges.

PNNL's staff expertise is focused on the areas of decision science, risk analysis, economics, systems engineering, decision support systems, operations research, policy analysis, social and behavioral science, statistics, and safety analysis. This capability enables the development and application of cutting-edge decision and risk analysis; safety, impact, and risk assessments; making resilient decisions under uncertainty; alternatives analysis; strategic process/systems improvements; and operational decision support. Additional modeling and analysis capabilities include socioeconomic modeling, market and policy analysis, techno-economic modeling and analysis, regional/national energy simulation, and cost-benefit analysis and uncertainty analytics. The team's breadth and depth of decision and risk analysis expertise fosters flexibility in assembling dynamic, multidisciplinary teams to develop science-based strategies for minimizing risks to individuals or the public, program life cycles, facility designs and operations, and the environment at the local, state, regional, national, and global levels.

Staff that support this capability at the Laboratory are located in several locations in Richland, including ISB1, ISB2, the Engineering and Analysis Building, MATH, and the National Security Building, as well as the PNNL offices in Portland, Oregon, and Seattle, Washington. They are recognized in the areas of nuclear and alternative energy; operational safety review and risk assessment; technology testing, evaluation, and performance assessment; technical and programmatic risk assessment; geo-spatial decision analytics and visualization; geointelligence; nuclear proliferation risk modeling; knowledge management and data reuse; multi-organizational collaboration decision support; distributed decision-making for power grid reliability; energy policy and regulatory development/deployment; appliance and commercial equipment energy efficiency codes and standards; and feasibility analyses of technology, siting, policy, and tax structures for energy technology deployment. Leadership in safety assessment, probabilistic risk assessment methodology development and application, environmental impact assessment, and analyses and feasibility assessments for nuclear, geothermal, hydropower, and other sustainable energy technologies, such as hydrogen-powered vehicles, are specific strengths. Current stakeholders that primarily utilize our capabilities include DOE (EERE, OE, EM, FE, and NE), NNSA, DHS, DoD, EPA, BPA, and NRC.

Health: Staff, portfolio, and equipment are good. However, 33 percent of staff are early career and another 17 percent are retirement eligible; recruitment and retention remain a matter to watch.

Engineering

Biological and Bioprocess Engineering

Leveraging the capabilities in biological and bioprocess engineering, PNNL is developing technologies and processes that create opportunities from ecological and economic liabilities by sustainably converting biomass and other carbon- containing waste materials into fuels and chemicals. Potential carbon feedstocks include food wastes, sewage sludge, municipal solid wastes, plastics, industrial wastes, and lignocellulosic materials (e.g., corn stover and wood wastes), as well as fungi and algae. This capability is strengthened through collaboration with Laboratory expertise in catalysis and reaction engineering; separations, process engineering, and flowsheet development; materials science; and techno-economic modeling. The capability also benefits from strong collaboration with external partners through the WSU-PNNL Bioproducts Institute and several DOE BETO consortia, including the Chemical Catalysis for Bioenergy Consortium, Feedstock-Conversion Interface Consortium, Bioprocessing Separations Consortium, Agile BioFoundry Consortium, and the Joint Bioenergy Institute.

PNNL successfully applies its capabilities in biological and bioprocess engineering to explore hydrothermal liquefaction for conversion of wet feedstocks to products, hydrotreating of biocrude and bio-oils to fuels, conversion of biomass-generated alcohols to jet fuels, and conversion of intermediates to chemical products. PNNL's bioprocess engineering capabilities span high-throughput and combinatorial catalyst screening, to benchtop reactors, to foundry-scale reactors, for next-generation conversion technologies. PNNL houses unique indoor, climate-controlled raceway ponds and photobioreactors that can cultivate microalgae strains under conditions that simulate outdoor ponds at any geographic location in the world. The capability also includes a unique Biomass Assessment tool that can quantify potential fuel production from microalgae and waste feedstocks.

This capability primarily supports the research mission of EERE's Bioenergy Technologies office. Current research spans from enzyme and microbe engineering to produce desired bioproducts from organic wastes, to fundamental understanding of the molecular interactions involved in conversion processes, to pilot-scale operations that demonstrate process technologies, paving the way for technology transfer to industry for commercial application. A recent example of the Lab's success in technology transfer leveraging this capability is the PNNL-developed alcohol-to-jet process that has been licensed to LanzaTech to enable the production of jet fuel from alcohol derived from industry flue gases. Through the PNNL-LanzaTech partnership, the jet fuel has been certified by the American Society for Testing and Materials for commercial use, and the first transatlantic flight utilizing a waste-gas derived jet fuel was flown by Virgin Atlantic.

Health: This capability remains stable, and technical accomplishments such as the development of the alcohol-to-jet process continue to receive national attention (2020 IRI Technology Achievement Award). Publication and patent records are solid. The pending retirements of several senior technical experts requires more aggressive succession planning, and a hiring plan to address this challenge has been developed. Availability of office and lab space is a growing concern in BSEL. Plans to decommission high hazard HT/DC research in PDL-W will relieve some safety concerns. Although this capability is primarily supported by one DOE office, there are an increasing number of additional research sponsors.

Power Systems and Electrical Engineering

PNNL has internationally recognized capabilities spanning the entire electric power grid. Staff at PNNL have deep expertise in the grid's transmission and distribution networks, reliability and resilience, smart grid and intelligent systems, distributed energy resources, market systems, and energy demand. PNNL develops innovative solutions to addressing emerging challenges facing today's power industry through better planning, operating, and controlling of modern power grids for enhanced resilience and reliability as well as decarbonization. Primary supporting disciplines include power system, electrical, and control engineering; computational science and software engineering; cybersecurity; data analysis; and mechanical engineering. With a focus on system- level issues, PNNL is the national leader in defining a decarbonized, resilient power grid of the 21st century, delivering innovative tools to enable unparalleled grid performance (resilience, reliability, security, transparency, efficiency, and sustainability) and new control and architecture paradigms spanning future demand and supply for unprecedented consumer engagement.

Key research areas include grid architecture, transmission and distribution system reliability and control analysis, power system protection, advanced grid data applications, computing and visual analytics, renewable resource integration, energy storage, distribution system modeling, power system economic analysis, and grid cybersecurity. PNNL's expertise in grid simulation and analytics enables high-performance grid monitoring and control at an unprecedented speed, from minutes to sub-seconds. For over a decade, PNNL has led the world in the development and application of transactive systems that combine economics and controls to enable distributed optimization and integration of distributed energy resources, including responsive loads, batteries, and renewable generation. PNNL's expertise in advanced control theory, application, and testbeds supports advancements in the development of new, distributed controls for the electric power system. PNNL's leadership in phasor measurement technologies supports broader national deployment, enabling unprecedented grid visibility and enhanced situational awareness. PNNL's one-of-a-kind, utility-grade control center infrastructure supports research in grid visibility, control, and resiliency, with the largest national repository of grid data and models to inform research.

This research is made possible with the use of the EIOC, the Interoperability Laboratory, and the Power Electronics Laboratory. These laboratories and facilities support world-class commercial tools, as well as PNNL-developed tools, including the following: the GridLAB-D™ open-source simulation and analysis tool for designing and operating power distribution systems, the GridAPPS-D open-source platform for advanced distribution system planning and operations application development, the GridPACK open-source package for parallelizing power grid simulations, the VOLTTRON™ open-source software platform enabling grid-interactive efficient buildings, the R&D 100 award-winning Dynamic Contingency Analysis Tool (DCAT) for enabling power grid cascading failure analysis, and tools for assessing power grid ramping capabilities with increased variable generation. These capabilities are supported by sponsors in OE, EERE (transportation technologies, hydrogen storage, building technologies, and fuel cell technology), DOE Office of Cybersecurity, Energy Security, and Emergency Response (CESER), ARPA-E, DHS, ASCR, DoD, the U.S. Department of State, and private industry.

Health: Aggressive hiring continued, with 30 staff hired over the past 12 months to support a diverse and growing portfolio of sponsors. PNNL continues to be assigned leadership roles on major DOE initiatives, such as NAERM, GMLC, and the Energy Storage Grand Challenge. While senior hires are helping to backfill key thought leaders who have retired, there is a continued need for both mid-career and additional senior hires. Office space pressure has been reduced by planned acquisition of additional space in Seattle and temporary work-from-home orders; future space sufficiency depends upon effective space management and implementation of lab-wide flexible work strategies. The EIOC continues to be a distinguishing capability to attract leadership roles in DOE programs, as does the transactive campus with the addition of thermal storage and new battery installations. Additional distributed grid assets (e.g., photovoltaics, energy storage, inverters, smart building loads, and advanced metering infrastructure) are needed to advance next-generation controls work at scale.

Systems Engineering and Integration

PNNL is internationally recognized for systems engineering and integration through the implementation of technology in real-world complex systems focusing on smart and robust nuclear and radiological security and energy systems optimization and integration. This core capability has solved some of the most challenging national problems by defining and interpreting complex technical requirements and translating them into fieldable solutions that address economic, social, policy, and engineering considerations. Using a structured approach to understand complex systems throughout their life cycle, PNNL applies its domain knowledge and experience in engineered systems simulation and modeling; system architecture and design; test, evaluation, and optimization; technology assessment, integration, and deployment; policy assessment and economic evaluation; and regulatory analysis, risk assessment, and decision support. This allows our staff to effectively take early stage research through the development and technology maturation processes and to deploy technical solutions that address our sponsor's most critical challenges.

PNNL proactively engages with other national laboratories and industry to define best practices for applying systems engineering in early stage R&D, and applies a graded approach to our systems engineering discipline that enables us to deliver solutions in a highly efficient, effective way. PNNL is known worldwide for effectively field-deploying international nuclear materials safeguards, nuclear and radiological security, and complex radiation detection systems. PNNL is also known for leadership in integrated building energy technologies, including advancing solid-state lighting, advanced building control, and building-grid integration technology. Further, PNNL is recognized nationally for the rigorous analyses that support building energy code development and enable DOE to fulfill statutory requirements related to appliance standards. Lastly, PNNL is widely known for advancing national power grid reliability and smart grid technologies.

Staff members are housed in facilities that include the Systems Engineering Building (SEB), EIOC, System Engineering Facility, 2400 Stevens, Engineering Development Laboratory, APEL, Radiation Detection Laboratory, and the Large Detector Test Facilities. The Systems Engineering and Integration capability is funded through programs in BES (design and operation facilities), BER, HEP, NP, EERE (buildings and transportation), EM (waste processing and nuclear materials disposition), OE (infrastructure security and energy restoration), FE (carbon and co-sequestration), NNSA (nonproliferation and safeguards), DHS (radiation portal monitoring and critical infrastructure and analysis), NRC, EPA, and DoD.

Health: Staff, portfolio, infrastructure, and equipment are all in good shape; there is some need for additional high bay space and dedicated facilities for testing and evaluation.

Chemical Engineering

PNNL's chemical engineering capabilities translate scientific discovery into innovative, first-of-a-kind processes to solve tough energy and environmental challenges for DOE and other stakeholders. PNNL develops materials, unit operations, and integrated chemical processes at scales ranging from molecular interactions to engineering-scale experiments to full- scale demonstrations that can be transferred to the sponsor or to industry for commercialization. PNNL's competency in this area includes chemical engineers, mechanical engineers, materials scientists, and chemists specializing in disciplines that include catalysis and reaction engineering, gas and liquid phase separations, heat exchange, process intensification, fluid dynamics and mixing, thermal- mechanical modeling, flowsheet development and modeling, and techno-economic analyses. Nuclear waste treatment (from milligram to ton-scales) is another area of expertise, encompassing slurry transport and mixing, glass melting, advanced rheology, and fluid dynamics for complex multiphase systems.

Examples of how PNNL successfully applies its chemical engineering capabilities include the invention and development of affordable, scalable processes for CO_2 capture and utilization; waste carbon conversion to fuels and products; catalytic automobile emissions control; novel heat pumps to increase energy efficiency; magnetocaloric liquefaction of hydrogen and other gases; micro-channel-based reactors and separations systems for high efficiency chemical conversions and solar natural gas reforming; and the development and application of software to predict the thermal and structural performance of spent nuclear fuel storage and transportation systems. Working in collaboration with academia, industry, and other national laboratories, PNNL has a leadership role in high-impact national programs, such as DOE AMO's Rapid Advancement in Process Intensification Deployment (RAPID) Institute, BETO/VTO's Co-Optimization of Fuels and Engines Consortium, and VTO's Cross-Cut Lean Exhaust Emission Reductions Simulation (CLEERS) initiative.

This core capability supports sponsor-funded research by DOE-SC (BES), as well as many of DOE's Applied Energy Offices (EM, EERE, FE, and NE), NNSA, and ARPA-E. PNNL's Chemical Engineering core capability is also leveraged in support of research funded by DHS and DoD. Current research focus areas include biomass and fossil fuel conversion to fuels and chemicals, as well as subsequent fuel upgrading; CO_2 capture from point and distributed sources; nuclear waste processing and immobilization; and cost-effective start-up and operation of the Hanford Waste Treatment Plant.

Health: Publication record continues to be strong, with increasing numbers of articles in high-impact journals. Equipment is adequate, though appropriate lab space, to include high bay space, continues to be tight and puts future capability growth (e.g., the development of a catalysis process development unit) at risk. Attracting diverse and qualified candidate pools to fill job vacancies is a challenge in this area, though the quality of new hires remains high.

Nuclear Engineering

PNNL has expertise in complex irradiation systems that support materials science, tritium production, advanced fuel modeling, and reactor production analysis. Research staff members have broad and deep technical skills across the full spectrum of nuclear engineering disciplines, including reactor physics, mechanical design, thermal- mechanical analysis, fluid dynamics, heat transfer criticality safety, nondestructive evaluation, and robotics, as well as materials science and microscopy. PNNL applies these skills in radiological facilities (e.g., 325RPL) to characterize and understand irradiation effects on materials through post-irradiation examination, and to make precise measurements and analyses that enable nuclear archeological assessments. In addition, PNNL has experimental testing capabilities that enable the design, development, and fabrication of advanced, accident-tolerant fuel for commercial reactors and low-enrichment fuel for research reactors, as well as the design, modeling, fabrication, and deployment of complex irradiation tests to evaluate nuclear materials.

PNNL is specifically recognized for the development of the Graphite Isotope Ratio Method, which is the world's most accurate estimation tool for graphite reactor operational history, and has a deep expertise in proliferant plutonium production, from reactor irradiation to plutonium metal. This year, a significant effort went in to expanding our support for NNSA's defense programs. PNNL is the design authority for tritium production targets, and this year, we successfully addressed significant quality assurance program concerns that could impact tritium supply. The combination of thermal, nuclear, and structural skills is also used to evaluate spent nuclear fuel storage and transportation options. PNNL is currently testing high burn up spent nuclear fuel to assure the continued safe dry storage at nuclear power plants across the nation.

A wide range of sponsors rely on PNNL's nuclear engineering capability. These include BES, who relies on PNNL to understand the benefits of modeling interfacial dynamics in radioactive environments and materials. The NRC relies on PNNL expertise to evaluate and confirm the thermal performance of nuclear systems as well as develop new techniques for nondestructive evaluation to extend the life of existing reactors. This strong knowledge base and expertise in the commercial nuclear industry enables the design of targets for isotope production and fuel performance modeling to develop or evaluate fuels for use in NRC-regulated commercial or research reactors. PNNL's nuclear engineering capabilities also support NE's missions and objectives, including the Versatile Test Reactor program, based on our historical expertise with the fast reactors. NNSA's defense programs rely on nuclear engineering to understand the production of materials for the nuclear deterrent, most notably tritium. NNSA's Office of Defense Nuclear Nonproliferation supports the understanding of future reactors and their impact on nuclear proliferation.

Health: Aggressive hiring over the last 12 months has brought on high-quality staff at all levels; however, we still have demand for more, especially with enhanced clearances. The current portfolio, while strong, is operationally focused and needs to be expanded/balanced with more research. Equipment is of high quality but is operating at full capacity. Some additional infrastructure needs at 325RPL (e.g., recapitalizing acid-compatible glove boxes and fume hoods, general building maintenance) have been identified.

User Facilities and Advanced Instrumentation

Environmental Molecular Sciences Laboratory

As one of BER's national scientific user facilities, EMSL leads molecular-level discoveries for BER and DOE that translate to predictive understanding and accelerated solutions for national energy and environmental challenges. Our vision is to provide a predictive understanding of dynamic molecular transformations underpinning biological and ecosystem functions. Research in EMSL focuses around three science areas: 1) Functional and Systems Biology; 2) Environmental Transformations and Interactions; and 3) Computing, Analytics, and Modeling. Within each of these thematic areas, EMSL scientists partner with users from around the world to explore critical questions in BER relevant science.

The **Functional and Systems Biology** area focuses on understanding and harnessing enzymes and biochemical pathways that connect protein structures and functions to complex phenotypic responses through a deep understanding of interactions within cells, among cells in communities, and between cellular membrane surfaces and their environment for microbes and plants. This understanding encompasses multiscale experimental observations, metabolic reconstruction, and modeling leading to improved strategies for designing plants, fungi, and microbes for biofuels and bio-based products, as well as unraveling the complexities of carbon, nutrient, and elemental cycles within cells and their immediate environment.

The **Environmental Transformations and Interactions** area focuses on the mechanistic and predictive understanding of environmental (physiochemical, hydrological, biogeochemical), microbial, plant, and ecological processes in above- and below-ground ecosystems, the atmosphere, and their interfaces. EMSL provides the experimental, data analytics, modeling, and simulation expertise to investigate the cycling, transformation, and transport of critical biogeochemical elements, contaminants, and atmospheric aerosols to test, improve, and validate model predictions or identify sources of model uncertainty. Coupled experimental and modeling approaches will accelerate understanding of the mechanisms and dynamics of processes, their interdependencies, and feedbacks at molecular to ecosystem scale.

The **Computing, Analytics, and Modeling** area focuses on combining advanced data analytics and visualization and computational modeling and simulation with state-of-the-art experimental data integration to develop a predictive understanding of biological and environmental systems. Our cohesive approach to integrating experimental and computational methods advances predictive approaches to biodesign for biofuel/bioproduct production and accelerates research to understand the molecular mechanisms underlying biological and hydro-biogeochemical processes controlling the flux of materials (e.g., carbon, nutrients, and contaminants) in the environment.

PNNL is recognized for its ability to conceive, design, build, operate, and manage world-class scientific user facilities, and is known internationally for its advanced instrumentation designed to accelerate scientific discovery and innovation. As an example, PNNL demonstrated this ability with the development, design, construction, and deployment of the 21T Fourier-Transform Ion Cyclotron Resonance (FTICR) mass spectrometer. As new capabilities are developed, special calls for first science applications promote rapid and effective utilization of these new tools. EMSL is active in leveraging its capabilities with other DOE user facilities to maximize the scientific community's ability to address critical challenges in biology, environment, and energy. As an example, EMSL jointly sponsors user calls with JGI and ARM through BER's FICUS initiative. The EMSL-JGI FICUS calls have been used to maximize DOE's genomic/transcriptomic and other ’omics capabilities, as well as EMSL's chemical and physical measurements for breakthroughs in systems biology. The EMSL-ARM FICUS call enables investigation of aerosol processes or aerosol-cloud interactions by studying the physical, chemical, optical, and microphysical properties of aerosols, including biological particles to develop a process-level understanding of the formation, transport, and evolution of aerosols and their impact on warm and cold cloud formation, and ultimately improve Earth system models. EMSL continues to explore other mechanisms to maximize the value and reach of the facility by partnering with other user facilities via the FICUS initiative, such as the BES-funded High Flux Isotope Reactor/Spallation Neutron Source. EMSL also collaborates with other user facilities through the new Society for Science at User Research Facilities.

Health: The quality of staff and the research portfolio are both strong. Research equipment health remains strong. A strategic equipment reinvestment plan is in process, which will guide future equipment acquisition. The EMSL roof is nearing the end of its useful life and plans for replacement are in process. Planning is in process for the use of space that will be available when Physical and Computational Sciences Directorate (PCSD) staff move to the ESC. Additional planning for renovations to the HPC space for future expansion of BER computing capabilities are in process focused on cooling and electrical upgrades to accommodate the increased demands.

ARM User Facility

The world's premier ground-based observations facility for atmospheric science research, ARM is a DOE user facility that provides a global network of instrumented fixed-location, mobile, and aerial observatories for obtaining cloud and aerosol measurements, as well as precipitation, solar and thermal radiation, surface heat and moisture, and meteorological conditions. ARM observatories are deployed to diverse meteorological regimes around the world where there are critical science questions and deficiencies in global-scale models. Fixed-location observatories are in the U.S. Southern Great Plains, the North Slope of Alaska, and Graciosa Island in the Eastern North Atlantic. Diverse data sets are being incorporated into integrated products for evaluating high-resolution atmospheric process models and large-scale Earth system models, such as the DOE E3SM Model.

To accelerate model development and associated atmospheric process studies, ARM is working to bridge the scale gap between ARM observations and global Earth system models by expanding capabilities at ARM observatories. The first test of this new strategy has been at the Southern Great Plains observatory, where ARM has developed a framework that combines high-resolution model simulations with ARM observations. The ARM observations provide three-dimensional constraints to the model as well as a test of model output. The combination of the ARM observations with the high-resolution model output and associated diagnostics provides a more complete representation of the ARM site domain, enabling broader use of the data by the scientific community. ARM is now preparing to implement this modeling framework to study deep convection. This second application of the modeling framework will make use of measurements from the Cloud, Aerosol, and Complex Terrain Interactions (CACTI) field campaign, held in Argentina from October 2018–April 2019.

ARM continues to deploy mobile facilities and the AAF as approved through the user proposal process. In FY 2021, the first and second ARM mobile facilities will be deployed in the continental United States. The first facility will be deployed near Houston, Texas, and will focus on the interaction of aerosols and deep convection. The second facility will be deployed in the Rocky Mountains, near Crested Butte, Colorado, and will focus on the interaction of atmospheric processes and mountain hydrology.

The AAF is undergoing a period of change, as the G-1 aircraft, which served ARM from 2010–2018, has been retired and the process of implementing a new research aircraft is underway. To replace the G-1, PNNL has followed the CD process (DOE O 413); following CD-2/3 approval, PNNL purchased a Challenger 850 regional jet in May 2019 and placed a contract for the modification of this aircraft in June 2020. The modification project includes the addition of mounting points for scientific instruments and an extensive reworking of the aircraft interior to provide power, communications, mounting systems for research equipment, and workspace for researchers. In addition, the team, in conjunction with the Port of Pasco and other regional partners, has obtained new hangar space to support the new aircraft as well as a mid-size UAS. The aerial facility team moved into this space in August 2020.

PNNL leads the development of UAS capabilities within ARM. PNNL manages and operates a very capable mid-size UAS, the ArcticShark, that can carry payloads of up to 100 pounds as high as 18,000 feet for periods of up to eight hours. The ArcticShark will undergo modifications and testing this year in preparation for research flights focused on aerosols at the ARM Southern Great Plains observatory.

PNNL is responsible for the overall technical direction of ARM's scientific infrastructure through leadership of a collaboration among nine DOE laboratories. PNNL has lead responsibility for a variety of facility components, including the management and operation of the AAF and related operations, technical leadership for various instruments and data product development processes, and communications. This capability is funded by BER.

Health: The Challenger 850 modification contract is in place and underway. There have been some challenges posed by travel restrictions associated with COVID-19; however, the modification project is on track for completion in the first quarter of CY 2022. A capability development plan for the ArcticShark has been approved and work is underway to prepare the mid-size UAS for research flights. The aerial facility team has moved into the new hangar that will serve both the Challenger 850 and ArcticShark. The radar engineering team continues to seek high bay space and field test sites to support radar maintenance between deployments. The team has identified an interim solution for high bay space. The portfolio is good and staffing is good, with the exception of radar analysis support. An interim solution has been implemented for that function and a hiring effort is underway.

Science and Technology Strategy for the Future/Major Initiatives

Scientific Vision

PNNL advances the frontiers of knowledge, taking on some of the world's greatest science and technology challenges. Distinctive strengths in chemistry, Earth sciences, biology, and data science are *central to our scientific discovery mission. PNNL's research lays a foundation for innovations that advance sustainable energy through decarbonization and energy storage and enhance national security through nuclear materials and threat analyses.*

PNNL's signature strengths in scientific discovery, sustainable energy, and national security (Figure 2) are summarized below. They are followed by a discussion of our six Major Initiatives, which are the focus of our strategy.

Infrastructure

Overview of Site Facilities and Infrastructure

PNNL is based in southeastern Washington State, in the city of Richland, with buildings on the Laboratory's main campus and in the 300 Area of the Hanford Site. PNNL also conducts operations in Sequim, Washington, and satellite locations in Seattle, Washington; Portland, Oregon; and College Park, Maryland.

The PNNL Richland Campus Master Plan is available at
https://www.pnnl.gov/sites/default/files/media/file/2017CampusMasterPlan.pdf.

The PNNL Sequim Campus Master Plan is available at
https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-29685.pdf.

To maximize mission impact for DOE, PNNL's facilities and infrastructure planning is underpinned by six goals:

- Maintain a ready-to-serve, mission-ready campus
- Increase federal ownership of the campuses and facilities and reduce dependance on third-party leasing
- Leverage local support for utility infrastructure and services, fire, police, and emergency response capability
- Invest in facilities and infrastructure to increase resiliency and maintain current low deferred maintenance
- Recognize that the COVID pandemic has changed our understanding of the future of work and incorporate this in our facility and infrastructure planning
- Achieve NZERO emissions with no loss in resiliency at both our campuses.

Mission-Ready, Federally Owned Campuses. The real property assets at PNNL represent nearly 2.4 million gsf in 86 buildings and approximately 550 acres of land (see Table 4). DOE is in the final stages of acquiring all contractor-owned facilities, the capstone of a five-year agreement between DOE and Battelle to transfer ownership of this real property. The final transition of facilities and land in Richland and Sequim will be completed in FY 2022.

PNNL is aggressively reducing its dependance on leased facilities. The PNNL Richland Campus and adjacent areas include 18 leases totaling ~880,000 gsf. PNNL is expecting to reduce Richland lease holdings by more than 70 percent, representing just 11 percent of the total gsf of the PNNL Richland Campus. Appendix 4 provides more detailed lease information.

Leveraged Utilities. The utilities for the PNNL Richland Campus are provided by the city of Richland and are well maintained. In coordination with the city of Richland, PNNL recently assumed operational control of the Hanford 300 Area water and sewer systems and will take over the natural gas system operations during FY 2022. The city of Richland has an agreement with each individual contractor in the 300 Area to support electrical service. Additionally, PNNL will soon transition all emergency services support to the city of Richland. The city of Richland is constructing a new city fire station adjacent to PNNL's core campus to serve this need.

At the PNNL Sequim Campus, current sewer and water needs are serviced by septic sewer and potable well water. These services will be transitioned to local municipalities over the next three years. The city of Sequim provides emergency services to the PNNL Sequim Campus.

Planning for Investments in Facilities and Infrastructure. PNNL's campuses and facilities have been well maintained and boast an average building age of 28 years, with a very low deferred maintenance backlog resulting in an overall condition index of 94. In planning future investments, PNNL is guided by an understanding of the needs of our Major Initiatives (see Section 4.0) and by cues from our ICM review of the health of our core capabilities (see Section 3.0 and Appendix 1 for discussion of process and results). Any areas of concern identified through ICM are evaluated for the most efficient solution in the context of mission alignment and optimized functionality, reliability, utilization, and operating costs.

The Hybrid Workplace. The COVID-19 pandemic has had far-reaching impact on how PNNL is thinking about, and planning for, its future, with consequent implications for its facilities and infrastructure. By embracing several core principles, we believe that we can increase our ability to deliver for our sponsors; retain our sociable culture; improve hiring, retention, and diversity; and benefit from an increased presence in other geographic locations (e.g., sponsor colocation). The core principles we are using to guide the design and implementation of what will be a new and more flexible work environment for our staff are as follows:

- Delivering exceptional mission impact for our sponsors and the nation
- Creating a shared sense of culture and belonging
- Embracing flexibility in where and when people work
- Equipping leaders to lead distributed teams.

PNNL envisions creating a new model that allows for flexible work environments and location requirements to support the changing needs of staff and provide them with an improved quality of life. This model will accommodate a new distribution of on-site, hybrid, and virtual workers. All staff, regardless of location, will benefit from the technological, physical, and sociological enhancements to our campuses that will be necessary to ensure the success of our model—better communication, increased attention to mentoring, and enhanced work location flexibility.

The implementation of the hybrid workplace will have a dramatic effect on our physical campus and configurations of workstations within our facilities. One immediate challenge will be planning for the accommodation of those hired during the pandemic but not yet situated on the physical campus. PNNL has increased its hiring to address growth in many areas of research—net direct head count growth in FY 2019 and FY 2020 was nearly 7 percent and 6 percent, respectively, and projections for FY 2021 and FY 2022 show continued FTE growth of 6 percent per year.

An additional challenge lies in taking advantage of our new thinking about the hybrid workplace to reassess our need for leased space. Prior to the impact of the pandemic, PNNL was actively pursuing the acquisition of additional office space through leasing and new construction. Consistent with our hybrid workplace planning and principles, we have created a new Campus Realignment Project, which includes modifying existing workspaces to match the needs of on-site, hybrid, and virtual workers. These changes are allowing for new projections of office space needs, which are now significant enough that we have placed our office space expansion and acquisition plans on hold, with the exception of our space in Seattle (which will continue to be in high demand). The Campus Realignment Project will entail a series of realignment pilots showcasing new workspace options, including hoteling/hotdesking office space;

collaborative, activity-based spaces; and in-person/remote meeting experiences. The pilots will include technology (software and hardware), furniture, and possibly a re-architecture of specially selected spaces. Existing spaces in facilities across the campuses will be configured to support shared office space (e.g., hoteling and hot desking). These efforts are expected to free up 10 to 15 percent of existing space on campus to support current and future needs. During FY 2022, PNNL will be in position to evaluate the results of the campus realignment efforts and their impact on future facility investment decisions.

It is unlikely that lab-centric facilities will be altered as significantly by the Campus Realignment Project, due to researchers' need to be near their laboratories—delivery for our sponsors is our first principle. Thus, in lab-centric areas, such as the 300 Area, we envision an unabated need for additional office space.

Net-Zero Emissions and Energy-Resilient Operations (NZERO). PNNL has begun development, in consultation with DOE, of a Laboratory-wide initiative to achieve NZERO emissions with energy resiliency at our campuses. This goal is challenging but can be achieved through the successful demonstration and deployment of advanced sustainability technology. Our NZERO initiative will address *reducing* energy consumption, *replacing* carbon-based fuels and eliminating other greenhouse gas emissions, ensuring the *resiliency* of operations, and establishing PNNL as a NZERO *research* testbed. This testbed will support technology demonstrations with transparent, integrated, data-rich information streams for use by partners and stakeholders. Our vision is to serve as a national demonstration of the feasibility for achieving the administration's climate and energy goals and accelerate progress toward these goals through government-industry partnerships.

PNNL is uniquely positioned among DOE laboratories to take on this challenge because of the following:

- Our footprint is geographically and operationally diverse.
- We are already well-instrumented and transactive-controls-ready.
- Our energy usage is relatively low compared to other national labs.
- We have a large and diverse portfolio of expertise in clean energy research and technology development, coupled with a strong track record of partnering with industry for deployment.
- Our facilities and infrastructure are well maintained with the lowest deferred maintenance among the national laboratories.
- We align with and will leverage Washington State's commitment to provide 100% clean energy to the state.

We intend to eliminate emissions of all Scope 1 and 2 greenhouse gases in aggregate (measured as CO_2 equivalent emissions). We will eliminate direct emissions as a top priority and will eliminate on-site fossil fuel use at an early stage. We will fully eliminate indirect emissions resulting from electricity consumption by substantially reducing the amount of energy we consume and by changing the sources of that energy. In addition, while our initial focus will be on Scope 1 and 2 emissions, we will track, monitor, and incentivize the reduction of Scope 3 emissions—those indirect emissions resulting from other activities.

We will control emissions for all facilities and operations at Richland, Sequim, and other PNNL locations, including both owned and leased facilities. Note that the NZERO goal applies to the entirety of PNNL rather than to each facility or location in isolation. Our initiative does not envision the purchase of credits or offsets, since such steps do not directly accelerate technology development and adoption.

PNNL's strategy with respect to this initiative includes a variety of infrastructure investments and the integration of innovative technologies into existing infrastructure and operations. Through aggressive, near-term investments and deployment of associated operational strategies, initial planning efforts indicate PNNL's emissions can be reduced up to 50 percent over the next three to five years. Complimentary to the reduction of emissions, resiliency will be enhanced by substantially reducing the amount of energy required to operate PNNL. Most substantially, near-term actions to reduce emissions include, but are not limited to, the following:

- Electrify building heating sources and on-campus transportation to eliminate carbon-based fuel
- Upgrade facilities and infrastructure (e.g., HVAC, heat recovery, and lighting)
- Deploy advanced system analytics, automated controls, and fault detection to optimize operations and further reduce energy needs
- Leverage our energy storage R&D for applications to operations across PNNL campuses.

In parallel, and in the near term, we intend to transform PNNL into an ideal site to conduct research and demonstrate new technologies—both those developed by the Lab and those explored with third parties. Longer term, our efforts will focus on incorporating distributed renewable power generation (both on- and off-site); increasing energy storage capacity; and realizing the full impact of transactive operational controls deployment, improved campus resiliency, and emissions reduction through partnerships with regional organizations, local and national companies, energy system operators, and other stakeholders. We see these partnerships as opportunities for deliberative action to improve environmental justice, for example, through our relationships with Tribes on the Olympic Peninsula and/or by leveraging utility partnerships to better serve rural communities in Eastern Washington.

Each of the plans associated with the PNNL's Ten-Year Campus Strategy (described below) incorporate investments for, and are aligned with, PNNL's goal of achieving NZERO.

Campus Strategy

In partnership with our Pacific Northwest Site Office (PNSO), PNNL is developing and executing a 10-year campus strategy representing a new wave of campus transformation. Our strategy includes two funded capital line-item projects that will substantially advance our capabilities in chemical catalysis and battery breakthrough technologies.

The Energy Sciences Center – Reinventing Chemical Catalysis

The ESC will be a DOE-SC science laboratories infrastructure (SLI)-funded $90M line item. It will house basic and applied research programs in an ~139K gsf facility consisting of 52 laboratory modules, 200 workstations, and additional collaboration space. The ESC is under construction and is scheduled for completion in late FY 2021.

The ESC will support the Condensed Matter Physics and Materials Science, Applied Materials Science and Engineering, Chemical and Molecular Sciences, Chemical Engineering, and User Facilities and Advanced Instrumentation core capabilities.

Grid Storage Launchpad – Grid Control and Energy Storage at Massive Scale

The mission of the GSL, a DOE-OE funded project, is to validate and accelerate next-generation energy storage materials and technologies through collaboration across the entire energy storage community, including other DOE labs, academia, and industry. PNNL is constructing the GSL, which received CD-2/3 approval in March 2021. The $77M project is scheduled to break ground in Q3 of FY 2022, and will serve as a collaborative energy storage R&D facility for the nation, providing an 85,000-square-foot facility designed for safely testing energy storage systems under realistic grid operating conditions.

Following completion of the GSL (Q4 of FY 2023), PNNL will consolidate the Laboratory's footprint onto the PNNL Richland Campus by vacating a third-party leased facility. PNNL is currently analyzing the most appropriate option.

The GSL will support the Chemical and Molecular Sciences, Condensed Matter Physics and Materials Science, Applied Materials Science and Engineering, Systems Engineering and Integration, and Power Systems and Electrical Engineering core capabilities.

New Campus Strategy Objectives

In addition to the capital construction described above, PNNL is pursuing five campus strategy objectives to assure that the laboratory remains well-positioned for its future. PNNL is evaluating an increase to indirect Facility and Infrastructure funding beyond FY 2023 to address emerging needs and support projected Lab growth. As the campus strategy matures, PNNL will consider off-cycle requests to initiate projects to support our mission.

F&I Objective 1: Facility Capabilities in Support of Molecular Microbial Phenomics

A recent BER workshop report highlights a common gap in researchers' ability to characterize and predict biochemical pathways and the function of microbes from single cells to soil microbial communities that absorb and change phenotype due to environmental perturbations. To address these gaps, PNNL is proposing a new BER research capability for M^2P. The M^2P would allow the following:

- High-throughput automated single-cell communal isolates and soil microbial experimental culturing capabilities
- Multimodal characterization of microbial gene function in single cells and communities at speed and scale
- Annotation of biological function through coupled AI/ML-driven observation, experimentation, and analyses.

This objective would support PNNL's Chemical and Molecular Sciences, Biological and Bioprocess Engineering, Biological Systems Science, Climate Change Science and Atmospheric Science, and User Facilities and Advanced Instrumentation core capabilities.

F&I Objective 2: Demonstrating Sustainable Marine Energy Systems

Accelerating the development of marine energy requires dedicated facilities to evaluate new materials in marine environments, control systems for integrating marine power into specific applications and communities, and accessible field-testing locations to accelerate the device testing cycle and inform environmental assessments. These new capabilities and facilities must be able to integrate onshore laboratory testing and characterization under realistic marine conditions with marine test beds equipped with the state-of-the-art data collection, analysis, and visualization capabilities.

As DOE's only marine science laboratory, PNNL is uniquely situated to provide R&D in support of coastal and ocean-based technologies; however, some replacement/refurbishment/expansion of existing facilities on the PNNL Sequim Campus is required. These include the following:

- Advanced underwater test beds in multiple locations
- A data collection and analysis portal with innovative visualization capabilities
- Wet laboratories to enable foundational research and testing of novel materials
- High bay space for systems engineering and assembly
- Waterfront capabilities for loading and unloading pilot-scale systems onto research vessels

- Conferencing and collaboration space with in-person and online facilities.

These improvements would support PNNL's Earth Systems Sciences and Engineering, Systems Engineering and Integration, and Power Systems and Electrical Engineering core capabilities.

F&I Objective 3: Secure Facility Test Bed for Convergent Technologies, including 5G, Radio Frequency, and Artificial Intelligence

Critical energy infrastructure in the United States, and the DOE facilities that conduct research, development, and analysis to defend it, are under constant attack by adversaries seeking to disrupt operations and acquire U.S. knowledge and innovation. Safeguarding the security and resilience of U.S. infrastructure and of the classified environments and data used to prevent, detect, analyze, and respond to threats against it requires transformative new capabilities to address a growing landscape of technical surveillance dangers.

To mitigate the risk, a new infrastructure protection capability is needed to harness the integrated power of advanced computing, data analytics, AI/ML, and radio frequency exploitation, including advanced wireless communications modalities such as 5G and beyond. PNNL is proposing to construct federally owned Enhanced Security Facilities that would include the following:

- Multidisciplinary teaming at the intersection of science and security fields
- A physical environment that bridges research and production missions
- Experimental testbeds, including flexible laboratory spaces that can be rapidly reconfigured to adapt to emerging threats.

This activity would support the Nuclear Engineering, Systems Engineering and Integration, Decision Science and Analysis, Cyber and Information Sciences, Systems Engineering and Integration, and Advanced Computer Science, Visualization, and Data core capabilities.

F&I Objective 4: Extend the Life and Nuclear Mission Capabilities of the Building 325 Radiochemical Processing Laboratory Facility

The most important nuclear challenges facing the United States include the domestic production of nuclear material; safely storing, managing, and dispositioning radioactive waste; developing signatures that can be used to determine whether a facility is conducting proliferation activities; and forensics of nuclear and other radioactive material to determine the origin and history of materials. Multidisciplinary R&D will be required in each of these areas to overcome the challenges. Research in these critical areas requires nuclear facilities. Nuclear facilities across the complex are mostly subscribed, and over half are more than 40 years old. While the overall asset condition of 325RPL is Adequate, the condition index of the facility is at 89, identifying the need for significant investments to bring the facility up the PNNL standard of 95.

PNNL is planning for a lifecycle extension of the 325RPL facility that is crucial for long-term support of these critical research challenges. 325RPL was designed and constructed in 1953 and is in the 300 Area of the Hanford Site. It is one of only two remaining DOE-SC Hazard Category II non-reactor nuclear facilities. Life cycle extension for 325RPL is required to address the aging infrastructure and space configurations to continue to meet mission needs and operate safely; modification to the 325RPL will include the following:

- Refurbish and expand 325RPL's aging and undersized ventilation system
- Refurbish or replace beyond useful life plumbing and electrical
- Refurbish deteriorating exterior
- Replace roof at end of useful life
- Renovate 1950's-era laboratories, including replacement glove boxes, fume hoods, lab spaces, and instrument suite
- Refurbish hot cell infrastructure

These improvements would support the Nuclear Engineering, Chemical Engineering, and Nuclear and Radiochemistry core capabilities.

F&I Objective 5: Extend the Life of 300 Area Radiological Facility Capabilities, Roads, and Utilities

PNNL occupies multiple buildings in the 300 Area of the Hanford Site that support important missions, including 325RPL; the Life Sciences Laboratory, which conducts work in characterizing and monitoring aquatic and terrestrial ecosystems as well as geophysical methods for monitoring field-scale and regional phenomena; and the Radiological Calibrations Laboratory, which provides testing and calibration of a large variety of radiological instrumentation, dosimetry, and radiation effects research. Key infrastructure and building systems that are managed by PNNL are reaching the end of their useful life and need replacement. PNNL has agreement (through PNSO) with DOE's Office of Environmental Management (EM) to occupy these Hanford 300 Area facilities for an extended period; the continued reliability of the systems in these facilities is paramount to their safe operation.

Modifications to the 300 Area would include the following:

- Replace the aging primary water lines to prevent catastrophic water leaks
- Refurbish and expand the 300 Area buildings' aging and undersized ventilation systems
- Convert end-of-life heating systems to energy-efficient technology to support the NZERO initiative
- Reroute the road that crosses the PNNL Site and is used to deliver decommissioned Naval reactor compartments to the Hanford Site; it currently intersects culturally sensitive land and should be rerouted around this area to reduce the risk of inadvertent environmental impact and avoid future mitigation liability.

These 300 Area facilities support multiple core capabilities, including Biological Systems Science, Nuclear and Radiochemistry, Nuclear Engineering, Chemical Engineering, Environmental Subsurface Science, and Chemical and Molecular Sciences.

Site Sustainability Plan Summary

Fundamental to the science and technology outcomes that PNNL delivers every day is a commitment to sustainability—a serious responsibility. Sustainability at PNNL encompasses environmental stewardship in our operations, as well as how the Laboratory demonstrates social responsibility and advances economic prosperity—all in a manner that delivers lasting benefit to our sponsors, community, and the nation.

From innovative best practices in sustainable operations to environmentally focused scientific breakthroughs, PNNL is committed to making the world a better place to live for many generations to come. In FY 2020, despite the unprecedented disruptions and challenges of the ongoing COVID-19 pandemic, staff at PNNL have remained productive. Key accomplishments and initiatives in advancing PNNL sustainability are highlighted below.

Reducing Energy Use

In March 2020, PNNL moved into curtailed operation to combat the COVID-19 pandemic and transitioned over 90 percent of PNNL's nearly 5,000 staff to telework. Since then, building operations have been modified to ramp up outside air flow to deliver maximum fresh air into applicable buildings following the Centers for Disease Control and Prevention (CDC) guidance. However, due to much reduced plug loads, PNNL was able to achieve an overall reduction in energy intensity of approximately 5 percent compared to FY 2019. Figure 10 provides PNNL's total energy use (in million British thermal unit [MMBtu]) in FY 2020, as well as the projection through FY 2032, assuming that net zero emissions and energy resilient operations (NZERO) are achieved by 2030.

Reducing Water Use Intensity

By the end of FY 2020, PNNL reduced its water intensity by 64.6 percent compared to the FY 2007 baseline and achieved an 8.9 percent year-over-year usage reduction compared to the revised FY 2019 potable water usage. This is a 10 percent year-over-year reduction in the water use intensity (WUI). This accomplishment was achieved primarily due to water conservation and efficiency efforts.

Sustainable Building

Currently, PNNL has 11 (or 517,841 gsf) of 21 (or 1,149,480 gsf) applicable buildings compliant with the guiding principles issued by the Council of Environmental Quality (CEQ). This is 52 percent by building count, or 45 percent by total square footage.

PNNL has committed that all new construction, major renovations, and alterations of buildings greater than 10,000 gsf will comply with the guiding principles. PNNL started construction on the ESC project in early calendar year (CY) 2020. This facility will co-locate chemists, materials scientists, and computational scientists to advance catalysis and material syntheses for energy application. The ESC building will be PNNL's next sustainable building compliant with the 2016 guiding principles and will be equipped with controls and sensors enabling Smart Labs operations.

Additionally, PNNL has begun the design of a GSL building to consolidate and enhance the grid energy storage research capability. This building will also be designed to meet the 2016 guiding principle requirements.

In FY 2021, PNNL began the development of a Laboratory-wide initiative that will result in NZERO emission and energy-resilient operations. The objectives of the NZERO initiative will be a critical element in the planning and design of PNNL's facilities and infrastructure investments.

PNNL is on Track to be 50001 Ready

In FY 2020, PNNL signed an agreement to support DOE's *50001 Ready Cohort* initiative. This *50001 Ready* Energy Management System (EnMS), when implemented fully, will improve PNNL's ability to continually identify, monitor, track, and improve energy conservation measures. PNNL is positioned to obtain the *50001 Ready* recognition from DOE by the end of 2021 or early 2022.

Elevating Energy/Water Resilience through Technical Resilience Navigator

DOE's Federal Energy Management Program (FEMP) Technical Resilience Navigator (TRN) provides a systematic approach to examining resilience needs and goals, assessing on-site energy and water systems, evaluating risk, identifying resilience gaps, and developing and prioritizing solutions to resolve those gaps.

In FY 2020, PNNL was selected by the Federal Energy Management Program to pilot its TRN tool to determine the effectiveness of the methodologies and provide lessons learned/improvement opportunities. PNNL seeks to utilize the TRN process as a means of reviewing and improving its existing resilience posture. As a secondary objective, PNNL plans to share the lessons learned with other DOE sites. The TRN pilot is scheduled to be completed in FY 2021.

Better Building Smart Labs Accelerator Partner

PNNL participated in DOE's Better Building Smart Labs Accelerator Partner Program. In FY 2019, PNNL developed a Smart Labs evaluation tool to help with consistent review and qualifying buildings and laboratory spaces as "Smart Labs." To date, PNNL has qualified one building and 40 laboratory spaces using. the PNNL Smart Labs checklist. In FY 2021, PNNL plans to align the Smart Labs evaluation process with the Energy Independence and Security Act (EISA) commissioning/retro-commissioning requirements as a continuous improvement effort.

PRINCETON PLASMA PHYSICS LABORATORY

Lab-at-a-Glance

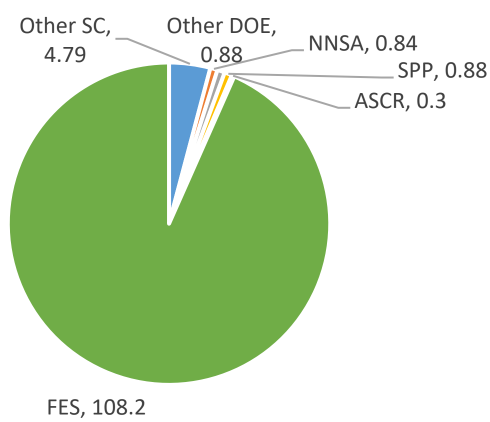
Location: Princeton, NJ
Type: Single-program Laboratory
Contractor: Princeton University
Site Office: Princeton Site Office
Website: www.pppl.gov

- **FY 2020 Lab Operating Costs:** $115.89 million
- **FY 2020 DOE/NNSA Costs:** $115.01 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $0.88 million
- **FY 2020 SPP as % of Total Lab Operating Costs:** 0.8%

Physical Assets:
- 90.7 acres and 32 buildings
- 763,000 GSF in buildings
- Replacement Plant Value: $835.2 M

Human Capital:
- 577 Full Time Equivalent Employees
- 9 Joint Faculty
- 39 Postdoctoral Researchers
- 53 Graduate Students
- 37 Undergraduate Students
- 312 Facility Users
- 35 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

The U.S. Department of Energy's (DOE) Princeton Plasma Physics Laboratory (PPPL) is a collaborative national center for fusion energy science, basic sciences, and advanced technology. The Laboratory has three major missions: (1) to develop the scientific knowledge and advanced engineering to enable fusion to power the U.S. and the world; (2) to advance the science of nanoscale fabrication for technologies of tomorrow; and (3) to further the development of the scientific understanding of the plasma universe from laboratory to astrophysical scales.

PPPL's expertise in fusion and plasma science and the role it plays in the DOE missions are reflected in PPPL's five core capabilities:

- Plasma and Fusion Energy Sciences
- Systems Engineering and Integration
- Large Scale User Facilities/Advanced Instrumentation
- Mechanical Design and Engineering
- Power Systems and Electrical Engineering

The Laboratory's highest priority is the successful construction of the National Spherical Tokamak Experiment Upgrade, a world-leading compact fusion experimental user facility. PPPL is also partnering in the ITER Project to prepare for U.S. participation in the first burning plasma. As the only DOE national laboratory with a Fusion Energy Sciences mission, PPPL aspires to be the nation's premier design center for the realization and construction of future fusion concepts. In addition, the Laboratory is evolving, broadening its expertise to more effectively contribute to the economic health and competitiveness of the U.S. by serving as a national leader in computation, nanofabrication, surface science, and technology. Indeed, PPPL aims to drive the next wave of scientific innovation in plasma nanofabrication technologies to maintain U.S. leadership in this critical industry. Princeton University and PPPL develop the workforce of the future by educating and inspiring a diverse cadre of world-class scientists, engineers, and operations staff to serve the Laboratory and the national interest.

Core Capabilities

The Princeton Plasma Physics Laboratory (PPPL) has five DOE-designated core capabilities, two emerging core capabilities, and one proposed new capability that enable the vital role of the Laboratory in executing DOE's missions, as well as in aiding the development of industry-driven science initiatives:

1. Plasma and Fusion Energy Sciences;
2. Systems Engineering and Integration;
3. Large-Scale User Facilities/Advanced Instrumentation;
4. Mechanical Design and Engineering;
5. Power Systems and Electrical Engineering;
6. Computational Science (beyond plasma simulation)*
7. Condensed Matter Physics and Materials Science*
8. Chemical and Molecular Science**

*Emerging
**Proposed New

PPPL has proactively strengthened and reinvigorated capabilities 2-5 for the NSTX-U Recovery Project by recruiting from both private industry and other national laboratories, and through closer interaction with experts from other national labs during project reviews. The totality of PPPL's integrated science and engineering capability make it uniquely equipped for development with Universities and industry in the pursuit of the next generation of fusion concepts, innovations, and designs.

PPPL has been at the forefront of developing numerical capabilities for fusion prediction, analysis, and design, and for plasma simulation, in general. PPPL's world-leading capabilities in diagnosing and understanding plasmas will support the next generation of nanoscale fabrication, which are central to the development of technologies of many *technologies of tomorrow*. However, these technologies require a multidisciplinary set of capabilities that PPPL is committed to strengthening and growing.

PPPL's unique capabilities in diagnosing and understanding plasmas will support the next generation of industrial plasma processing. Through the activities outlined below, PPPL is increasing efforts to strengthen and/or diversify into research areas embodied in these additional core capabilities mentioned above, which are further described later.

Plasma and Fusion Energy Sciences

PPPL has made history as a world-leading experimental and theoretical plasma physics and fusion facility, with depth and breadth of research that is still unparalleled in the U.S. or the world. This uniquely positions PPPL to lead and coordinate the multidisciplinary research needed to advance the goals of FES, and to prepare students and staff for leadership in the field.

As such, PPPL and Princeton University staff have been instrumental in community planning activities since FY 2020, both as participants and in leadership roles. The program committee of the community planning process (CPP) includes six members affiliated with PPPL or Princeton University, including one of the co-chairs of the process. Staff at PPPL and Princeton University were fully engaged in the CPP process and the writing of the final report, completed in 2020. Successfully designing, constructing, and operating a world-leading "next-generation facility"—a recommendation in the final report—will require PPPL's long-standing and diverse expertise in fusion energy sciences, experience and capacity for executing projects within the DOE environment, and close involvement with major international projects.

Two efforts in 2020, which culminated in 2021, followed on from the CPP report. The first was a FESAC subcommittee tasked to flesh out details of the CPP report and produce a true strategic roadmap for the U.S. fusion program. Further, a National Academy of Sciences and Engineering panel was tasked with developing the strategy for "Bringing fusion to the grid." The panel was comprised of representatives from national laboratories, universities, and the electric power industry. The final report was issued in February 2021. PPPL had representatives on both panels, with a PPPL researcher chairing the NAS panel.

The Laboratory continues to explore the plasma processes that take place in the universe; the high-temperature, high-pressure magnetically confined plasmas required for fusion energy production; and the use of plasmas in technological applications, including the synthesis and modification of materials. PPPL conducts research on experimental facilities located at PPPL, including the National Spherical Torus Experiment Upgrade (NSTX-U), the recently upgraded Lithium Tokamak Experiment – Beta (LTX-β), the Magnetic Reconnection Experiment (MRX), the Low-Temperature Plasma (LTP) Laboratory, and the Facility for Laboratory Reconnection Experiment (FLARE). In addition, PPPL staff members are leading significant research programs at DIII-D (San Diego), the superconducting long-pulse facilities W7-X (Germany), KSTAR (South Korea), and EAST (China), as well as smaller research collaborations at MAST-U (UK), JET (UK/EU), ST-40 (UK), ASDEX Upgrade (Germany), LHD (Japan), and WEST (France).

PPPL's researchers contribute computational plasma physics and theory expertise toward the development of Whole Device Modeling (WDM) applications for the DOE Exascale Computing Project, as well as for Scientific Discovery through Advanced Computing (SciDAC) Centers. Initiatives in plasma- material interactions, such as nanomaterial synthesis, plasma processing, and plasma-surface modification, uniquely qualify PPPL to lead in the science behind the trillion-dollar industry that uses plasmas to create their products.

Noteworthy updates illustrating increased integration between fusion and plasma physics, computational science, and engineering analysis and design include:

- New tools capable of simulating flows and heat transfer using Computational Fluid Dynamics (CFD) were successfully employed to create numerical models of plasma-facing components (PFCs), with complex cooling structures. These were applied to the design and optimization of the diagnostic modules for ITER. Thermal analysis included nuclear volumetric heating as well as surface heating distribution on the front face. Results of thermal analysis were used as a thermal load for non-linear elastic plastic structural analysis.
- The Fluid dynamics model was expanded to include magnetohydrodynamics (MHD) capability, allowing analysis of the flows of conducting liquids in magnetic fields, such as Tritium breeding blankets. Electromagnetic equations are solved in the liquid metal, as well as in the solid components of the structure and plasma. The capability to model transition through all four phases of matter was tested. This allows for model complex phase-transition events in fusion devices. Solid metallic PFCs can undergo transient melting in response to high heat flux events such as large edge-localized modes (ELM),

unipolar arcs and disruptions. Changes in surface morphology caused by the motion and possible destabilization of the resulting melt layer can lead to a considerable degradation of the PFC longevity and heat-handling properties.

Systems Engineering and Integration

PPPL is well positioned to lead the systems engineering and integration of new fusion facilities to incorporate innovative designs for reduction of capital costs and risk mitigation. Systems Engineering and Integration principles are ingrained in PPPL's daily work processes to include the engineering staff and technicians for design to include field integration, with consideration for technical risk and failure modes throughout the engineering lifecycle. This creates a force multiplier in implementing more efficient systems, implementation cost as part of the design and establishing better lines of communication within the workforce.

Systems engineer begins to incorporate the lessons learned from successful complex systems changing the current systems engineering paradigm of trying to predict requirements of systems that are years from operation. Rather, use of provide high-level system requirements at the conceptual design phase to provide technical trade studies while focusing on key tenets, i.e., safety, reliability.

The INCOSE Vision 2025 includes using virtual engineering simulation and visualization into an integrated model-based approach versus the traditional model-based systems engineer (MBSE) process.

PPPL establishes a virtual engineering environment that incorporates modeling, simulation, and visualization to support all aspects of systems engineering by enabling, prediction, analysis, optimization and capture complex emergent behaviors. This virtual engineering environment will address improving the systems engineering process by including the theoretical foundation of fusion systems to advance the state of the practice.

PPPL's systems and design engineering expertise positions PPPL to assume a leadership role in designing and establishing a virtual engineering environment. The is quite valuable to enhance the planning, design and integration of research and development activities leading to the conceptual design of a fusion power plant. This environment focuses on the increased interaction and communication while between physics, engineering, analysis and CAD. This provides some of the following capability:

- Quick-turn scoping studies with feedback loops between engineering
- Semi automation and automation of workflows
- Conduct performance and sizing requirements for different models
- Cost considerations as a parameter
- Engineering and capturing the interfaces between models with the subject matter experts

There is a potential to establish a public-private partnership with industry to develop a commercial environment removing some of the risk and providing the interfaces between components of the environment.

Part of the virtual engineering includes virtual/augmented reality. This can be used to add data in near real-time on simulated plasmas in a short time step should be included to address as remote maintenance, to avoid exposure to hazardous environments; and the importing of data from diagnostics and instrumentation associated with test stands, prototype efforts, experiments, or modeling results. Establish experiments to establish a proof of concept to capture. The utility of using this technology.

Large-Scale User Facilities/Advanced Instrumentationn

PPPL's large facilities and extensive capabilities for plasma production, confinement, control, and measurement systems make it an ideal site for research development and collaborations. PPPL specializes in technologies to safely heat, fuel, control, and exhaust plasmas at temperatures as high as 550 M°K, with a broad application and uses beyond NSTX-U.

Technologies that are being developed as prototypes for future devices include flexible neutral beam injection and ion cyclotron range of frequency (ICRF) waves that can be used for both heating and current drive.

Gas injection at supersonic speeds will be tested as a means to efficiently fuel the deep core. Real-time plasma control methodologies are being developed that will allow for control of the plasma, and tailoring of plasma profiles, to maintain stable, high-performance plasmas for their entire lifetime. An Impurity Powder Dropper (IPD) and Impurity Granule Injector that have shown success on domestic and international facilities will be employed to mitigate heat flux and control edge instabilities. Liquid lithium component prototypes will be tested as a basis for a more expansive liquid lithium divertor that would be a transformative solution to heat flux mitigation in compact, high-temperature devices.

Research on NSTX-U and LTX-beta, in particular, has led to exploration of how innovative wall coatings, such as lithium, can reduce wall recycling and lead to enhanced plasma confinement. Evidence from both machines indicates at least 50% higher plasma confinement can be achieved. Further, the testing of liquid lithium components in both devices are critical to developing a transformative path to controlling power fluxes escaping the plasma, and this will allow for operation of high-performance, long-pulse discharges.

NSTX-U's active plasma control development group is developing real-time plasma control algorithms to be applied to the lifetime of the NSTX-U discharge, as well as a critical set of real-time diagnostics to serve as sensors in these algorithms. The objective is to produce, and be able to control in real-time, long-pulse, high-performance plasmas that may be prototypical of those in next-step devices.

Other updates of note are:

- For NSTX-U, several new diagnostic capabilities that will provide measurements to enable real- time plasma control have been or are being deployed on NSTX-U. These include:
    - real-time measurements of the plasma toroidal rotation velocity via charge exchange recombination spectroscopy, and
    - measurements of the electron temperature and density via Thomson scattering.

  Other new capabilities include upgrades to the material analysis probe to allow improved analysis of material samples that are exposed to the plasma and upgrades to the fission chamber neutron detectors for improved reliability.
- The first absolutely calibrated Ly-alpha measurement has been developed and deployed on DIII- D to determine the neutral density and ionization source in the plasma. PPPL and MIT developed the instrument using additive manufacturing and a novel on-site compact vacuum calibration chamber.
- LTX-β has resumed operation to provide higher magnetic field, neutral beam injection, and enhanced diagnostics. PPPL and collaborating institutions will investigate plasma confinement with a liquid lithium boundary with more relevant plasma parameters and separate control of the plasma heating and plasma particle source.
- The FLARE collaboration facility installation has begun and enables world-leading studies of reconnection of magnetic fields in plasma.
- Recently, the use of the IPD that was commissioned on the Large Helical Device (LHD) Japan in FY 2020 has led to the observation of a novel improved confinement regime. Electron temperature increases of up to 50% accompanied by increases in ion temperature and suppression of density fluctuations across the full plasma cross-section are observed with boron powder injection. Analysis is ongoing to understand this new operational mode.

Mechanical Design and Engineering

PPPL has implemented a design approach, using systems engineering techniques, to ensure that requirements are identified as early as possible, and that the design is verified throughout its evolution by a series of reviews. The NSTX-U Recovery project benefited from this approach, with well-documented designs leading to successful CDE-2, 3a and 3b reviews.

Engineering processes and procedures have been updated to align with the PPPL quality program. The Laboratory's Quality Assurance Program Description has clearly defined roles for engineering in design verification, validation and implementation.

The engineering shops at PPPL were upgraded with multiple state-of-the-art multi-axis CNC machines. Machinists with specialized training were hired to operate these machines. PPPL is now able to produce large-scale, complex prototypes and components, and build parts in large quantities in response to occasional urgent needs.

Virtual engineering will be an important capability for the design of the next generation of fusion experiments, and the Engineering Department is establishing a strong presence here. Integrated simulation and workflows for optimized design, with the optimization integrating physics and engineering considerations, are being developed. The designs of the MUSE stellarator and, to a greater extent, the ARPA-E permanent magnet stellarator, will drive and benefit from these capabilities. Initial use of integrated simulation capability for other programs such as ITER diagnostics to establish workflows as part of system design will be available.

Analytic capability, already strong, is increasing. Enhanced computing power has made the application of nonlinear features in finite element analysis more common. Multiphysics capabilities of commercially available codes are used more often. Computational fluid dynamics is being used more often, for example in the analysis of complicated water-cooling systems for ITER first wall components. And magnetohydrodynamic analysis is being developed for the design of liquid metal components. Cloud computing capability, and a new supercomputer at Princeton University, will support these large-scale analyses.

These capabilities will make PPPL Engineering a leader in many areas, including:

- Completion of NSTX-U Recovery and support of operations, including the development and
- use of "digital twins,"
- Collaboration with other institutions in design and manufacture, such as on COMPASS-U, ITER, WEST, and JT-60SA,
- Leading the effort to design and build a fusion pilot plant,
- Developing liquid metal plasma-facing components,
- Helping PPPL's research into semiconductors and nanotechnology

Power Systems and Electrical Engineering

PPPL offers both the physical infrastructure and the technical capabilities for meeting the extraordinary power system demands intrinsic to fusion energy research machines.

As part of the Metuchen-Trenton-Burlington (MTB) project, PSE&G is replacing its 138kV lines with 230kV. PSE&G is maintaining the 138kV service to PPPL, near the Plainsboro Substation, by installing a new 230/138kV (550 MVA) autotransformer. This transformer has been selected in conjunction with the Laboratory, to support the future experimental load requirements. The capacity of the main switchyard transformers is sufficient to support the NSTX-U power load and auxiliary experimental system loads for the planned 10-year run of NSTX-U.

The Laboratory has two main "age groups" of electric power distribution. Group 1 consists of electrical equipment installed to support the initial operations of the Laboratory in the late 1950s and early 1960s. Group 2 equipment was installed in the late 1970s to support the TFTR period of operations and continues to provide the electrical power distribution for NSTX-U. While NSTX-U will continue to be the largest power demand for the

Laboratory, it still used significantly less than that of TFTR, for which the D-Site experimental power system was originally designed.

Generally, the priority over the next 10 years is to replace the 60-year-old equipment of the Group 1 electrical distribution system, including a new transformer for supplying alternate experimental power to C-Site. The capacity of this transformer will be sized to account for the present and future loads of the C- Site experiments. The loads considered include LTX-beta and the RF loads supporting NSTX-U. The work for this replacement is predominantly covered by PPPL's CIRR project.

Anticipated, future developments to support this capability include:

- expansion of power conversion engineering staff to enhance systems engineering capabilities, integrate fusion design activities, facilitate advances in fusion technology, and reduce the development risk in future designs through virtual, modern engineering practices; and
- expansion of radio frequency (RF) engineering staff to continue enabling research in low- temperature plasma (LTP) material interaction for industrial applications.

Emerging and Proposed New Core Capabilities

PPPL's unique capabilities in diagnosing and understanding plasmas will support the next generation of industrial plasma processing. PPPL is increasing efforts to progress and/or diversify into research areas embodied in three core capabilities:

- Computational Science
- Condensed Matter Physics and Materials Science
- Chemical and Molecular Science

In recent decades, one of the two goals of the Fusion Energy Sciences program in the United States has been to build the knowledge needed to develop a fusion energy source. This knowledge is generated by the careful design and study of experiments and simulations. Interpretation of what we observe in fusion experiments requires computation, and thus the knowledge we have about fusion as an energy source is literally encoded and expressed in whole-device models of fusion systems. In this very real sense, fusion energy science is computational science. Recognizing the centrality of computation to the Laboratory, FES, and wider DOE missions, a new Associate Laboratory Director for Computational Science position was created and filled in 2020. Subsequently, a new Computational Sciences Department (CSD) was established, focusing on six distinct areas: software engineering, high performance computing, data science and learning, algorithms and applied mathematics, integrated modeling, and, looking to the future of computing, quantum information science.

The Laboratory aims to extend its capabilities and expertise in nanofabrication science, especially in the context of low-temperature plasma science. Nanofabrication science in this context necessarily involves **condensed matter physics and materials science** since the purpose of nanofabrication technology is to modify materials that will be used in solid state electronic or quantum devices. In order to lead the new initiatives in nanofabrication for advanced electronics and Quantum Information Science, PPPL hired a new Associate Laboratory Director for Low-Temperature Plasma-Surface Interactions (LTPSI), as well as an expert in Quantum Information Science. These individuals are collaborating closely with existing PPPL staff with LTP expertise, as well as with industry and several Princeton University departments (PRISM, Chemical and Biological Engineering (CBE), Electrical Engineering, and Physics).

PPPL is also proposing a new, closely-related core capability in **chemical and molecular science** associated with understanding and control of plasma chemistry. This core capability is related to PPPL's new efforts in developing plasma nanofabrication science and technology for materials that will be used in solid state electronic and quantum devices.

The Laboratory expects to establish these three new core capabilities over the next five years.

Science and Technology Strategy for the Future/Major Initiatives

The Laboratory has three related missions:

1. The first is to develop the scientific knowledge and advanced engineering to enable fusion to power the U.S. and the world. PPPL's highest priority is the successful recovery and operation of its User Facility, NSTX-U, an innovative experiment that could lead to a reduced cost route to commercial fusion power. PPPL is also exploring the science of novel advanced fusion concepts and technologies with computer simulation and targeted experiments. The Laboratory is collaborating with private fusion companies and foundations to move fusion science and technology toward market viability.
2. The second mission is to advance the science of nanoscale fabrication for technologies of tomorrow. Nanoscale fabrication for microelectronics and eventually sub-nanoscale fabrication for quantum systems is central to the U.S.'s future economic security and competitiveness. PPPL expertise is highly sought-after by industries dependent on plasmas to synthesize and fabricate the nanoscale structures in their products. Industry needs have facilitated many new partnership opportunities for the Laboratory. These partnerships and expanded research opportunities have allowed PPPL to grow an attractive, diverse, multi-purpose R&D portfolio. PPPL's future as a multi-purpose laboratory will lead to growth in staffing, in the number of active experiments, and in the cross-fertilization of research programs as depicted in the 10-year timelines below.
3. The third mission is to further the development of the scientific understanding of the plasma universe from laboratory to astrophysical scales. The Laboratory's unparalleled capability in plasma physics is being employed to gain a predictive understanding of fundamental plasma processes that underlie important problems in astrophysics and space physics. A collaborative experiment, FLARE, is being constructed to unravel the mysteries of magnetic reconnection that powers many natural explosive events. The next frontier is to leverage investments in exascale fusion simulation to model ultra-relativistic kinetic plasma processes at the heart of multi-messenger astronomy, a window into the most mysterious and violent processes in the known universe.

PPPL is developing a diverse cadre of scientists for the nation's Science, Technology, Engineering, and Mathematics (STEM) talent pool, with graduates of its Ph.D. program in leadership positions at DOE national laboratories, research universities, and business and industry. Leveraging the resources of its M&O contractor, Princeton University, PPPL has access to funded, specialized research centers and institutes, as well as world-renowned scientists in multidisciplinary fields. Achieving the Laboratory's missions will require scientific diversification and growth, including new funding sources beyond FES. The following five strategic initiatives guide the evolution of the Laboratory in meeting DOE's program goals, as well as expansion of strategic, multi-sector partnerships over the next decade.

Infrastructure

Overview of Site Facilities and Infrastructure

The 90.7-acre Princeton Plasma Physics Laboratory is situated on Princeton University's 1,750-acre Forrestal Campus located in Plainsboro Township, New Jersey. This land, punctuated by dense woods, brooks, and nearby streams, has been leased to the DOE for operation of the Laboratory. The Laboratory is surrounded by several hundred acres of undeveloped land, including protected wetlands, and is conveniently proximate to both Philadelphia and New York City.

The Laboratory has a workforce and user population of approximately 750 and utilizes 763k gross square feet (GSF) of the Princeton University Forrestal Campus, 32 government-owned buildings. There are currently no leased buildings or facilities. PPPL updated its land lease agreement with the DOE on April 1, 2019, extending the lease through 2056. There were no other real estate transactions during FY 2020 and there are no current plans for transactions in FY 2021.

The major utility systems at PPPL include:

- Electrical distribution,
- Potable water,
- Non-potable water,
- Chilled water,
- Steam generation and distribution,
- Natural gas,
- Fuel storage,
- D-Site dewatering system,
- Sanitary sewer system,
- Fire systems,
- Computing infrastructure, and
- Telecommunications.

Primary 13 Primary 138 kilovolt (kV) power is provided by the local electric utility company. Ensuring the reliability and capacity of these utilities and systems is essential to mission readiness, as well as execution of PPPL's expanded vision.

All of PPPL's buildings and trailers are currently categorized as "Operating". All of PPPL's Other Structures and Facilities (OSF) are also categorized as "Operating" with the exception of one OSF asset, MG Free Cooling Ext. Pipe (Property ID # 7132030301, 400 linear feet).

Infrastructure Data Summary

Total Building Assets	**30**
Total Other Structured Facilities (OSF)	27
Total Deferred Maintenance 2019 ($)	**$70.7M**

As discussed in earlier sections, PPPL is embarking on significant mission expansion and requires the infrastructure that enables this strategy of multi-purpose science initiatives, public/private projects, and the associated population growth. Condition assessments have identified 62% of PPPL's buildings to be Substandard and Inadequate. PPPL relies on the completion of major SLI projects to provide the new and improved spaces necessary to safely support current research and operations. Nearly $12 million of the current General Plant Projects (GPP) portfolio is in construction, with another $7 million in design. The Laboratory has received CD-1 approval of more than $200 million in SLI Projects. CD-1 milestones for both the Princeton Plasma Innovation Center (PPIC) Building and the Critical Infrastructure Recovery & Renewal (CIRR) projects were approved in the second quarter of FY 2021. The CD-1/2/3 DOE Independent Project Review was successfully conducted in the second quarter of FY 2021. These projects will provide expanded scientific capability, enhance PPPL's resiliency, and improve efficiency with renewed utility infrastructure that provides increased data capabilities to leverage artificial intelligence for operations.

FY 2021

Condition	Buildings	Sq. Footage
Adequate	14	377,088
Substandard	10	287,462
Inadequate	8	98,512

Figure: Building Condition

The only gross square foot reductions under consideration at this time are associated with the SLI construction of the PPIC. PPIC will demolish two existing, "inadequate" buildings (Theory Building and the Administration Building), and the CIRR project will replace significant original infrastructure systems such as Electrical, HVAC, Chilled Water Generation, Underground Utilities, and IT. These systems, while not buildings, carry Deferred Maintenance (DM). Recovery and repair of these systems will reduce DM and dramatically improve the various systems' availability, reliability, and capability. A key factor for building assessments to reach an "Adequate" rating is having addressed the identified Repair Needs and DM. PPPL's campus strategy addresses these elements with the goal of producing Adequate Overall Asset Conditions on all Real Property Assets. PPPL has no underutilized buildings, and spaces currently suitable for personnel have reached capacity. The recent investment in a space management program has yielded opportunities for PPPL to identify areas for future transformation and better use of space.

Campus Strategy

PPPL plays a key role in the delivery of strategic goals outlined by FES, as well as general governmental goals for Science and Technology leadership in the development of *technologies of the future*. As the leading national laboratory for future fusion concepts, PPPL is actively working with universities and industry partners to further develop an expert understanding of plasma and its applications to new technologies, which are central to U.S. economic health, security, and competitiveness. Many industries, such as the microelectronics industry, utilize plasmas to synthesize and shape the materials in their products. These industries are actively proposing and initiating new partnership programs with PPPL researchers, which further underscores the need for additional investment in flexible, robust, and reliable infrastructure that will foster ground-breaking research occurring both on-site and remotely.

To support these efforts, as well as new, expanded opportunities across science disciplines, PPPL's campus must evolve to enable this vision. The campus strategy goes beyond the goal of providing reliable, efficient systems in new and planned facilities, and aims to position PPPL infrastructure as a strategic asset that adds value to the research experience. As PPPL continues to grow its expertise and staff in support of industry-driven plasma research, user facility expansion, and increasing opportunities for national and international collaboration, it becomes even more critical that the campus grows to meet those needs to provide safe, modern, efficient facilities and infrastructure.

The FY 2021 Maintenance and Repair (M&R) budget has been allocated higher than FY 2020 funding levels, but still well below the recommended 2% of replacement plant value (RPV). While PPPL continues to replace and modernize existing legacy infrastructure with GPP and SLI investments, further funding is needed. When PPIC and CIRR are completed, these projects will have replaced old, inefficient buildings (one 40+ years old and one 62+ years old); provided a new modern research building with nominal maintenance needs and high operating efficiencies; and replaced/modernized ~$80M in building systems and general plant infrastructure. These building systems and associated general plant infrastructure are well beyond their useful life and were not designed to accommodate the current and future needs for modern research. The Tritium System Demolition and Disposal (TSDD) project will recover thousands of square feet of usable space and free-up the FuRTH test cell, making this national asset available for public/private partnerships as discussed in previous sections.

While DM is rising, the effects of the aforementioned SLI infrastructure replacement projects (PPIC and CIRR) will result in reductions to DM once these projects are constructed. The GPP pipeline of projects is critical to sustaining, modernizing, and maintaining PPPL existing infrastructure. The campus strategy is currently at a pivotal point in which new science diversification plans have been defined.

Infrastructure – Core Capability Gap Analysis

Adequate, modern, and flexible laboratory space is required to foster innovation for efficient project management, as well as extensive collaboration between theorists, experimentalists, and engineers. PPPL looks forward to the completion of current projects – the PPIC, CIRR, and TSDD – to provide needed and currently unavailable scientific capability, to co-locate scientific staff populations, and to resolve functionality and reliability issues; however, further planning and assessment is ongoing with regard to specific infrastructure capabilities that will support growth in research and development and a more nimble state of readiness for future Laboratory opportunities within the DOE, as well as advanced industries. Most of PPPL's spaces were designed and built in the late 1950s and lack the physical capabilities and infrastructure to support modern research and anticipated research advancement. These spaces do not have sufficient floor area or volume to support the development of new fusion concepts or diagnostics for at-scale large fusion experiments.

Existing lab spaces are fully occupied or oversubscribed and do not support needs for joint collaborations using large-scale data sets. Adjacent office spaces that enable researchers to benefit from collaboration with subject matter experts in computational science, machine learning, artificial intelligence, exascale computing, data management, data acquisition, simulation, imaging, visualization, and modeling also are not currently available. Further, the present space is inadequate for the current ventures in microelectronics, nanofabrication research, and associated diagnostics, all of which require substantial foundations and ceiling height. Existing space is not reconfigurable and does not contain the environmental controls needed for smaller-scale diagnostic development. While opportunities are being pursued with Princeton University relative to microelectronics, nanofabrication, and Quantum Information Sciences (QIS), the Laboratory must aggressively renew the existing campus in order to provide the needed environment for current and projected growth.

PPPL's five existing core capabilities, two emerging capabilities, and one newly proposed, as well as the five strategic initiatives defined in Section 4, have informed the gap analysis in the table below. The listed Planning Objectives map PPPL's intent to reduce the risks currently delaying advancement of the strategic initiatives, and will support continued growth in established, emerging, and proposed new core capabilities.

<table>
<tr><th>Planning Objectives</th><th>Increase User Facility Reliability/Capability</th><th>Advance Technologies of Tomorrow</th></tr>
<tr><td>Gaps/ Risks</td><td>NSTX-U lacks adequate infrastructure to support users of an active user facility.
• Construct PPIC to offer modern lab spaces, collaboration spaces, and office spaces to both attract and support a long-term user base.
• Implement the CIRR project to update electrical distribution, HVAC systems, the communications distribution network, chilled water generation, and other critical utility services.

PPPL lacks adequate space for liquid lithium component research required to explore reduced cost of fusion in NSTX-U and next-step fusion devices.
• Pursue development leading to construction of Liquid Metals Development Laboratory with accompanying engineering and technical staff to safely develop and prototype liquid metal plasma-facing components (PFCs).</td><td>PPPL lacks modern lab and research space, equipment, and clean rooms to (1) advance nanofabrication research and to (2) pursue new Quantum Information Science (QIS) and low-temperature plasma (LTP) R&D:
• Design and construct PPIC to offer modern lab spaces, collaboration spaces, and office spaces for continued and/or new QIS and LTP research, and to provide space for diagnostics, fabrication, and testing.
• Complete TSDD project and rebrand and reclaim the Fusion Research Technology Hub (FuRTH) Test Cell space and unique attributes for use by private industries.
• Design and construct a new FuRTH collaboration building adjacent to the reclaimed FuRTH Test Cell to support external partners and growing R&D staff.
• Support partnerships for work at PRISM.</td></tr>
<tr><td>Impacted Science Initiative</td><td>1, 3, 4</td><td>2, 3, 4, 5</td></tr>
<tr><td>Impacted Core Capability</td><td>1, 3, 5, 6*</td><td>1–4, 6*, 7*, 8**</td></tr>
</table>

Science Initiatives

1. Rebuild NSTX-U, advance ST as a reduced-cost fusion concept
2. Develop new low-temperature plasma applications, nanofabrication for microelectronics, QIS, and sustainability
3. Optimize ITER burning plasmas and design next-step fusion devices including pilot plants
4. Improve fusion through innovations in 3D shaping, boundary composition, and magnets
5. Understand the plasma universe from the lab to the cosmos

Core Capabilities

1. Plasma and Fusion Energy Sciences
2. Systems Engineering and Integration
3. Large-Scale User Facilities/Advanced Instrumentation
4. Mechanical Design and Engineering
5. Power Systems and Electrical Engineering
6. Computational Science (beyond plasma simulation)*
7. Condensed Matter Physics and Materials Science*
8. Chemical and Molecular Science**

Planning Objectives	Enhance Laboratory Operational Reliability/ Safety	Enhance Laboratory Operational Efficiency	Diversify PPPL's Research Portfolio
Gaps/ Risks	To enhance Laboratory operational reliability and safety, PPPL must implement the CIRR project, to update electrical distribution, HVAC systems, the communications distribution network, chilled water generation, and other critical utility services. To participate in ITER and next-step fusion devices, reliable computing infrastructure and remote collaboration technology are required: • Partner with Princeton University for use of High-Performance Computing Resource Center (HPCRC); upgrade and relocate current computing systems to support exascale computing. • Design and construct PPIC's Collaboration and Visualization Hub (CVHub). • Build a dedicated data center supporting data mirroring applications requiring reliable and secure PPPL-managed data access.	To provide vastly improved sustainability, resiliency, safety, and efficiency, PPPL must implement PPIC and CIRR. Existing, usable building spaces and offices are oversubscribed and cannot accommodate the staff growth necessary for mission execution: • Design and construct PPIC to provide additional, flexible, mobile infrastructure to accommodate changing needs, and to provide space for diagnostics and actuators for FLARE, and a PM Stellarator, superconducting magnet research, and fabrication and testing space. Existing spaces are not able to co-locate or "cluster" collaborators and mission-focused research teams: • Construct a new building adjacent to the reclaimed FuRTH Test Cell to accommodate internal and external user growth and provide proximity to experiments. PPPL does not offer enough space to accommodate large collaborations: • Remodel existing spaces, including auditorium, for immediate and safe use for all groups. • Design and construct PPIC, which includes modern designs for collaboration space.	PPPL lacks space for new staff, external partners, and users of different science disciplines: • Design and construct PPIC to offer modern lab spaces, collaboration spaces, and office spaces. • Construct a new building adjacent to the reclaimed FuRTH Test Cell to accommodate internal and external user growth and provide proximity to experiments.
Impacted Science Initiative	3, 4, 5	2, 3, 4, 5	2, 4, 5
Impacted Core Capability	1, 2, 3, 6*	1, 3, 5, 6*, 7*, 8**	1–5, 6,* 7*, 8**

*Emerging **Proposed New

Based on this gap analysis, the Laboratory has identified the infrastructure priorities necessary to close these gaps and support mission readiness.

The Princeton Plasma Innovation Center (PPIC)

PPPL's immediate program needs also include modern laboratories, collaboration space, and office spaces to accommodate growth in scientific and engineering staff, as well as visiting scientists. PPIC will not offer new spaces in time for existing and near-term, emerging research, but will accommodate these user groups, as well as additional students and external partners at the time of its anticipated opening in FY 2026. The modern laboratory spaces and clean rooms are vital for continued work in nanofabrication research, and necessary to *advance technologies of tomorrow* through collaboration with external, private partners, who expect and need these modern, state-of-the-art resources and spaces. These spaces satisfy needs for:

- microelectronics fabrication and R&D;
- clean room(s) and environmental controls;
- modeling activities; and
- materials and surface analysis equipment.

The above-mentioned building specifications will be particularly important to the development of the proposed new core capability of Condensed Matter Physics and Materials Science and to advancement in LTP and QIS device research. Labs will also require sufficient space and radiological shielding for the calibration and operation of large magnetic fusion X-ray diagnostics. These spaces will need to be stable, reconfigurable, and vibration controlled.

Scientific staff also will depend on the availability of Princeton University laboratories and partners to support research that cannot currently be conducted on site until PPIC is available.

Critical Infrastructure Recovery & Renewal (CIRR)

To improve our mission readiness and position PPPL for long-term growth, the CIRR Project will replace significant original infrastructure systems, such as Electrical, HVAC, Chilled Water Generation, Underground Utilities, and IT. Replacing and updating these systems will dramatically improve the various systems' availability, reliability, capability, and resiliency. Incorporating modern, efficient equipment and systems will both increase PPPL's sustainability and decrease the current deferred maintenance (DM).

PPPL's New Liquid Metals Development Laboratory

In preparation for NSTX-U, active research in prototyping liquid metal plasma-facing components (PFCs) is taking place with Galinstan in smaller-scale devices. However, to support NSTX-U's major future program in flowing liquid metals, a space to safely explore the use of lithium in quantities as great as 50 pounds will be needed. A conceptual physics design of NSTX-U in-vessel liquid metal systems was initiated in FY 2021. Future integrated physics and engineering design will drive NSTX-U liquid metal system requirement, and this, in turn, will inform the design and eventual construction of the liquid metals laboratory. Small, standalone structures, or sufficiently large plots of empty land and adjacent power supplies are currently being investigated for the location of this new experimental building. With the completion of defined program needs, a proposed new, or remodeled structure will be encased in stainless steel designed to the National Fire Prevention Association (NFPA) 484 standard to ensure operational safety.

Remote Collaboration Center (RCC) and Computational and Visualization Hub (CVHub)

The PPIC will introduce use of the new Remote Collaboration Center (RCC) and Computational and Visualization Hub (CVHub), which will provide remote research capabilities for collaborations on international projects (ITER, W7-X, etc.) and visualization of exascale computing results, respectively. While the PPIC will open its doors in FY 2026, the completion of the RCC and CVHub do not come in time to meet the needs for near-term domestic and international collaboration.

Further, the nation's experience with pandemic response has demonstrated that capabilities for extensive, reliable remote research connections are essential for maintaining project schedules and the safety of staff. Even before the COVID-19 pandemic, improved and enhanced remote collaboration capabilities were becoming increasingly necessary to support Virtual Engineering initiatives and collaboration of researchers around the world. COVID-19 concerns, jeopardized project schedules, and halted domestic and international travel have accelerated these needs. PPPL proposes three key projects to enhance remote meeting capabilities to improve overall productivity. The primary funding for these spaces is GPP, GPE, or Program funding to provide the audio-visual systems required to provide remote collaboration capabilities in the spaces below:

1. Upgrade an outdated, underutilized control room (B205) to a modern display wall capability that will enhance the sharing of results and ideas between remote groups and serve as a remote control room for experiments.
2. Create a second remote collaboration room, one that can serve as a smaller prototype for the ITER collaboration room before PPIC's RCC is in operation.
3. Upgrade the MBG Auditorium to make it fully interactive for remote participation and safety.

PPPL's Fusion Research and Technology Hub (FuRTH)

PPPL's vital, growing external partnerships – research programs sponsored by private industry and/or a number of foundations – are not supported by PPPL's current campus layout or available infrastructure. These partnerships must be fostered to continue supporting efforts for national competitiveness in meaningful collaboration toward the development of technologies of the future. FuRTH is envisioned to support formal public/private partnerships, to further enable advancements of fusion technologies. The Fusion Research and Technology Hub (FuRTH) would consist of the existing TFTR test cell, surrounding work area, and a new collaboration office building on D-Site to support science, engineering and operations collaborators.

The test cell space, created through completion of the Tritium System Demolition and Disposal (TSDD) Project, make available a shielded, concrete space measuring 148' x 115' x 54.' This high-value infrastructure will support PPPL's initiatives to grow and diversify its R&D portfolio. Removal of the neutral beam boxes in the Test Cell, as well as the Tritium process systems in the basement below, will provide valuable experimental space for PPPL's industrial partners, especially local fusion start-ups. The TSDD project is now underway with expected completion in FY 2023.

The newly available facility will provide refurbished, ventilated, air-conditioned, humidity-controlled, industrial space for fusion experiments in what had once housed one of the largest fusion experiments in the world. The design of the space provides extensive shielding for experiments producing radiation from fusion reactions and enables construction and maintenance of large experiments with heavy components. The structurally robust space, with a thick concrete roof, a crane capacity of 110 tons, nearby critical infrastructure (e.g., electric distribution systems), and high bay areas, is well suited to support a range of future uses. In addition to supporting the development of new technology partnerships, this space may also be well-suited for the near-term construction of the half-period section (one-sixth of the magnets required for a three-period device) of the permanent magnet project.

The FuRTH office building is proposed to be constructed adjacent to the Test Cell to *enhance laboratory operational efficiency* and *diversify PPPL's research portfolio*. Its proximity to the active experimental areas will offer flexible, transient office space and proper security controls, following the successful completion of the Physical Access Control System (PACS) project, to accommodate on-site private industry research partners. This new building will provide two stories of working spaces to accommodate:

- researchers and technicians employed by these collaborating companies;
- PPPL researchers and operations staff supporting this research;
- additional PPPL staff necessary for supporting growth of research programs; andprovide much needed, and timely, swing space as staff is displaced to construct PPIC.

Site Sustainability Plan Summary

PPPL has institutionalized a comprehensive approach to fulfilling the requirements of Presidential Executive and DOE Orders applicable to the DOE's operational efficiency and sustainability goals. The DOE sustainability goals are fully integrated into PPPL's ISO14001-certified Environmental Management System (EMS) as EMS objectives and targets.

PPPL's FY 2020 Scope 1 and 2 Greenhouse Gas (GHG) emissions were 78.1% below the FY 2008 baseline. This is primarily due to reduced fugitive sulfur hexafluoride (SF6) emissions from experimental power systems and reduced energy usage from the curtailment of onsite staffing in response to the COVID-19 pandemic. Scope 3 GHG emissions were 38.8% below the FY 2008 baseline primarily due pandemic limits on travel, lower site electricity usage and associated transmission & distribution (T&D) losses, and reduced employee commuting resulting from curtailed onsite operations.

PPPL maintains a robust waste diversion program that achieved a combined recycling rate of 72.9% for solid waste (52.7%) and construction waste (93.1%) in FY 2020. PPPL continues efforts to facilitate the purchase of environmentally preferable products through Lab-wide subcontracts and by enhancing sustainable acquisition guidance and resources available to employees. On-site renewable energy and high-performance building improvements continue to be emphasized in the Laboratory's Campus Plan.

The new PPIC building will be constructed with implementation of High Performance and Sustainable Building provisions during design of the facility.

Figure: Artist's rendering of the new entry to PPPL with the Princeton Plasma Innovation Center (PPIC)

PPPL's total energy consumption for goal subject and excluded assets decreased in FY 2020 compared to the FY 2019 by almost 7%. PPPL's Potable Water Intensity (Gal/GSF) for goal subject and excluded assets decreased 23% in FY 2020 compared to FY 2019. When comparing FY 2020's Potable Water Intensity to the FY07 baseline, PPPL's water intensity decreased 54%, exceeding the 40% reduction goal. PPPL entered a period of curtailed operations in early March 2020, and the reduced onsite activity favorably influenced the site's energy and water performance.

PPPL ensures efficient management of its vehicle fleet through its annual vehicle & mobile/heavy equipment justification process and established Local Use Objectives (LUOs) for each vehicle. PPPL emphasizes the use of alternative fuels in its fleet management program and several pieces of heavy- mobile equipment including a 15-ton forklift, backhoe, skid-steer loader and off-road utility vehicles. A recent Parking Study has identified potential locations for longer-term deployment of EV charging stations and investigations on initiating some early installations are ongoing, with broader deployment being considered as part of the CIRR Project. PPPL continues to explore opportunities to enhance its environmentally sustainable practices as it advances and diversifies research initiatives in fusion energy science, basic sciences, and advanced technology.

As seen in the chart below, the decrease in electric usage is linked to HEMSF-NSTX-U, which was last operational in 2016. NSTX-U's projected electric usage will increase concurrent with planned operations. The electric usage of the Princeton Plasma Laboratory Computing Center (PPLCC) is expected to double by FY 2024 due to the anticipated expansion in research computing needs to support the Laboratory's growth and diversification.

SLAC NATIONAL ACCELERATOR LABORATORY

Lab-at-a-Glance

Location: Menlo Park, CA
Type: Multi-program Laboratory
Contractor: Stanford University
Site Office: SLAC Site Office
Website: www.slac.stanford.edu

- **FY 2020 Lab Operating Costs:** $474.2 million
- **FY 2020 DOE/NNSA Costs:** $450.1 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $22.8 million
- **FY 2020 SPP as % Total Lab Operating Costs:** 5.1%
- **FY 2020 DHS Costs:** $1.3 million

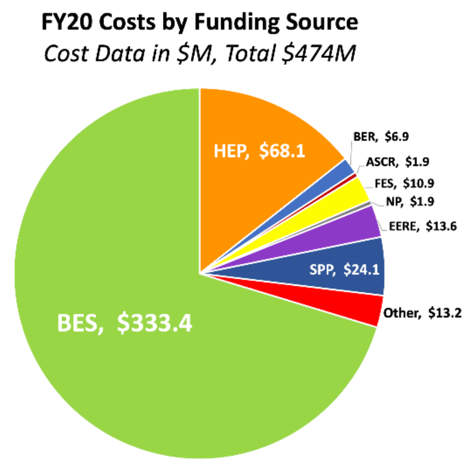
Physical Assets:

- 426 acres and 150 buildings
- 2.35M GSF in buildings
- Replacement Plant Value: $3.1 B
- No Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:

- 1,592 Full Time Equivalent Employees (FTEs)
- 22 Joint Faculty
- 240 Postdoctoral Researchers
- 255 Graduate Student
- 77 Undergraduate Students
- 1,589 Facility Users
- 16 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

SLAC National Accelerator Laboratory is a vibrant multi-program laboratory that pushes the frontiers of human knowledge and drives discoveries that benefit humankind. We invent tools that make those discoveries possible and share them with scientists all over the world. Our research helps solve real-world problems and advances the interests of the nation. To date, four Nobel Prizes have been awarded for research done at SLAC.

SLAC sits on 426 acres of Stanford land in the heart of Silicon Valley and is managed by the University for the U.S. Department of Energy (DOE). This unique partnership and support advances the work of the Laboratory, providing infrastructure, capabilities and expertise that amplify our impact across shared areas of focus, including sustainability research and industries of the future. SLAC runs five joint research centers with Stanford, and together we educate and develop the U.S. scientific workforce in key technological areas.

SLAC is the world-leading laboratory in X-ray and ultrafast science owing to our almost six decades of expertise developing critical accelerator concepts and technologies and to our two user facility light sources: The Stanford Synchrotron Radiation Lightsource (SSRL) and the Linac Coherent Light Source (LCLS).

LCLS is the world's first hard X-ray free-electron laser (XFEL) and a revolutionary tool for chemistry, materials sciences, biology, atomic physics, plasma physics, and matter in extreme conditions. SLAC is commissioning the upgrade to LCLS, LCLS-II, and developing a second upgrade, LCLS-II-HE, each of which will provide a major jump in capability and ensure the U.S. maintains its leadership for years to come.

SLAC started nearly 60 years ago as a place to discover fundamental particle and forces. Today, we deploy our scientific talent and technology from mile-deep caverns to an orbiting satellite in the search for dark matter, dark energy and the fundamental nature of the neutrino. SLAC manages the construction of the world's largest digital camera, which will produce panoramic images of the complete Southern sky once installed at the Vera C. Rubin Observatory in Chile.

As stewards of renowned user facilities, SLAC hosts, supports, and collaborates with more than 4,000 U.S. and international researchers – including many students – at SSRL, LCLS, the Facility for Advanced Accelerator Experimental Tests (FACET), and the Stanford-SLAC and National Institutes of Health (NIH)-funded cryogenic electron microscopy (cryo-EM) facilities.

SLAC's location in Silicon Valley and our connections with DOE, Stanford, and other leading research centers speed our progress. Through continued diversification of our research programs, SLAC aims to strengthen our impact, specifically exploring applications of our user facilities and core capabilities that support the broader DOE mission, the mission of other federal agencies, and expansion of our collaboration with industry.

Core Capabilities

The SLAC National Accelerator Laboratory's (SLAC's) mission is founded on unique user facilities, research capabilities, and scientific expertise, and the Laboratory provides science and technology stewardship to the following six U.S. Department of Energy (DOE) core capabilities:

1. Large-scale User Facilities / Advanced Instrumentation
2. Accelerator Science and Technology
3. Chemical and Molecular Science
4. Condensed Matter Physics and Materials Science
5. Particle Physics
6. Plasma and Fusion Energy Science

Large-Scale User Facilities/Advanced Instrumentation

SLAC operates three DOE Office of Science (DOE-SC) user facilities: the Linac Coherent Light Source (LCLS), the Stanford Synchrotron Radiation Lightsource (SSRL), and the Facility for Advanced Accelerator Experimental Tests upgrade (FACET-II). The Laboratory also operates the joint DOE-National Aeronautics and Space Administration (NASA) Fermi Large Area Telescope (LAT) mission and is a major partner in several particle physics and astrophysics instrument projects.

LCLS. LCLS uses a 15 gigaelectronvolt (GeV) linear electron accelerator to create X-ray pulses a billion times brighter than previously available at synchrotrons. Up to 120 pulses are delivered per second, each one lasting just femtoseconds, or quadrillionths of a second – a timescale at which the motion of atoms can be seen and tracked. LCLS takes X-ray snapshots of atoms and molecules at work, revealing fundamental processes in materials, technology, and living things. Snapshots can be strung together into movies that show chemical reactions or phase changes in materials as they happen. These movies allow scientists to study important proteins at room temperature, in some cases even while they are active. Each of the seven experimental stations is equipped with a suite of specialized diagnostics to help scientists gather a wide range of data, from telltale signatures of electrons and ions to the intricate patterns left by crystallized samples probed by the X-ray laser.

Megaelectronvolt (MeV) Ultrafast Electron Diffraction (UED) instrument (now integrated with LCLS user operations). SLAC has established the most advanced UED facility in the world – an instrument with a 100 -femtosecond time resolution. With the addition of a terahertz (THz) to mid-infrared pump source and a three-fold increase in repetition rate to 360 hertz (Hz), the UED facility continues to make performance improvements that expand our ultrafast science capabilities.

SSRL. SSRL is an X-ray synchrotron-based. Its 3 GeV, high-brightness third-generation storage ring, upgraded in 2004, operates at 500 mA in top-off mode, with high reliability and low emittance. SSRL's extremely bright X-rays allow researchers to study our world at the atomic and molecular level, leading to major advances in energy production, environmental remediation, nanotechnology, new materials, biology, and medicine. SSRL provides unique educational experiences and serves as a vital training ground for future generations of scientists and engineers. SSRL operates 25 X-ray beamlines with 33 experimental stations where scientists from a broad user community can perform outstanding research in a safe environment. SSRL operates approximately nine months each year with very high reliability, delivering more than 97 percent of scheduled X-ray beam time.

SSRL's accelerator research and development program is aimed at improving the performance and reliability of the accelerator complex, including decreasing its emittance and allowing operation with pulses in the few-picosecond range. In addition, SSRL is adding undulator beamlines in strategic areas, allowing it to expand high-throughput characterization and *in situ* and *operando* studies of materials synthesis, growth, and assembly, as well as multimodal methods for time-resolved catalyst characterization to meet the needs of academic, national laboratory, and industrial users. The new beamlines will form additional bridges to LCLS, as does the addition of the undulator Beam Line 12-1. This new beamline, which targets micro-beam macromolecular crystallography, forms a structural biology gateway between SSRL and LCLS and will allow integration of multimodal imaging with the cryo-electron microscopy and cryo-electron tomography (cryo-EM/cryo-ET) facilities at SLAC.

Cryo-EM/ET. SLAC operates one of the world's leading centers for cryo-EM research and technology development; the seven state-of-the-art instruments can image single particles with no need for crystallization and make 3-D images through cryotomography, all at near-atomic resolution. The Stanford-SLAC cryo-EM facility, which provides access to SLAC and Stanford researchers and external collaborators, operates four of the instruments. Three others are made available to the scientific community at S^2C^2. The recently funded Stanford-SLAC CryoET Specimen Preparation Center (SCSC) will add to the growth in available technologies. Adding these new capabilities, when coupled with programs at the SSRL and LCLS end stations, will allow researchers to use a multi-pronged approach, and over a range of time and length scales, to investigate the structure and function of biological materials. The current focus is on addressing research needs related to COVID-19, and meeting the associated challenges in drug design, drug resistance, vaccine development, and other relevant areas of critical research.

Facility for Advanced Accelerator Experimental Tests (FACET). See "Accelerator Science and Technology" core capability below.

Particle Physics facilities and instruments. See "Particle Physics" core capability below.

Advanced instrumentation. SLAC is an international leader in the development of advanced instrumentation and computational tools to serve the needs of our current and future scientific mission areas. The Instrumentation Division within the Technology and Innovation Directorate nurtures a broad suite of SLAC's core expertise in system level design of instrumentation. This system level approach leverages our expertise at all levels of instrumentation including traditional and quantum sensor design, ASICs and discrete front-end electronics, RF processing techniques, FPGA and digital ASIC design. The Division's capabilities span concept innovation through engineering, design, fabrication, testing, and deployment of their technologies. The Division is recognized world-wide for quality and innovation in detectors and instrumentation that are central to SLAC's research in high energy physics and X-ray science funded by DOE-SC. The Instrumentation Division also conducts research for NASA and other U.S. government agencies and collaborates with industry to drive American innovation.

Funding for this core capability primarily comes from DOE Basic Energy Sciences (DOE-BES) and DOE High Energy Physics (DOE-HEP). Other sources include DOE Biological and Environmental Research (DOE-BER), DOE Fusion Energy Sciences (DOE-FES), Laboratory Directed Research and Developments (LDRD) investments, and Strategic Partnership Projects (SPP) from NIH. SLAC's efforts support the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23, 24, 25, 26). (Data Analytics at the) Exascale for Free Electron Lasers project (ExaFEL) is supported by the Exascale Computing Project (SC 17, 20), a joint project of DOE-SC and DOE National Nuclear Security Administration (DOE-NNSA), which is responsible for delivering a capable exascale ecosystem that includes software, applications, and hardware technology in support of the nation's exascale computing imperative.

Accelerator Science and Technology

SLAC is the premier electron accelerator laboratory in the U.S. and one of the top accelerator laboratories in the world. Our research in accelerator science and technology spurs innovation in accelerators across the globe, enabling the development of bright X-ray sources – both FEL and synchrotron light sources – as well as ultrafast electron diffraction (UED) and ultrafast electron microscopy (UEM). These advances strengthen SLAC's core capabilities in materials science, chemical and molecular science, and plasma and fusion science. In partnership with Stanford, SLAC operates a renowned accelerator education program, one of just a few in the nation. Accelerator Science and Technology at SLAC encompasses the broad areas described below.

Free-electron laser R&D. The LCLS-II and LCLS-II-HE upgrades are implementing superconducting accelerator technology to increase the FEL pulse repetition rate from 120 Hz to 1 megahertz (MHz). In contrast to the pulsed superconducting European X-ray Free Electron Laser, the LCLS-II SRF linac will operate in a highly stable continuous wave (CW) mode and will deliver uniformly spaced bunches at rates of up to 1 MHz. The FEL R&D program aims to achieve complete control of the X-ray beam's spectral and temporal properties, which is critical for reaching the full discovery potential of LCLS, LCLS-II and LCLS-II-HE. The R&D program has been highly successful in making a continual stream of new tools and technologies available to our scientific users. These include: development of seeding to narrow the spectrum within a single X-ray pulse; generation of higher-power and shorter FEL pulses; generation of multiple colors and multiple pulses; and advancements in techniques, diagnostics, and optics for both ultrafast science and cavity-based X-ray FELs. Most recently, the X-ray laser-enhanced attosecond pulse generation (XLEAP) program has demonstrated high power sub-femtosecond pulses in the soft X-ray regime, along with the diagnostics needed to confirm those pulse lengths. A SLAC LDRD funded project recently demonstrated the optics feasibility and alignment precision of an FEL scale cavity with the first ever hard X-ray ringdown measurements in a 21m round-trip Bragg cold cavity.

MeV-Ultrafast Electron Diffraction (UED). SLAC's MeV-UED R&D program has led to a new paradigm in ultrafast electron scattering, producing a broad array of scientific opportunities in material science and chemical dynamics. To enable grand-challenge science and broaden the scientific reach of UED, the program is developing a new generation of ultrafast high-brightness electron beam and detector capabilities to enable larger coherence length, improved temporal resolution, and direct electron detection with micron-scale electron beams. This will broaden the scientific reach of MeV-UED into the realms of bioscience and liquid-phase dynamics with improved time resolution, capability for direct electron detection and pump-probe at kHz acquisition rates.

High-brightness electron beam generation. SLAC recently launched a comprehensive R&D program on high-brightness beam generation. A high-brightness electron beam at the undulator is a key component for generating coherent hard X-rays; improving the brightness by a factor of four would nearly double the FEL spectral coverage. High brightness beams are also critical for future experiments in UED / UEM and plasma wakefield acceleration (PWFA). The R&D program includes detailed start-to-end simulations to solve problems that degrade beam emittance. The program is developing SRF electron sources and plasma-based sources critical for the success of future X-ray experiments, UED / UEM, and particle colliders.

Facility for Advanced Accelerator Experimental Tests (FACET). SLAC plays an internationally unique role in the development of beam-driven PWFA. To maintain our leadership in this increasingly competitive field, we are now transitioning FACET-II to operations by optimizing beam configurations and experimental hardware. FACET-II will be the only facility in the world capable of providing 10 GeV electron and positron beams for accelerator science R&D, with the primary focus on investigating key challenges presented by PWFA-based positron-electron colliders and fifth-generation light sources as outlined in the DOE Advanced Accelerator Development Strategy Report.

Research into intense beams and machine learning is an important part of the R&D program at FACET-II which provides unique opportunities to test the limits of existing theories. This line of research is expected to develop enabling technologies for next generation facilities including a potential follow-up facility to FACET-II. The science case for a facility co-locating extremely compressed 30GeV electrons and positrons, multi-Petawatt optical lasers and X-ray FEL for accelerator R&D is being developed with the involvement of a broad community.

Advanced RF accelerator technology. In the area of RF accelerator technology, new developments are enhancing the capabilities of existing DOE accelerator facilities (e.g., THz accelerator beam manipulation for femtosecond bunch compression), along with new initiatives from electron, hadron, and radionuclide medicine to X-ray, gamma-ray and deuteron sources for national security to materials processing (discussed in section 5.2.1). Our DOE-HEP stewardship programs have developed extremely high-efficiency high-intensity linac and deflector designs for electron and ion beams. We continue to develop our start-to-end simulation capabilities for accelerators and apply novel algorithms to model the RF sources. New superconducting thin-film deposition tools integrated with our nanofabrication facilities and cryogenic testing equipment will allow us to design innovative RF linac topologies, which demonstrate remarkable improvements in performance for both normal-conducting and superconducting RF accelerators. To leverage the breadth of this activity across DOE-SC – e.g., supporting the mission of revitalizing the domestic industrial accelerator technology base – we are evaluating the facility improvements needed to integrate this capability and secure our global leadership position in accelerator science, technology, and engineering.

Educating the next generation of accelerator physics leaders. The renowned SLAC-Stanford accelerator education program benefits from the science and engineering challenges we tackle and our unique set of accelerators and test facilities, where graduate students and postdocs can acquire hands-on experience needed to further their careers.

In its 25-plus years of operation, the education program has produced more than 60 PhDs in accelerator physics – 32 from Stanford and about 30 from other universities and institutions. Eleven of the 30 recipients of the American Physical Society thesis award in beam physics completed their graduate research at SLAC. Today the program includes 14 graduate students in accelerator physics and engineering and five Stanford University faculty.

Funding for this core capability comes from DOE-BES, DOE-HEP, SPP customers, and LDRD investments. The core capability supports the DOE-SC mission in scientific discovery and innovation (SC 2, 22, 23, 24, 25, 26).

Chemical and Molecular Science

SLAC's research program in chemical and molecular science focuses on understanding chemical catalysis at a fundamental level and observing chemical reactions on their natural timescales – at the frontier of ultrafast chemical science. Developed over the past decade, SLAC's core capabilities in these areas are widely recognized for their quality and innovation, and for their distinctive role within the broader American scientific enterprise. Both of these research areas benefit greatly from having SSRL, LCLS, and their associated expertise close at hand.

Chemical catalysis. Understanding chemical catalysis at a fundamental level is a scientific frontier with enormous impact on energy transformation, storage, and management. SLAC is a world leader in using theory to provide a quantitative and predictive understanding of key problems in catalysis under realistic reaction conditions. Recently, SLAC has used this strength, in strong collaboration with experiments, to achieve a step-by-step understanding of how carbon dioxide (CO_2) can be converted into valuable chemicals and fuels through electrochemical reduction, along with an understanding of how to devise new catalysts for this process. At the same time, we have expanded our expertise in synthesizing catalysts, characterizing their properties, and testing their performance. The ability to probe the properties of catalysts at SSRL is an integral part of this work. Stanford faculty are strongly involved in our research approach through the SUNCAT Center for Interface Science and Catalysis (SUNCAT), contributing expertise in catalyst synthesis, characterization, and testing.

Ultrafast chemical science. The movements of atomic nuclei and electrons that drive chemical reactions take place on attosecond to picosecond timescales – billionths to quintillionths of a second – and to understand those fundamental processes, we need to observe and measure them on these timescales. SLAC's ultrafast science research program collaborates with LCLS on this effort, enhancing the impact and success of both. The program also benefits from our partnerships with Stanford, including the joint institute with Stanford, the Photo Ultrafast Laser Science and Engineering Institute (PULSE). The scope, depth, and experimental capabilities of SLAC's ultrafast chemical science program are unique in the U.S., and similarly comprehensive programs are being rapidly developed elsewhere in the world, particularly in conjunction with new XFEL facilities opening abroad.

Complementing the experimental methods available at LCLS and LCLS-II, SLAC's extensive laboratory facilities allow scientists to observe and measure processes down to femtosecond and attosecond timescales. In addition, our experimental program is influenced and enhanced by strong collaboration with theory and simulation. We collectively apply these diverse methods to study fundamental physical concepts that govern chemistry and explore how powerful lasers interact with matter.

Funding for this core capability comes from DOE-BES (SC 2, 21, 22, 23). Selected LDRD investments are supporting scientific discovery and innovation.

Condensed Matter Physics and Materials Science

Condensed matter physics and materials science at SLAC evolved hand-in-hand with the development of SSRL as one of the first synchrotron light sources to address the electronic and structural properties of matter. Our current research program continues to focus on key scientific problems that can be addressed through our X-ray user facilities – SSRL and LCLS – along with our world-class materials synthesis, characterization, and theory activities.

The Laboratory's researchers partner with Stanford and industry to pursue frontier issues in the assembly and design of materials, their collective quantum dynamics, and their ability to transform energy. Each of these lines of research addresses DOE's missions in science, energy, and security. One focus – assembling low-dimensional materials and interfaces at the nanoscale level to give them novel collective properties – is particularly rich in opportunities to study mission-relevant grand challenge problems.

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SLAC scientists partner in this work with Stanford on initiatives such as the Precourt Institute for Energy and the development of a new school for sustainability, which fosters outreach activities for energy science education and training, helping to develop the next generation of talent.

SLAC scientists have been working with SSRL and LCLS to develop and use X-ray beamlines, and they lead the implementation of SLAC's ultrafast materials science strategy. Many principal investigators use SLAC's light sources and UED facility to pursue important scientific lines of inquiry identified in recent Basic Research Needs workshops and roundtable reports. They have contributed important content to DOE-BES reports, helping to set the scientific agenda in the fields of quantum materials, synthesis and tool science, ultrafast science, and quantum computing.

Materials science will continue to offer major research targets in the areas of quantum materials, interfaces, and energy materials, and for users of SSRL and LCLS. With the advent LCLS-II, a golden age of scattering and spectroscopy is emerging, bringing unprecedented opportunities for understanding, designing, and manipulating materials at nanometer to micrometer length scales, and femtosecond to picosecond timescales. Advanced scattering, spectroscopy, and microscopy play pivotal roles both in exploring the electronic, geometric, and excited-state properties of crystals, surfaces, interfaces, and complex nanoscale assemblies of atoms and molecules, and also in teasing out how their physics evolves in response to temperature, pressure, electric and magnetic fields, and other external factors. This exploration is not only of fundamental scientific interest, but also essential for designing new materials with properties tailored for technological applications – ranging from energy transformation and storage, to quantum information – that are crucial for the nation's economic well-being and energy security.

Funding for this core capability comes from DOE-BES, with related support from Energy Efficiency and Renewable Energy (DOE-EERE) and LDRD investments. It serves the DOE-SC mission in scientific discovery and innovation (SC 2, 21, 22, 23).

Particle Physics

SLAC is a world leader in exploring the frontiers of particle physics and cosmology. Our comprehensive suite of underground, surface, and space-based experiments addresses some of the most compelling questions in the field today: what is the nature of dark matter, dark energy, and the neutrino? How did the universe evolve? What is the nature of matter at the most fundamental level, and how did it affect the evolution of the universe? In pursuit of these fascinating questions, which are a vital part of the DOE mission, we have built a renowned theory group and a high level of expertise in building instruments, detectors, and facilities and managing large-scale projects. We continually find ways to apply these tools and develop new ones needed to expand the frontiers of discovery.

SLAC is using these capabilities to build the Large Synoptic Survey Telescope (LSST) camera for the Vera C. Rubin Observatory, which will conduct an unprecedented survey of the Southern sky. SLAC continues to expand its core capabilities in designing and building state of the art detectors and cryogenic readout, with continued investment in liquid noble time projection chambers to study fundamental properties of neutrinos and to advance the search for dark matter. SLAC has started the construction process of the detector microfabrication facility to further develop our core capability for fabricating superconducting quantum sensors and devices. The thrusts include: quantum sensing using previously impossible probes of fundamental physics enabled by sensitivity better than the standard quantum limit, or quantum sensor supremacy; quantum simulation to probe fundamental physics, such as black hole duals, and the scrambling of quantum information; and quantum transduction to enable entanglement in quantum ecosystems, allowing scaling of sensing and simulation to different length scales and more degrees of freedom. These capabilities are critical for the future of quantum information science (QIS), dark matter, fabrication of sensors and readout for the Cosmic Microwave Background Stage 4 (CMB-S4) project, and fundamental physics, generally; they will also have broader societal impact in such areas as biomedical imaging, drug discovery, and the development of new materials.

Advanced quantum devices. Our quantum program has several thrusts that will be enabled by the detector microfabrication facility that we are now building with Stanford support; it will be a new capability for the DOE complex and allow us to produce superconducting devices on a large scale. Our thrust in "quantum supremacy" involves developing much more sensitive quantum sensors to carry out previously impossible probes of fundamental physics. Quantum simulation explores fundamental physics, such as the details of black hole pairs, as well as the scrambling of quantum information. Finally, quantum transduction enables entanglement in quantum ecosystems, allowing sensing and simulation at a broader range of length scales and with more degrees of freedom. The ability to do these things is critical for the high energy physics programs in QIS, dark matter new Initiatives (DMNI), for which we are developing the Dark Matter Radio M-cubed detector, and studies of the cosmic microwave background radiation, as well as enabling technology for future research in fundamental physics. It will also have a broad impact on society in areas such as biomedical imaging, drug discovery, and the development of new materials.

Large-scale microfabrication of superconducting devices. We are playing a major role in building the CMB-S4 project supported by our expertise in designing and building arrays of superconducting devices and readout systems. Along with responsibility for the superconducting readout system for CMB-S4, the detector microfabrication facility will provide science grade wafers, a core element of the project. These technical contributions combined with earlier work in the Background Imaging of Cosmic Extragalactic Polarization (BICEP) cosmic microwave background (CMB) program will allow us to use CMB-S4 data to contribute to studies of cosmic inflation, neutrino masses, gravitational lensing and the evolution of galaxy clusters.

ATLAS detector systems. The ATLAS (A Toroidal LHC Apparatus) experiment at the Large Hadron Collider is exploring teraelectronvolt (TeV) mass scales and beyond for elucidating the properties of the Higgs and discovering new particles and interactions. For the High Luminosity-Large Hadron Collider (HL-LHC) project, SLAC is leading the assembly of the ATLAS inner tracker pixel detector system, as well as studies of pile-up and jet reconstruction. SLAC also has a major role in the construction of the silicon inner tracker, which is the most important detector subsystem in these planned upgrades. We contribute infrastructure and expertise in several key areas, including 3-D and complementary metal oxide semiconductor (CMOS) pixels, strip detectors, and high-speed data transmission and readout. SLAC will assemble the U.S. pixel staves using a newly commissioned coordinate measurement machine in our Building 33 cleanroom.

Time projection chambers for neutrino research and dark matter. SLAC's two major neutrino programs – the Enriched Xenon Observatory (EXO) search for neutrinoless double beta decay (NDBD) and the Deep Underground Neutrino Experiment (DUNE) experiment to study neutrino oscillations – are powered by our expanding expertise in liquid noble time projection chambers (TPCs), associated high-speed readout and purification systems, and machine learning analysis reconstruction techniques. SLAC and Stanford led the development of EXO-200, which established world-leading NDBD limits and made the first observation of the related two-neutrino process. Its success positions us to play a leading role in the next NDBD program to better determine the relative masses of the three neutrino types and whether they are their own antiparticles, which has been given a high priority by the Nuclear Science Advisory Committee. One of the leading candidate technologies is nEXO, a multi-ton scale-up of EXO-200. For DUNE, SLAC has a leading role in developing the project's near detector, particularly a system of modularized liquid argon TPCs that is now a core part of the near detector concept. Our Liquid Noble Test Facility (LNTF) is being used to build and test prototypes for this concept. With SLAC now leading the mechanical design of prototype modules, the LNTF will play a critical role in the process leading to a final design of the near detector, which has a conceptual design report in final stages of preparation and a preliminary design report to follow in about a year. The LNTF and our experience in building the LUX-ZEPLIN liquid xenon time projection chamber to search for dark matter provides a critical core capability to lead a G3 dark matter experiment, which is the subject of the ongoing Snowmass community study.

Readout electronics. SLAC has also been developing readout electronics for liquid noble gas detectors in which several functions are pipelined into a single application-specific integrated circuit (ASIC), which will be deployed within the cryogenic environs of the readout plane. Putting all the circuits in one chip minimizes power consumption, increases reliability by reducing the number of interconnections and external components, and reduces the overall costs for the final application. This approach also makes it possible to use these chips in applications where system components must be minimized to reduce background contamination. A single ASIC, with minor modifications, meets requirements for both nEXO and DUNE. The first DUNE version was received in 2019, and after modifications to correct a few deficiencies, a version optimized for nEXO has just been received. Systems testing using the ICEBOX and ProtoDUNE cold box are expected this year, and we expect the field of potential technologies for DUNE to be narrowed down in early 2021.

Funding for this core capability comes from DOE-HEP and DOE Nuclear Physics (DOE-NP), as well as SPP from the National Science Foundation (NSF) and NASA, and LDRD investments. SLAC's efforts serve the DOE-SC mission in scientific discovery and innovation.

Plasma and Fusion Energy Science

The SLAC program in plasma and fusion energy sciences exploits the Laboratory's unique combination of high-power lasers and LCLS, which has launched a new era of precision in high energy density (HED) science by probing ultrafast changes of matter in extreme conditions. Fusion science research drives new technology developments in 100Hz repetition rate and high-power petawatt-class lasers and develops the physics of energetic phenomena and radiation sources, which is important for astrophysics and technical applications.

X-ray studies of HED plasmas. Our frontier research programs in plasma and fusion energy sciences focus on high-pressure and high-temperature plasmas. LCLS X-rays measure the characteristics of warm dense matter states with an accuracy that can support or refute competing theoretical models. These studies provide critical experimental tests of physics models that are important for the design of full-scale fusion experiments and they provide understanding of structural, transport, and radiation physics properties of fusion plasmas. These programs were recently expanded through new capabilities at LCLS that include an eight pulse multi-bunch mode and THz probing of electrical conductivities of matter in extreme conditions.

Theory and simulation. Another major research area is the development of ways to use high-power, short-pulse lasers to accelerate particles in plasmas. Our experimental efforts are coupled to a theory program that uses 3-D particle-in-cell modeling of HED plasmas. It can resolve the femtosecond timescales and sub-micrometer spatial scales needed to explore advanced particle acceleration, ultrafast X-ray probes, and laser-produced fusion neutrons. Our calculations result in a new understanding of radiation sources and predictions have led to the demonstration of the 1st order Fremi acceleration process that can lead to very high particle energies relevant to explaining the origin of cosmic rays**.**

The HED program has created a new theory group funded by a DOE-FES Early Career Award. The program is expanding SLAC's footprint in the simulation of HED phenomena, exploring new scientific frontiers that our HED facilities – in particular the upgrade of the LCLS Matter in Extreme Conditions (MEC) experimental station – are making accessible. We expect to make major advances by using novel machine learning tools to model experiments at realistic scales of time and space.

High-resolution diagnostics and technology. We have demonstrated ultrafast pump-probe experiments on warm dense matter, achieving unprecedented precision. These experiments are made possible by investments in a diagnostics and technology program aimed at achieving high-resolution measurements in space, time, and energy. We are also developing cryogenic targets for high-repetition-rate studies of liquid hydrogen, deuterium, and other important materials for fusion research. In addition, the program has demonstrated novel probe techniques such as THz transmission measurements that are unique to ultrafast studies of dense plasmas.

HED facilities. As the MEC upgrade at LCLS moves toward Critical Decision-1 approval, we are optimizing the layout of laser drivers and diagnostic and target capabilities to keep our world leadership role in this area. This upgrade includes a new separate underground hall and access tunnel beyond the Far Experimental Hall to provide the required space and radiation shielding for petawatt- and kilojoule-class laser drivers that have been endorsed by the 2020 Brightest Light Initiative and the 2020 Division of Plasma Physics Community Planning Process reports.

Funding for this core capability comes from DOE-FES and LDRD investments and serves the DOE-SC mission in scientific discovery and innovation.

Science and Technology Strategy for the Future / Strategic Initiatives

SLAC contributes to meeting the nation's critical scientific and technological challenges through our diverse research programs, world-leading user facilities, strong relationship with Stanford, and Silicon Valley connections. The six ongoing strategic initiatives that focus our efforts and help us attract the world's best scientists and engineers as researchers, technology innovators, and facility users are:

- **Lead the world in X-ray and ultrafast science** by solving the most difficult problems in chemistry, materials sciences, biology, and plasma physics using the ultrashort, ultrabright pulses of coherent X-rays produced by LCLS and the future LCLS-II and LCLS-II-HE
- **Foster a frontier program in the physics of the universe** through our search for dark matter, our work to understand dark energy, and by probing the fundamental nature of the neutrino
- **Transform high energy density science** by leading the world in advanced experimental capabilities that enable measurements with unprecedented spatial, temporal, and spectral resolution, and advanced modeling of plasma under extreme conditions
- **Drive biological and bio-inspired science for sustainability** by applying our state-of-the-art integrative, multi-modal X-ray, cryo-EM/ET, expanded imaging, and computational program to advance discovery and innovation in biology, bioenergy, materials, and environmental sciences
- **Advance quantum information science across DOE** by integrating key scientific programs and technologies to deliver unique capabilities and further emerging applications of QIS
- **Innovate massive-scale data analytics** to meet the unprecedented needs of our user facilities, which will allow us to amplify the impact of SLAC programs on the DOE-SC mission

Our vision, strategic initiatives, core capabilities, and expertise set the foundation for the Laboratory's continued growth, ensuring the advancement of scientific discovery across the spectrum of grand challenges identified by the DOE, the nation, and the world.

Infrastructure

Overview of Site Facilities and Infrastructure

SLAC executes six DOE core capabilities on a 426-acre site leased from Stanford. DOE and Stanford signed an initial land lease agreement in 1962 and renewed it in 2010 for 33 additional years. As part of this agreement, DOE and Stanford identified 25 acres on three separate parcels as opportunities for Stanford to consider removing from the ground lease. We recognize these areas in our land-use planning. Stanford manages SLAC and supports the Laboratory’s science and infrastructure development. Stanford and SLAC are strongly linked through academic and mission ties.

As documented in the Facilities Information Management System (FIMS), SLAC’s total real property inventory comprises 358 assets: 171 buildings, 161 other structures and facilities (OSFs), and 26 trailers. The most common land use of these properties is “mixed-use,” which includes offices, laboratories, research facilities, and support structures. Approximately one-fourth of the square footage is dedicated to tunnels and unique experimental facilities. The largest real property assets are the Klystron Gallery and the corresponding accelerator housing supporting our 2-mile-long accelerator.

The utility infrastructure that serves as the backbone of SLAC’s facilities and science mission includes electrical power, chilled and hot water, domestic water, fire protection systems, low-conductivity water (LCW), storm water, sanitary sewer, natural gas, telecommunications, and compressed air.

The average age of SLAC-operated facilities and infrastructure is 39 years, with 37 percent of assets built more than 50 years ago. Cognizance of our infrastructure's current state is critical as we look toward the upcoming decades of developing new science. We must evaluate the current status of our real property inventory and take the appropriate strategic actions to revitalize and modernize our Laboratory’s infrastructure. Investments must support utility resiliency and redundancy in the laboratory's utilities infrastructure, provide flexible and collaborative science and support spaces for a new era of working environments, and modernize existing facilities to support existing and new science missions.

Campus Strategy

This section lays out the campus strategy, as summarized in **Error! Reference source not found.**, which provides a map locating SLAC’s 10-year planned facility and capital infrastructure investments. This section also includes both required and supplementary summary tables and discussion of current and future priorities that support the Laboratory’s mission and strategic initiatives.

The unprecedented combination of challenges in the past year put SLAC’s preparedness strategies to the test. Due to systems already in place, we were able to meet a cascade of challenges including the COVID-19 pandemic, widespread wildfires, and utility provider (PG&E) public safety power shutoffs intended to prevent further wildfires. Throughout these ongoing crises, the Laboratory has also maintained preparedness for other potential human-made or natural disasters, such as social unrest or a major earthquake. SLAC leadership demonstrated adaptability and flexibility as each new major threat to continuity of operations emerged. SLAC’s ability to meet each of these crises underscores the importance of maintaining capabilities and planning for resilience and adaptability.

The work conditions imposed by the pandemic have dramatically accelerated implementation of technologies that allow remote collaboration and forced rethinking the on-site/off-site requirements for much of the personnel. This will leave a significant imprint on planning future workspaces. Mandated requirements to shelter-in-place and practice social distancing have shown that many types of work can be effectively accomplished remotely. When work requires on-site collaboration, adaptable spaces are needed, and particularly for activities that can only be performed on-site. These require a more flexible use of infrastructure, including laboratories, instruments, and tools, which should be available on an as-need basis. We have begun a “Future of Work” initiative to examine and implement a range of measures to provide this type of flexibility, with infrastructure responsiveness playing a major role. This is being supported by a member of Stanford’s School of Engineering and graduate students, using human-centered design. Several use cases are evaluating processes and outcomes for the spectrum of telework.

The following sections describe the campus strategy as it evolves to deliver highly reliable, efficient, and effective infrastructure – both on campus and for support activities occurring off site. The SLAC Long-Range Vision Plan (2015) provided a blueprint for physical infrastructure that continues to guide SLAC’s support of DOE’s science mission over the long term. An update of this plan, scheduled for release in 2022–2023, will be developed in partnership with DOE and Stanford. The strategy for achieving a joint long-range vision includes a near-term focus for the next 5–10 years to address current capability gaps, and a broad vision for what will enable future science over the span of the next 15–20 years. Both direct and indirect infrastructure investments will be leveraged to close gaps and maintain mission-ready facilities today and into the future.

SLAC's infrastructure investment strategy focuses on optimizing the use of current assets, modernizing facilities to provide flexible and adaptive spaces, and synchronizing stewardship of operations and maintenance in support of current and future science missions. Our three campus strategy goals are:

- Revitalize and modernize our utility infrastructure backbone to provide flexible and resilient delivery of utilities, support strict operational tolerances, and ensure mission readiness;
- Provide a variety of flexible and adaptive spaces for diverse groups to work collaboratively and explore science opportunities; and
- Modernize, consolidate, and repurpose existing facilities to enable our strategic initiatives and encourage efficiency.

Error! Reference source not found. provides a location map of SLAC's 10-year planned programmatic and institutional investments and includes projects supported by Stanford. Each project is listed under the campus strategy goal it meets, illustrating how various investments are leveraged for a unified infrastructure vision. Over the years, DOE programmatic and Science Laboratory Infrastructure (SLI) support has been instrumental in transforming the Laboratory's physical character through new infrastructure systems benefiting scientific programs and continued fit-out of laboratory spaces. SLI support has been essential in addressing severely degraded aging critical electrical and cooling water systems through general plant projects (GPP). In addition to this support, SLAC has also significantly increased the institutional infrastructure budget every year for the last five years and has been able to fund such small- and mid-scale projects as roof renovations, underground leak repairs, and replacement of underground cooling water piping, electrical infrastructure, and cooling tower modernization.

The investments described in the following sections show how our campus strategy optimizes systems for life cycle, systems management, operations, and maintenance, and how sustainability is integrated into each project.

Campus Strategy Goal 1: Revitalize and Modernize Utility Infrastructure

Utility resiliency and reliability are essential for meeting the requirements of user facilities, scientific instruments, laboratories, and experimental equipment with extreme criticality tolerances and operating parameters. With expanding workforce demands and emerging research, revitalizing and modernizing aging infrastructure is a must, and coincides with developing means of addressing emerging threats and operational risks. While many operational risks have been addressed, continued degradation of original electrical power and cooling water systems presents an ongoing threat to current and future science missions.

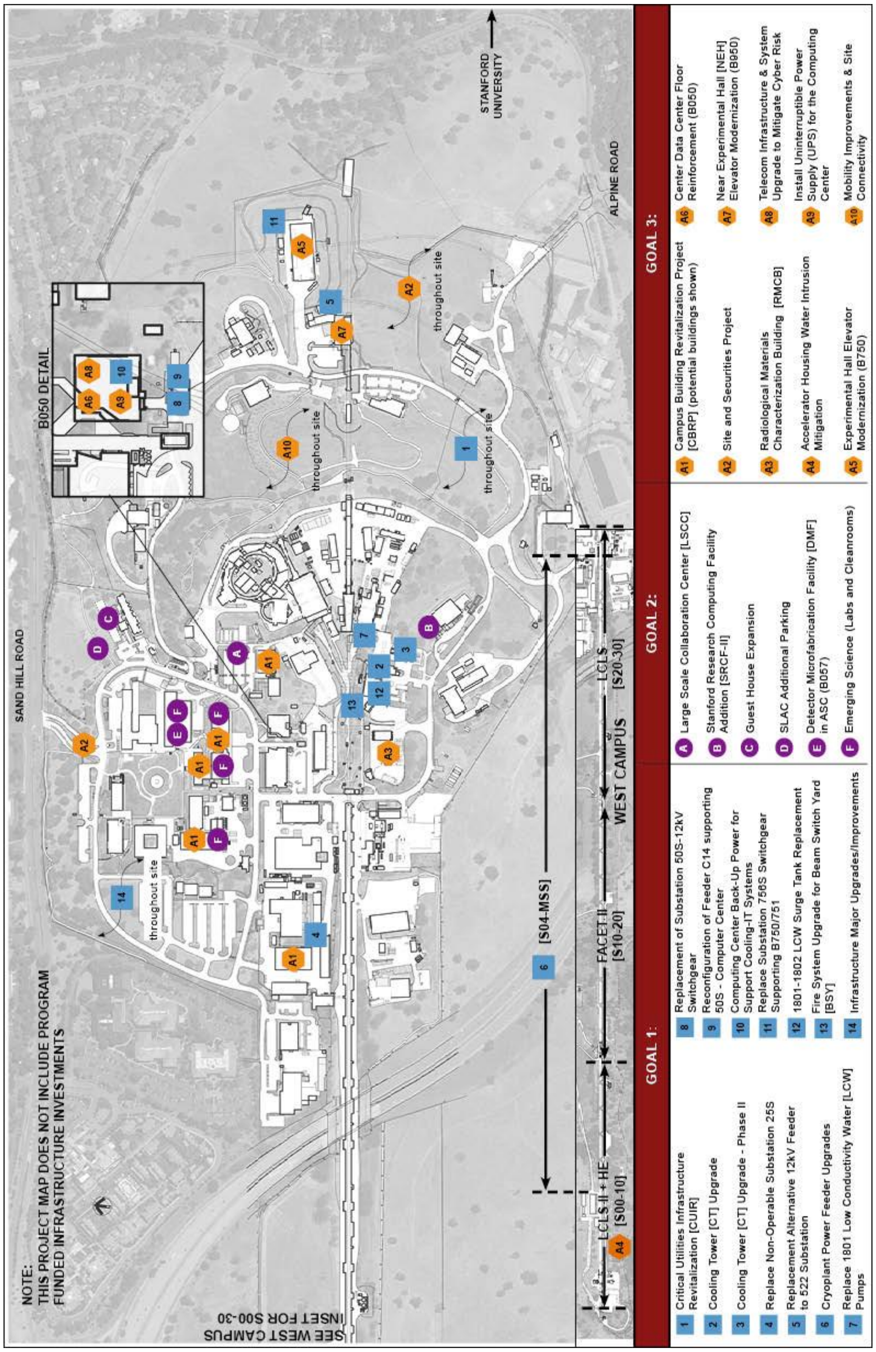


Figure 2: SLAC's 10-Year Planned Facility and Infrastructure Investments

Electrical Power

Continuous and reliable power delivery is critical to the science mission. Power is delivered to SLAC by means of a DOE-owned 5.4-mile 230-kV transmission line located near wildfire-prone dense vegetation in steep terrain, and near residential development outside the leased area. Mitigating these risks involved coordinating with the utility provider, PG&E, to install fault protection devices and to carry out an aggressive vegetation clearing project and vegetation management plan for these power lines. Three years of extensive vegetation management along the primary 230-kV transmission line has mitigated much of the risk, and the focus is now on continuing to work with PG&E to ensure the resiliency and availability of our secondary power source, a 60-kV transmission line.

Direct SLI-GPP investments in electrical substations and medium- and low-voltage equipment has modernized assets to improve electrical utility delivery and operational reliability for multiple accelerator systems housed in the two-mile-long linac. Such improvements decrease downtime due to required maintenance of outdated equipment or unplanned mishaps.

SLAC indirect investments are also underway on the electrical system. Results of an FY 2021 winter downtime assessment of the existing electrical duct bank infrastructure along the linac show that much of the original conduit is constructed of deteriorating bituminous fiber pipe. This material is deteriorating, beyond useful life, and poses a risk to pulling new cable in existing conduit. With existing conduit in use or obstructed, there is only one viable pathway for a dedicated feeder cable between our master substation and our new cryoplant. The existing configuration interconnects linac systems and some of the new infrastructure required for LCLS-II-HE. This places a priority on addressing immediate power reliability through both indirect infrastructure investments and acceleration of electrical work within the CUIR project scope to support linac operations and provide an electrical grid to deliver long-term stability and redundancy for power delivery. These actions support the resilience strategy for delivering reliable power to our facilities.

Cooling Water

Our next highest operational reliability risk is the sustainment of cooling water systems. An SLI-GPP for LCW systems was completed in FY 2020, and an SLI-GPP for the replacement of cooling tower cells is underway this year. The cooling tower project replaces aging cooling tower cells serving critical loads in the Beam Switch Yard, SSRL, LCLS experimental halls, and research end stations. Completing these projects enables the cooling tower system to be optimized from the current oversized 36 MW capacity to a more efficient and sustainable 12 MW system. These two projects will retire approximately $3.3 million of deferred maintenance (DM).

Through indirect investments, we recently completed a project to replace underground cooling water and above ground piping, along with associated infrastructure. This project reduces the overall failure risk for mechanical infrastructure and improves cooling water reliability for multiple accelerator systems along the linac. Institutional GPP (IGPP) funding to modernize original heat exchanger infrastructure has been prioritized.

Underground Utilities and Communications Infrastructure

Capability gaps contributing to operational risks also include the state of the following underground utility systems: sanitary sewer and lift stations, storm drainage, domestic water and fire protection, and natural gas. Much of this infrastructure is degraded and past its normal service life, and in some cases the utility services delivered have been reduced as a result of reduced system capability.

The computing and critical fiber optics communications network infrastructure is currently overloaded and will be modernized to support both current requirements and the additional capacity requirements that will be realized once new science projects such as LCLS-II, LCLS-II-HE, MEC Upgrade, and LSST, are operational. Modernization of this infrastructure will also improve SLAC's cybersecurity posture and response readiness.

Critical Utilities Infrastructure Revitalization

The above actions have already made a significant impact on mitigating risk; however, there is still a requirement to make a significant capital investment in our utilities that will occur through an SLI line item (LI) request for an infrastructure investment project. The projected CUIR budget is $189 million Total Project Cost (TPC), FY 2020 to FY 2030, and received its CD-0 Energy Systems Acquisition Advisory Board (ESAAB) in May 2019, and CD-1 is anticipated later this year. This project's primary objective is to close many of our infrastructure gaps by creating resilient, reliable, and robust infrastructure for science delivery in support of DOE's multi-program science missions.

Our utility system stewards have assessed the power, mechanical, water, instrumentation, and fire protection systems to identify single points of failure and poor or failed infrastructure to plan projects for this utility revitalization. These assessments were the basis for identifying projects and establishing risk mitigation plans to minimize potential infrastructure risks. In FY 2020, SLAC procured a utility system engineering design firm to develop the CDR and work with science liaisons, utility stewards, operations staff, and mission readiness planners to prioritize projects for a program of execution. The CDR will be completed in FY 2021 along with a cost-loaded schedule and other required documents for the DOE CD-1 independent project review (IPR) planned for summer 2021.

The project includes critical repairs, replacements, and modernization of site-wide electrical systems, underground domestic water and fire protection, sanitary sewer, storm drain, natural gas, mechanical, and compressed air, as confirmed by specialized assessments. The electrical utility component revitalization will provide a more resilient linac electrical grid that is interconnected and configured in a manner that minimizes science disruptions caused by power fluctuations and faults both at the local level and the regional level due to PG&E's public safety power shutoff program. Science drivers for the CUIR are as follows:

- Reduce electrical reliability risks to LCLS, LCLS-II, LCLS-II-HE, FACET-II, and future science projects. As mentioned above, parts of the investment are required for LCLS-II-HE start-up.
- Close infrastructure gaps in support of DOE's multi-program science missions by creating resilient, reliable, and robust infrastructure for science delivery.
- Revitalize critical utility infrastructure, resulting in higher reliability, redundancy, and operational utility efficiency to support site-wide science.
- Develop means of addressing emerging threats and operational risks.
- Leverage AI/ML in our utility systems to increase operational reliability, optimize systems, enable faster diagnostics and fine-tuning, and support analysis of complex scientific data sets, science research, and technology development through computing operations.

The highest priority scope items are organized into sub projects that maximize linkages and efficiencies between projects and minimize impact on science operations during construction. The planned program of execution comprises the following sub projects:

- Sub Project A is comprised of several pre-construction studies and assessments necessary for follow-on scope development. This includes design guidelines and performance specifications (DGPS), geotechnical/civil systems studies, electrical power and automatic transfer supervisory control and data acquisition (SCADA) studies, data and communication systems assessments, and cooling water demands study.
- Sub Project 1 includes the procurement of long lead time equipment; the construction and installation of a generator for cryoplant helium recovery in the event of a power outage; a new electrical substation, Substation K5B, to support future power requirements; and an electrical pathway for new electrical feeders down to Sector 4 of the linac.
- Sub Project 2 contains a new MSS transformer and MSS upgrades, as well as storm drain, sanitary sewer, and domestic/fire water work.
- Sub Project 3 consists of low- and medium-voltage work for the linac's motor control centers (MCCs), variable voltage substations, and low-voltage breakers; LCW work along the linac; domestic water; and design of the AI/ML system.

- Sub Project 4 includes replacement of waveguide, accelerator, and klystron systems equipment (mechanical and water pumps, motors, etc.) along the linac and installation of management systems data capture and controls for future development of AI/ML algorithms.

We will also leverage this major infrastructure investment by introducing AI and ML into facility operations and maintenance. The CUIR projects provide an opportunity to incorporate data collection sensors, control systems, and instrumentation to gather utility data that will be the foundation for developing site-wide AI/ML systems. Leveraging AI/ML will increase operational reliability, optimize systems, enable faster diagnostics and fine-tuning, and support analysis of complex data sets. AI/ML integrated into utility systems as part of CUIR will allow efficient and effective means for delivering resilient and reliable utilities for science research, technology development, and site-wide computing operations. In addition to underground civil infrastructure and electrical work, this project addresses vital cooling water system revitalization with increased capacity to support multiple science programs with cooling system controls, water mains, laterals, tower piping, and valve replacements. Timely delivery of these utility projects is essential for the continued success of DOE's science programs. Currently, the CUIR project is anticipated to reduce around 30 percent ($25 million) of SLAC's DM backlog.

Campus Strategy Goal 2: Flexible and Adaptive Spaces for Groups to Work Collaboratively

SLAC's campus vision and strategy advances our core competencies, including emphasizing collaboration on all science fronts. Creating opportunities for collaboration and increased productivity has become even more important as the pandemic made telework a necessity, and forms of telework will likely continue once the pandemic passes. This dynamic presents an opportunity for new designs that optimize the use of both interior and exterior spaces to expand the flexibility of all configurations, including teaming rooms, outdoor meeting areas, and touchdown spaces. The new opportunity also extends to design considerations for pedestrian traffic patterns. Enhancing collaboration opportunities across research areas and programs for SLAC's post-pandemic workplace design includes flexible workspaces, optimizing physical workspace locations and adjacencies, more flexible access to laboratories and tools, as well as operating scientific instruments remotely while supporting those activities on-site with reduced staff. The concept for touchdown and temporary workspaces has already proven successful in the Arrillaga Science Center, which hosts a range of laboratory and office support spaces that create opportunities for collaboration among the hosted programs and collaborators. The Science Quad is a central focal point for collaboration and serves as a natural outdoor meeting place for formal events and informal exchanges.

Large Scale Collaboration Center

The LSCC will provide a new model and concept for collaboration and represents the next logical step in a campus vision that provides collaborative spaces for developing new science programs. While the Arrillaga Science Center already delivers multi-mission laboratory spaces, the LSCC will support current and future science by providing a modern research collaboration and visualization facility for massive-scale data analysis that will enable interaction between disparate user groups. Extremely large data rates, up to a terabyte per second, will be generated from future operation of LCLS-II and LCLS-II-HE (DOE-BES, NIH), as well as large data streams from the Vera C. Rubin Observatory (DOE-HEP, NSF), FACET-II (DOE-HEP), SSRL (DOE-BES, DOE-BER), Cryo-EM (DOE-BER, DOE-BES, NIH), and associated DOE-ASCR activities. This drives the need for deep collaboration among users, local beamline and accelerator staff, and ML/AI scientists using advanced tools and complex simulation codes linked to HPC at SLAC and across the DOE complex.

Science drivers for the LSCC are as follows:

- Major science facility upgrades from 2020–2025 result in huge increases in data rate.
- Science innovation requires advances in computer science and ML.
- It will act as a focal point for harnessing this data to tackle the grand data challenge science questions.
- Collaborative office space is required for (1) development of key workflows, data extraction, online analysis, (2) data interpretation and impact, (3) improved experimental design, and (4) targeted source development.

- Multi-way flow of talent, ideas, and solutions between large-scale programs at SLAC to gain insight, innovation, and co-development.

The LSCC is being designed to explicitly enable data scientists and ML staff to address this need for real-time, massive-scale data analytics in our programs in X-ray and ultrafast science, physics of the universe, HED science, and bioimaging sciences. Multi-disciplinary teams will need to come together to work with the real-time data streams to optimize experiments as they are being conducted, ensuring efficient and effective use of the facilities and maximizing science output. With instruments taking data from detectors at rates that are orders of magnitude faster than today, scientists need AI/ML experts developing algorithms and capabilities for on-the-fly data reduction, real-time data analysis via HEC facilities for facility operation and novel data analysis. Massive data sets from our X-ray and cryo-EM facilities distributed over the site need operators and users to work together simultaneously to efficiently execute experiments. The LSCC will provide the collaborative space required for development of key workflows, data extraction, online analysis, data interpretation and impact, improved experimental design, and targeted source development. Early examples of a cross-functional approach have already produced remarkable results in the interpretation of complex images in a wide variety of situations through the application of ML and other AI methodologies.

Cross-fertilization of ideas is envisioned across all DOE-sponsored programs at SLAC, augmented by the further development of many active Bay Area laboratory partnerships and Silicon Valley industry collaborations.

The LSCC CDR was completed for the CD-1 ESAAB in November 2019: $58.4–$92.4 million, with a target building of $66 million TPC; FY 2019–FY 2026. In 2020, an LSCC focus group of future building occupants, scientific users, and laboratory leadership was formed to assist the architectural and engineering team in transforming the design so that it accommodates a completely new way of working in a dynamic facility optimized for collaboration. Taking into account lessons learned during the pandemic and with a focus on the future needs of the new science facilities, further design evaluation is currently underway. Focus group input is currently being implemented through design guidelines and performance specifications (DGPS) and used as the centerpiece for the request for proposal (RFP) to procure the design-build (D-B) contractor. Once the D-B contracting partner is selected and procured, the partner will collaborate with the LSCC project team to complete the final design and construction. This project will remove degraded trailers that currently occupy the project site boundary, resulting in a small DM reduction.

The LSCC will have the capacity to co-locate 100 to 150 personnel, enabling flexible collaboration between major programs to gain insight, innovation, and co-development. It is important to note that SLAC's population has been growing at 4 percent per year over the past five years, and the anticipated growth of the population by the time the LSCC is completed is 400 additional people. A new facility, in combination with improved design and efficiency of existing space, will be needed to support this level of growth.

Stanford Collaborative Projects

As demonstrated by the DOE-Stanford partnership in the Photon Sciences Laboratory Building / Arrillaga Science Center, Stanford remains a strong SLAC supporter and continues to drive the development of a "best-in-class" laboratory. SLAC continues to leverage this partnership to grow the Laboratory with key support facilities benefiting science programs, staff, and the user community. Such facilities already exist at SLAC with the SRCF and Stanford Guest House. We are now looking to expand these facilities for our current and future science needs.

Stanford Research Computing Facility Expansion

The SRCF expansion (SRCF-II), represents a Stanford commitment of circa $40 million to nearly double both the footprint (adding approximately 18,000 square feet of floor space) and peak power (from 3 MW to 6 MW) of the existing SRCF data center. Both SRCF and SRCF-II will support the SLAC-Stanford research community by hosting HPC infrastructure in an advanced, modern data center facility. This expansion is needed to support the Rubin U.S. Data Facility, enable real-time data extraction from LCLS-II and LCLS-II-HE, and provide support for science programs across SLAC and Stanford.

The expanded facility will be flexible enough for varying high density computing equipment loads within individual rows of racks, and it will be energy efficient with lower operational costs compared to traditional data centers. If built and approved for SLAC use by DOE, the SRCF-II could provide an optimally effective and efficient solution for DOE.

Stanford Guest House Expansion

The Stanford Guest House expansion is an approximately 47,000-square-foot, 120-room addition to the existing 108-room Guest House. This expansion will build on the existing success of the Guest House, keeping the characteristics that make it so popular with the SLAC user community. The Guest House was designed to provide low-cost short-term accommodation to visiting scientific users. The expansion project includes new interior gathering areas, conference areas, and guest amenities. The expansion will provide a vital asset to the Laboratory as user science programs continue to grow, with a concurrent need for hosting visiting scientists. Stanford is reviewing post-pandemic requirements for occupancy, number of rooms, and room design, with conceptual design to occur over the next couple of years.

Campus Strategy Goal 2: Modernize Existing Facilities to Support Laboratory Goals

The pandemic has forced changes in how we work and collaborate. Uncertainty now and in the future requires us to reimagine and rethink our workplace and how we adapt and accommodate new ways of working. The pandemic safety protocols are in place. When personnel resume work on-site, the requirement and expectation through the recovery is that the work environment will remain safe. While certain types of work may still be performed remotely, the focus of work performed on-site still require us to rethink how we operate the accelerator complex and execute user programs at LCLS, SSRL, FACET, Cyro-EM and other facilities. As such, modernizing existing facilities to support new ways of working will be critical to the Laboratory's future.

Just as new facilities are being designed to promote collaboration, synergy, and flexibility, projects that modernize existing buildings must also meet these goals. Office space consolidation may provide increased opportunity for repurposing or excessing obsolete facilities. As assets are modernized, adequate IT and security infrastructure must be incorporated to secure people, science, facilities, and equipment.

Over the last decade, direct and indirect funding was invested in the modernization of our most critical infrastructure. The next phase of building modernization focuses on major renovation of some of our most critical aging buildings that, despite best efforts, have become “substandard” in their ability to provide the capabilities and configurations required by current and future science initiatives. The functionality and flexibility of these buildings must be improved to enable the continued advancement of the science programs they support.

Campus Building Renovation Project

The Campus Building Renovation Project (CBRP) (FY 2025–FY 2029) will be an SLI LI modernization project to update aging laboratory and office spaces in existing buildings around the Science Quad supporting DOE’s multi-program missions. These facilities house infrastructure that enables the full life cycle of the Laboratory’s accelerator systems and also house engineering and scientific staff working on particle and X-ray detector systems, sensors, application-specific integrated circuits, and electronics for a broad range of advanced applications. Renovation of substandard laboratory and office spaces will modernize workflows, support growing programs, and help achieve SLAC sustainability goals through increased energy efficiency. Renovation of substandard office and laboratory spaces will modernize workspaces and align them with sustainability requirements.

Recent assessments identified these additional requirements for this project: heating, ventilation, air conditioning (HVAC) units, mechanical utilities, roofing systems, and electrical systems will be replaced or upgraded to align with current science mission needs and comply with the latest building and energy codes. These improvements will also enhance sustainability by reducing DM, currently documented at approximately $8.75 million for this project.

Site Security and Access Improvements III

The Site Security and Access Improvements III project ($11.3 million, FY 2023–FY 2026, with proposed funding by the DOE Safeguards & Security Program), represents the final phase of SLAC security projects and will complete the protection of DOE assets and enhance science collaboration across the Laboratory. The project will replace the main entrance gatehouse with a modern guardhouse and security dispatch center. This will reconfigure SLAC's main entrance and exit at Sand Hill Road to improve both safety for security officers and efficiency in verifying access badges.

The project will also install radiation portal monitors at SLAC's main entry and Alpine Road gates, which reduces the risk of accidental off-site transport of activated materials. Additional security gate improvements will substantially lessen the accelerator gated access area, converting the area around PEP Ring Road into a general access area for improved site-wide collaboration. The project will also secure critical buildings and accelerator tunnels using card readers and cameras for access control at all entry control points. Providing modern access control at these buildings will improve property and personnel security by providing site lockdown capability for threat situations in compliance with DOE Design Basis Threat requirements. This project will result in the demolition of the current undersized and ill-configured guardhouse.

Building Enclosures

The site-wide building enclosures ($19.8 million, FY 2023–FY 2024) is an SLI-GPP request to upgrade and modernize 1960s- and 1970s-era buildings across the site that support mission-critical science and support functions. These facilities have long supported laboratories, specialized shops, and office spaces but are now affecting operations because major building enclosure components are beyond their useful life. Building envelopes, including roofs, doors, windows, and exterior enclosure materials, are severely degraded. Several facilities have been identified that are strategically located for optimal use; however, the facility in its current configuration does not adequately support current science requirements. This project will improve overall workforce productivity in these buildings by repairing persistent water leaks and renovating facility systems to restore functionality.

Our campus strategy is driven by science needs and requirements – as well as funding sources – as shown in **Error! Reference source not found.**. Projects are executed to ensure delivery and mission readiness of our facilities and the process and project execution schedules must remain fluid to meet changing needs.

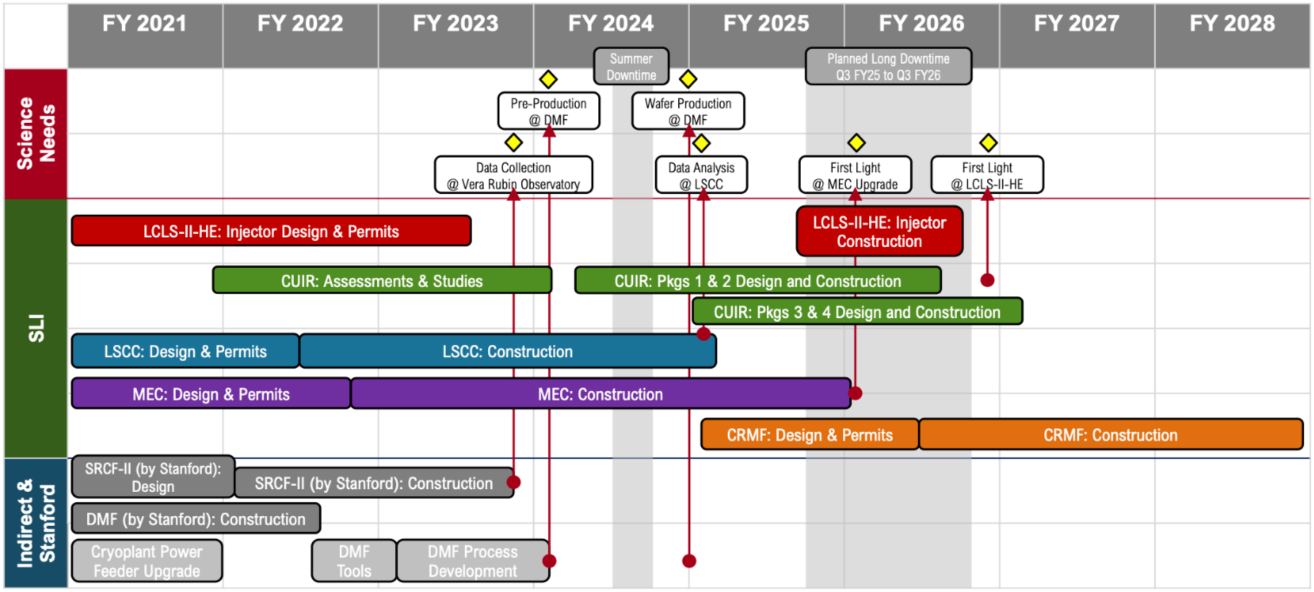


Figure 3: Infrastructure Projects Scheduled to Meet Science Requirements

Asset Management

This section provides an overview of SLAC's asset management efforts and contextualizes SLAC's integrated campus strategy. This includes characterizing the impact of the pandemic on the management of DOE assets and describing process improvements that increase the accuracy and granularity of real property data. SLAC's subject matter experts in real property and facilities rely on the data quality that is enforced through an annual DOE FIMS data validation conducted in close coordination with the local DOE site office. Also described are SLAC's most recent DM trends, maintenance investment index (MII), and replacement plant value (RPV). An analysis of other maintenance indices is provided. These on-going efforts affect the overall life cycle of assets and provide the basis for proactive short- and long-term actions that can be taken to achieve facilities stewardship.

Building and Space Management Pandemic Response

Instituting safety protocols and requirements for workplace health and safety during the pandemic called for collective action by Building and Space Management (B&SM) and Environment, Safety & Health (ES&H). As the potential for a pandemic became increasingly clear in February 2020, SLAC began implementing an immediate response by reconfiguring workspaces to lower the occupation density, instituting social distancing measures, installing hand sanitation stations, and setting up a hub to ensure cleaning supplies and personal protective equipment was available site-wide. As a Bay Area-wide shelter in place order was issued in mid-March, SLAC instituted measures to safely reopen mission-critical facilities. Rapidly transforming spaces critical to conducting research on the mechanisms that drive COVID-19 remained a top priority throughout.

Essential to reopening safely is an online "Health Check" application that screens for health status and potential exposure to COVID-19. Also implemented is a Buildings Readiness program that validates a facility as safe to occupy after temporary closure. Two formal COVID-19 training courses were developed and required for all staff prior to returning to the site and upon first returning to perform on-site work. These helped to describe and implement safety measures such as signage, space configuration, social distancing protocol, limited occupancy, face coverings, and "clean as you go" (CAYG) requirements. Building managers continue to be crucial in implementing a safe return to operations by ensuring Recovery Buildings Information Briefs are completed and maintaining buildings data information on occupancy and recovery efforts in a dashboard that leverages geographic information system (GIS) information. This ensures buildings are stocked with the appropriate cleaning supplies and materials. These ongoing efforts are essential for SLAC operations to continue and for personnel to be able to return safely.

FIMS Data Accuracy

As stewards of DOE’s physical assets, it is essential to monitor and maintain infrastructure inventory and provide current and accurate data regarding its mission, use, status, condition, operation, and maintenance. The DOE relies on the FIMS extensively to make investment and management decisions for real property. Complete and accurate information on real property assets is critical to DOE to manage facilities and satisfy such external reporting requirements as the Federal Real Property Profile. Facilities & Operations staff use this data to assess conditions and address needs for current and future infrastructure at the local level.

SLAC’s GIS has collected data from dozens of sources over the years, including CAD, aerial and drone surveys, ground surveys, LIDAR, and photogrammetry, and converted this information into internally accessible data to offer the most accurate and up-to-date thematic maps of the site. In recent years, Facilities & Operations leveraged this capability and began collaborating with GIS to provide geospatial illustrations of FIMS data. As a result, we have adjusted records in FIMS and created new ones. In 2020, 75 records were added to FIMS to better represent the real property assets in the field. The FIMS property record restructuring included the following utilities: electrical, domestic water, natural gas, sewer, storm water, hot water, and chilled water. Before 2020, these utility systems were captured by one property record per utility system.

The property record restructuring methodology aligns with the FIMS User’s Guide usage codes. For example, each lift station, sump pump, or substation now has an individual real property record. Likewise, pressure piping, gravity piping, and electrical cables each have an individual record. Furthermore, distribution piping and electrical cables are divided into service areas. The goal of this effort is to gain data granularity and accuracy of the overall systems, which enables planners to clearly identify where deficiencies exist and where maintenance or projects are required. FIMS data, such as operational status, overall conditions, mission dependency, and key plans in GIS layers, allows facilities planners and operators to analyze FIMS data and trends with greater clarity and make more strategic decisions about future planned investments. Real property data accuracy is a critical component of our toolkit to ensure a reliable infrastructure backbone. The 75 new asset records are summarized by type in the table below.

Summary of FIMS Asset Record Restructuring: New records added in 2020

	Asset Records		
	Legacy	New Added	Current
Site Electric	1	7	8
Site Domestic Water	1	3	4
Site Natural Gas	1	1	2
Site Sewerage	1	34	35
Site Stormwater	1	19	20
Hot Water	1	3	4

Chilled Water 1	5	6
Other New Footprint	3	3
New Asset Records Added (total)	**75**	
Legacy and New Records Combined (total)		**82**

Maintenance and Repair

Beginning with the third quarter of FY 2017, we began to recalculate the RPV of SLAC facilities using DOE models that take into account such factors as facility uniqueness and location in the San Francisco Bay Area. As a result of this and auto-escalation, RPV has increased, with a decrease in dependency on current plant values (CPV). Our reported RPV increased from $1.92 billion FY 2017 to $3.09 billion in FY 2020. The increase results from recalculating RPV for approximately 550,000 square feet of underground tunnel facilities and certain older buildings. To date, RPV calculations have been adjusted for 80 percent of facilities, and approximately 25 assets will be updated each year until adjustments for the remaining 73 assets (20 percent) are completed. We will review updates annually and gain DOE concurrence on the methodology, models, and factors used to adjust RPV. The overall objective for this RPV effort is to ensure that the indices arrived at are accurate.

DOE has historically assumed a “rule of thumb” maintenance target of 2–4 percent for the maintenance investment index (MII). MII is defined as the percentage ratio of actual annual maintenance (AAM) in relation to RPV as follows: MII=AAM/RPV. For FY 2020, our reported AAM was $20.3 million, and RPV was $3.09 billion, which results in a low MII. However, DOE’s Office of Asset Management (MA-50) now recognizes that this target is typically assumed in commercial industry but may not represent the type of industrial infrastructure within the DOE complex. For example, at SLAC there are many high-value, low-maintenance infrastructure items in the accelerator housing and experimental accelerator housing tunnels.

MII values were calculated separately for operational assets by property type: building, trailers, and two categories of OSFs (utilities and other). The results are summarized in the table below. Also provided is the condition index (CI) for each asset type, represented as the ratio of RN to RPV. While MII is low, the overall CI is relatively good when considered in relation to the average asset age, which is provided to tie maintenance investment to the relative condition of each asset category. It is important to note that SLAC prioritizes mission-critical assets in its resource allocation strategy. Currently, 13 percent (47) of our properties are categorized in operational standby condition, are not considered mission-critical, and typically have a very low AAM, which results in a lower MII in general for our site. Overall, as an integral part of SLAC’s campus strategy, continued investment in prioritized maintenance activities increased by 43.9 percent from FY 2016 to FY 2020 and by 26.8 percent from FY 2019 to FY 2020 alone.

The FY 2020 data illustrates our current largest maintenance investment is in assets with the lowest CI, namely OSFs utilities. Most of the Laboratory’s utility infrastructure is old and inefficient, which escalates overall maintenance and anticipated emergent repairs costs. Our request for SLI-LI CUIR closes infrastructure capability gaps in various civil, mechanical, and electrical utilities.

Generally, OSFs (Other) carries the lowest MII, as can be expected from high-value, low-maintenance facilities such as support structures that include retaining walls around the site, roads, and walkways. Although SLAC does not invest the typical industry standard for buildings (MII of 2 percent), these assets are managed to keep them in relatively good condition, as demonstrated by the average condition index of 93 percent. Mission-critical buildings deemed to be in “substandard” condition are included in our SLI-LI CBRP project request.

Maintenance Investment Index and Average Condition Index *by Property Type for Operational Facilities, $ in millions*			
	Buildings	**OSFs**	**Trailers**

			Utilities		Other			
AAM	MII	$10.31	0.41%	$9.67	2.00%	$0.31	0.34%	$.047	0.75%
RPV		$2,517		$484,.87		$91.26		$6.27	
Average CI (percentage)		93%		67%		71%		86%	
Average age (years)		39		41		40		26	
Source: FIMS Year-End Data FY 2020									

Deferred Maintenance Trends

In 2017, SLAC re-baselined its DM from $28.4 to $80.3 million by applying 2016 DOE-SC Infrastructure – Mission Readiness Working Group guidance. In continuation of this effort, starting in 2020, staff from 10 DOE-SC and Office of Nuclear Energy (DOE-NE) national laboratories collaborated to create a guidance document with the intent of enabling the national laboratories to develop site-specific internal procedures that will foster consistent reporting across all DOE-SC sites of values for RN, DM, and modernization of real property assets, such as buildings, trailers, and OSFs. SLAC utility stewards, who are subject matter experts responsible for assessing systems, used this methodology to validate their respective deficiencies and have continued to do so as is reflected in the values presented in the previous sections.

As an integral part of SLAC's campus strategy, reducing DM is a weighting factor that drives the development of projects that range from significant SLI-LI construction efforts to IGPP minor repair projects. The Mission Readiness team has enhanced "Work Induction" and "Project Implementation Manual" to close communication gaps among stakeholders and streamline these important processes. The Mission Readiness team also applied the "Projects Module" in the Condition Assessment Information System (CAIS) to accurately capture RN and DM associated with planned and active projects and retire such deficiencies when projects are completed. By recognizing the need to ensure our deficiency data's completeness and accuracy, in 2020 we conducted more in-depth condition assessments focused on our underground utilities and other infrastructure with limited access due to physical barriers preventing inspection. This aggressive approach to determine our utilities' condition contributed to an increase in DM after a steady decrease between 2018 and 2019, as evidenced by a DM of $79 million for FY 2020.

It is important to note that the DM value is subject to many variables in any given year. Each year, deficiencies are removed as minor and major projects are completed and added due to that year's Condition Assessment Surveys (CAS). FY 2020 CAS resulted in the addition of $3.2 million or 4.2 percent in DM from the previous year.

Our DM reduction in recent years included infrastructure investments in our electrical substations, accelerator housing, and the Klystron Gallery. Projects that will further reduce our DM in the near term include the cooling towers, LCW systems, associated heat exchangers, sanitary lift stations, electrical substations, electrical feeders, and building roofs. To reduce DM for maximum impact, we will leverage direct and indirect funding and SLI-LI requests to modernize our site. The combination of our planned maintenance activities, direct and indirect infrastructure investments, and the proposed SLI projects along with projects identified across SLAC's project portfolio discussed in section 6.2 should result in an anticipated 84 percent decrease of our current DM.

Site Sustainability Plan Summary

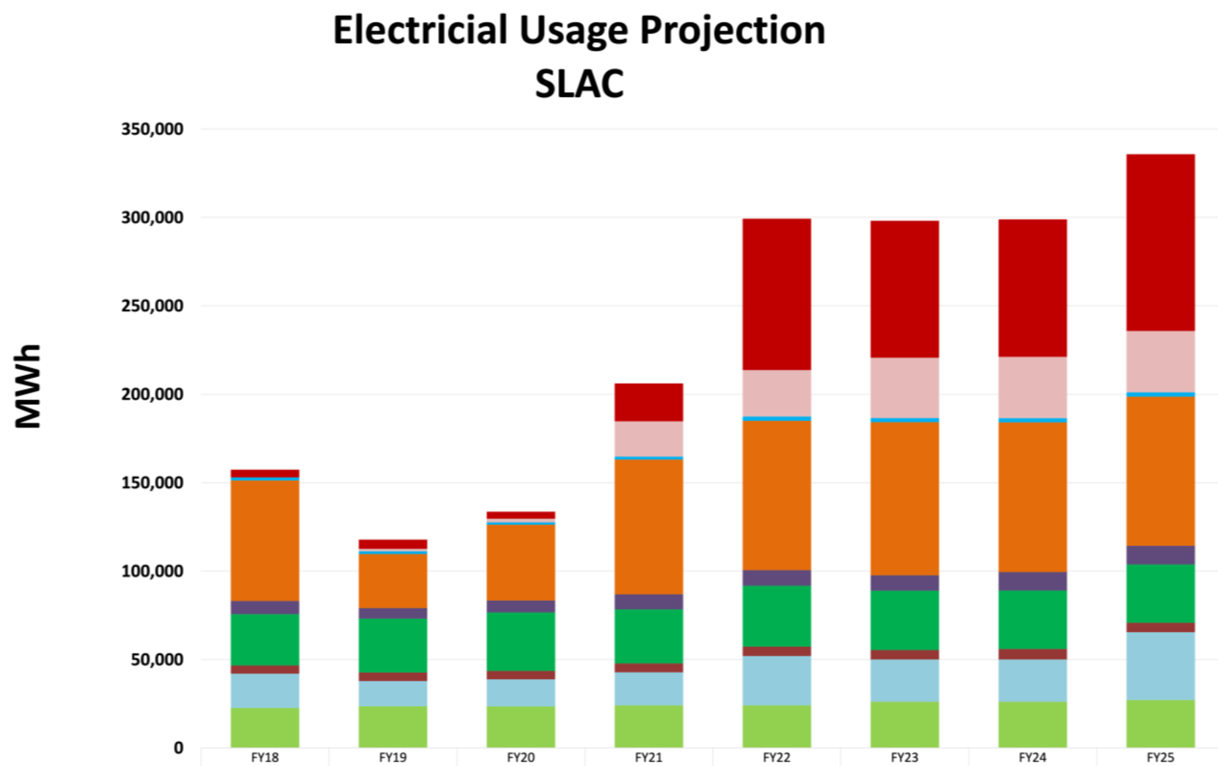
Sustainable design and efficiency are key campus strategy elements. Both are integrated into all design and revitalization efforts. The planned CUIR project proposes to add data collection elements as a foundation for developing data analytics to track, improve, and control energy efficiency.

SLAC's strategy for utility efficiency includes conducting building assessments, prioritizing opportunities based on life cycle cost effectiveness, and developing projects that optimize energy and water usage. Despite the limitations imposed by restricted access during the pandemic, energy efficiency projects were completed as follows:

- A detailed investigation of the first-floor laboratory ventilation system airflow duct noise in the Arrillaga Science Center resulted in identifying an airflow imbalance in the rooftop air handling units. Realignment reduced the fan speed by 40 percent, which is estimated to realize an energy savings of $10,000 per year.
- As part of the High Performance Sustainable Building (HPSB) commitment to maintaining efficiency, energy consultants were engaged to recommission operation of the thermal environmental conditioning (HVAC) and lighting operation in Buildings 52, 53, and 901. The implemented controls efficiently reduced electricity, cooling, and heating by $11,000 per year.
- Aged high bay lighting in Buildings 33 and 15 was upgraded to modern LED fixtures with a 10-year lamp life and wireless controls for efficiency, ease of maintenance, and safety. This replacement reduces electricity cost by over $9,000 per year.
- Native species requiring low water input were used to newly landscape the 10,000-square foot area around buildings bordering the SLAC Quad.
- SLAC received a 2020 DOE Sustainability Honorable Mention in the "Innovative Approach to Sustainability" category for SLAC's Swap program. This was a successful staff-led initiative to gather and re-use laboratory and office equipment that saved more than $24,000 while active in 2018 and 2019.
- Training on sustainability-related topics included a lunch-and-learn seminar attended by Facilities group project managers and the Building Inspection Office (BIO) staff.

13 percent, compared to last year, through energy saving setbacks. Water consumption in buildings was reduced by 40 percent. As soon as operations commenced, such as in the science-based laboratories in the Arrillaga Science Center, an increase in central plant cooling, heating, and gas consumption was observed. Increased electricity usage will become more pronounced with resumption of accelerator operations and commissioning LCLS-II in terms of megawatt hours (MWh), as indicated in **Error! Reference source not found.** below.

Greenhouse gas emission reduction is being pursued through the Western Area Power Administration (WAPA), on behalf of SLAC's participation in the electrical consortium, which is finalizing a contract on a long-term renewable energy power purchase agreement (PPA). Annually, 40,000 MWh is planned to be offset by solar power, which exceeds 100 percent of electricity used for office buildings. This model may serve as prototype for future consortium projects to increase SLAC's power sourced from solar.



	FY18	FY19	FY20	FY21	FY22	FY23	FY24	FY25
HEMSF LCLS-II	4,400	5,200	3,900	21,450	85,600	77,400	77,700	100,000
HEMSF FACET I/II	-	1,410	2,100	19,900	26,300	34,100	34,700	34,700
HEMSF HEP Test Fac.	1,700	1,500	1,300	1,660	2,400	2,400	2,400	2,400
HEMSF LCLS Accel	68,200	30,500	42,900	76,170	84,400	86,500	84,600	84,400
HEMSF LCLS Exp Fac.	7,400	6,100	6,800	8,610	8,800	8,800	10,500	10,500
HEMSF SPEAR3	29,000	30,400	33,000	30,480	34,500	33,500	33,000	33,000
HEMSF SSRL	4,700	4,800	4,800	5,060	5,300	5,300	5,900	5,300
Multi-prgm Support (Not Incl Goal Subj Bld.)	19,400	14,300	15,300	18,700	27,900	24,000	24,000	38,400
Goal Subject Bldg.	22,500	23,500	23,400	24,000	24,000	26,000	26,000	27,000

Figure: SLAC Electricity Usage Projection

THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY

Lab-at-a-Glance

Location: Newport News, VA
Type: Single-program Laboratory
Contractor: Jefferson Science Associates, LLC
Site Office: Thomas Jefferson Site Office
Website: www.jlab.org

- **FY 2020 Lab Operating Costs:** $161.7 million
- **FY 2020 DOE/NNSA Costs:** $160.2 million
- **FY 2020 SPP (Non-DOE/Non-DHS) Costs:** $1.5 million
- **FY 2020 DHS Costs:** $0 million

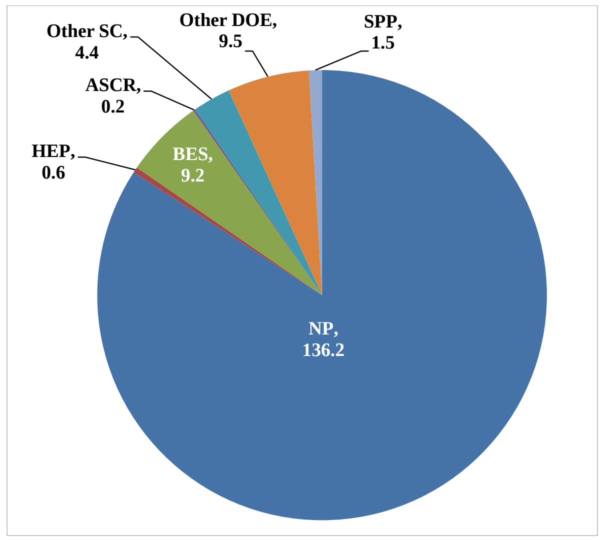
Physical Assets:

- 169 acres and 69 buildings
- 882,900 GSF in buildings
- Replacement Plant Value: $509 M
- 0 GSF in Excess Facilities
- 66,289 GSF in Leased Facilities

Human Capital:

- 744 Full Time Equivalent Employees (FTEs)
- 24 Joint Faculty
- 36 Postdoctoral Researchers
- 44 Graduate Student
- 21 Undergraduate Students
- 1,623 Facility Users
- 1,488 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



Mission and Overview

Thomas Jefferson National Accelerator Facility (TJNAF) is a world-leading research institution for exploring the nature of matter in depth, providing unprecedented insight into the details of the particles and forces that build our visible universe inside the nucleus of the atom. TJNAF was established in 1984 in Newport News, Virginia, and is operated by Jefferson Science Associates, LLC, for the Department of Energy's Office of Science.

Research at TJNAF reveals the fine details of the constituents of matter, from the familiar protons, neutrons, and electrons in the atom, to the lesser-known quarks and gluons inside the atom's nucleus. These studies are revealing how fundamental universal forces build and shape matter and are opening a window into matter's inner universe.

Enabling these studies is TJNAF's world leadership in the development and deployment of large-scale superconducting radiofrequency (SRF) technology. SRF technology powers TJNAF's flagship machine, the Continuous Electron Beam Accelerator Facility (CEBAF). The technological and research successes accomplished with CEBAF as a unique SRF particle accelerator have made possible a wide array of applications, from ever more powerful free-electron lasers for research to life-saving advances in nuclear medicine, and from impactful applications in industry to real-world solutions for protecting our nation's borders.

In support of its scientific mission, TJNAF maintains core capabilities and expertise in Nuclear Physics; Accelerator Science and Technology; and Large Scale User Facilities/Advanced Instrumentation. TJNAF is also exploring ways to capitalize on its expertise in the computational sciences to provide large-scale high-performance computing services to an array of research fields for accelerating and maximizing scientific insight in the future.

TJNAF actively partners with industry to advance critical technologies to benefit the nation. The lab is also investing in the next-generation STEM workforce. Its dedicated research facilities enable one-third of U.S. Ph.D.s in nuclear physics annually, and its outreach programs positively impact thousands of students and teachers while helping them build critical knowledge and skills for a brighter future.

Core Capabilities

Nuclear Physics

TJNAF is a unique world-leading user facility for discovery studies of the structure of nuclear and hadronic matter using continuous beams of high-energy, polarized electrons. The 2015 NSAC (Nuclear Science Advisory Committee) Long Range Plan clearly stated that its highest priority was to capitalize on this investment: "With the imminent completion of the CEBAF 12 GeV upgrade, its forefront program of using electrons to unfold the quark and gluon structure of hadrons and nuclei and to probe the Standard Model must be realized."

The CEBAF electron beam can be simultaneously delivered to the experimental halls at different energies. With the completion of the 12 GeV Upgrade the beam energy can be up to 12 GeV, converted to 9 GeV photons for experimental Hall D, and up to 11 GeV to Halls A, B, and C. Each experimental hall is instrumented with specialized experimental equipment designed to exploit the CEBAF beam. The detector and data acquisition capabilities at TJNAF, when coupled with the high-energy electron beams, provide the highest luminosity (10^{39}/eN/cm^2/s) capability in the world. The TJNAF staff designs, constructs, and operates the complete set of equipment to enable this world-class experimental nuclear physics program, in close collaboration with a large domestic and international user community of well over 1,600 users annually.

The CEBAF science program spans a broad range of topics in modern nuclear physics. Lattice Quantum Chromodynamics (LQCD) calculations predict the existence of new exotic hybrid mesons that can be discovered with the new 12 GeV experiments, and elucidate the nature of confinement. New phenomenological tools have been developed that produce multidimensional images of hadrons with great promise to reveal the dynamics of the key underlying degrees of freedom – a new science program termed Nuclear Femtography. A surprising connection between the role of nucleon-nucleon interactions and the quark structure of many nucleon systems discovered at TJNAF earlier, needs to be understood. Development of measurements of exceptionally small parity-violating asymmetries with high precision has enabled major advances in hadronic structure, the structure of heavy nuclei (through measurement of the neutron distribution radius), and precision tests of the Standard Model of particle physics, including a measurement of the electron's weak charge.

A comprehensive theoretical effort provides leadership across nuclear physics by pulling together state-of-the art theoretical, phenomenological, and computational approaches, including effective field theory techniques, QCD global analyses, and non-perturbative LQCD calculations. TJNAF deploys cost-optimized High Performance Computing for LQCD calculations as a national facility for the USQCD (a U.S. lattice gauge theory community) that complements DOE's investment in leadership-class computing. Computational techniques in LQCD now promise to provide insightful and quantitative predictions that can be meaningfully confronted with and elucidated by forthcoming experimental data. Those techniques also promise to calculate the structure of hadrons that are hard, if not impossible, to do scattering experiments with.

Excellent synergy exists between the TJNAF experimental, theoretical, and computing programs. The Joint Physics Analysis Center (JPAC) develops theoretical and phenomenological understanding of production and decays of hadron resonances, which helps bridge the analyses and interpretation of experimental data from TJNAF with the results of LQCD calculations. The Jefferson Lab Angular Momentum (JAM) collaboration pulls expertise in QCD theory, phenomenology, and high performance computing to develop new and better tools to help extract the 3D tomography of hadrons from TJNAF data. TJNAF was the first to make use of Graphics Processing Units for high performance computing based on heterogeneous architectures (for LQCD calculations) and continues this innovative approach to present needs, including wide embracement of Machine Learning and Artificial Intelligence in Nuclear Physics techniques.

The 2015 NSAC LRP recommends a "high-energy high-luminosity polarized EIC as the highest priority for new facility construction following the completion of FRIB." An independent assessment of the science case for EIC was undertaken by a committee of the National Academies of Science in 2016-18. The committee made their findings public in July 2018, strongly supporting the case for a U.S.-based EIC. Following the decision to select BNL as the site of the EIC, TJNAF actively worked with BNL to provide important expertise and capability to ensure successful implementation of the EIC, including taking responsibility of scope that benefits from TJNAF's long-time intellectual investment in the EIC, TJNAF's core expertise, and its wide international user community. TJNAF played a fundamental role initiating and expanding the international EIC User Group that has now grown to 1,266 individual members from 253 institutions in 34 countries, with a large contribution of TJNAF users.

TJNAF scientists are heavily engaged in the community effort and its phenomenological studies to refine the strong science case and help develop unique detection capabilities for the future EIC, including the year-long and user-driven Yellow Report Initiative. The purpose of this Yellow Report Initiative, initiated by TJNAF scientists, was to advance the state and detail of the documented physics studies in preparation for the realization of the EIC. The effort aims to provide the basis for further development of concepts for experimental equipment best suited for science needs, including complementarity of two detectors towards future Technical Design Reports (TDRs). TJNAF has consolidated its efforts in the development of the science program by forming an Electron-Ion Collider Center (EIC^2). Seminars, visiting fellows, and workshops will be among the components of this new center.

Accelerator Science and Technology

TJNAF has world-leading capabilities in technologies required for superconducting linacs:

- Complete concept-to-delivery of superconducting linear accelerators
- State-of-the-art SRF fabrication and assembly capabilities
- Unrivaled design, commissioning, and operations experience in large cryogenic plants
- World-leading polarized electron injector capabilities
- Low-level RF and controls
- Accelerator and large-scale control systems
- Accelerator operation and design

One of the key core capabilities of TJNAF is its capability in SRF system design and production. The SRF accelerator system consists of multiple integrated technologies with expertise spread throughout multiple disciplines and departments. TJNAF maintains collaboration and communication among all associated sub-systems essential to maintaining and enhancing SRF capabilities. System integration essential to an effective SRF system includes cavity fabrication and processing, cryomodules, low-level RF controls, high-power RF, cryogenics, software and hardware controls, and monitoring systems. Ensuring that each of these sub-systems maintains state-of-the-art capabilities is critical to maintaining a world-leading program in SRF accelerator system capabilities. To accomplish the mission, the SRF Institute must maintain a comprehensive set of expertise and facilities to support SRF technologies at TJNAF and be ready to respond to current and future needs of the lab, the DOE complex, and other partners. TJNAF's SRF Facilities occupy about 60,000 SF of contiguous space all under one roof, which includes over 30,000 SF of new work centers, 25,000 SF of renovated high bay assembly and test work centers, and about 5,000 SF for parts inventory and storage. A unique feature of the SRF facility is the ~800 m2 chemroom/cleanroom suite. This state-of-the-art facility is fully engaged to support LCLS-II HE, SNS PPU, critical fundamental SRF R&D, and future projects such as EIC, PERLE, and the ILC.

The Upgraded Injector Test Facility (UITF) underwent a series of Accelerator Readiness reviews and was fully commissioned in the fall of 2020. The UITF is now certified as an accelerator facility and is operational. During the initial phase of operations, TJNAF has completed a series of experiments to characterize the HDice polarized target, conducted commissioning studies for the new SRF "booster" cryomodule, to be installed in CEBAF during the 2022 shutdown, demonstrated next-generation LLRF controls performance in support of an AIP-funded project, and supported SBIR grants to study advanced polarimetry diagnostics. A new beamline for environmental applications, supported by LDRD funds, will be installed in the spring of 2021. The first experiment will be in collaboration with the Hampton Roads Sanitation District to study the effectiveness of e-beam irradiation to break down a ubiquitous solvent 1,4-Dioxane in wastewater. The facility will then be used to conduct the first ever testing with beam of Nb3Sn coated cavities operating at 4K. This work is supported by an Early Career Award.

Electron-Ion Collider (EIC) Design

The Accelerator Division, in partnership with the Physics Division and collaborators at other national laboratories, developed a design concept for a Jefferson Lab Electron Ion Collider (JLEIC). A design report for JLEIC was published in 2012, to respond to the energy and luminosity requirements of the EIC physics white paper. The JLEIC design team, composed of TJNAF personnel and strategic national and international collaborators, developed a pre-Conceptual Design Report (pre-CDR) in FY 2018 and FY 2019. These design efforts influenced and continue to influence the EIC project that started in FY20, with TJNAF as a major partner in the overall facility design and performance objectives. In particular, the portability of some key strengths of the JLEIC design were investigated and led to a possible increase of the luminosity of the BNL-based Electron-Ion Collider by nearly a factor of two at lower Center-of-Mass Energies. The design efforts were also instrumental to study the feasibility of a possible second Interaction Region design with somewhat increased crossing angle but a stronger emphasis of forward detection, to enhance science complementarity. These design optimizations are under further study now.

Large Scale User Facilities/Advanced Instrumentation

Experimental Nuclear Physics (funded by DOE SC – Nuclear Physics)

TJNAF is the world's leading user facility for studies of the quark structure of matter using continuous beams of high-energy, polarized electrons. With well over 1,600 users annually, of which roughly two-thirds are domestic, TJNAF supports what is generally considered the largest nuclear physics user community in the world. CEBAF is housed in a seven-eighths mile racetrack and was built to deliver precise electron beams to three experimental end stations or halls. The electron beam can be converted into a precise photon beam for delivery to a fourth experimental Hall D. Accelerator instrumentation is installed to deliver beams to all four halls simultaneously.

CEBAF provides a set of unique experimental capabilities unmatched in the world, as follows:

- Highest energy electron probes of nuclear matter

- Highest average current
- Highest polarization
- Ability to deliver a range of beam energies and currents to multiple experimental halls simultaneously
- Highest-intensity tagged photon beam at 9 GeV for exotic meson searches
- Unprecedented stability and control of beam properties under helicity reversal for high-precision parity violation studies

Hall D is dedicated to the operation of a hermetic large-acceptance detector for photon-beam experiments, known as GlueX. Hall A houses two high-resolution magnetic spectrometers of some 100 feet in length and a plethora of auxiliary detector systems, including the large-acceptance Super BigBite Spectrometer. Hall B is home of the CEBAF large-acceptance spectrometer (CLAS12) with multiple detector systems and some 100,000 readout channels. Hall C boasts two roughly 80-foot-long, high-momentum magnetic spectrometers that allow for precision scattering experiments, and has housed many unique large-installation experiments. Maintenance, operations, and improvements of the accelerator beam enclosure and beam quality, and the cavernous experimental halls and the multiple devices in them, are conducted by the TJNAF staff to facilitate user experiments. Important capabilities related to the experimental program include state-of-the-art particle detection systems, high-power cryogenic targets, polarized targets, high-speed readout electronics, and advanced data acquisition technology.

CEBAF Operations (funded by DOE SC – Nuclear Physics)

CEBAF is in the midst of a long shutdown to install a new 2K cold box, perform maintenance on the in-tunnel cryogenic transfer line system, refurbish warm girder segments between cryomodules to mitigate any potential particulate contamination, complete the first phase of an upgrade to the Injector for the parity program, and conduct extensive planned maintenance on many subsystems. The Energy Reach program will also install two refurbished cryomodules and remove one more to seed the refurbishment program. In late summer TJNAF will resume its primary mission of the 4-Hall 12 GeV Physics program. The multi-year CEBAF Performance Plan and Energy Reach programs are well underway and will continue to ensure TJNAF meets reliability goals and provide operational energy margin for the Physics program. In the following year the lab will complete the second phase of the Injector upgrade. As mentioned above, plans are underway to prepare technical reports that pave the way towards an increase in the CEBAF luminosity by 50% and to double the energy using FFA technology. With the completion of the 12 GeV Upgrade, firm plans in place for maintenance and energy reach as well as a vision towards the future, TJNAF will continue to be the world's premier experimental QCD facility.

Accelerator Technology (funded by DOE SC – Nuclear Physics, Basic Energy Sciences, High Energy Physics, DOD ONR, Commonwealth of Virginia, and Industry)

The ability to use the TJNAF Low Energy Recirculator Facility (LERF) as an accelerator R&D test bed for Energy Recovery Linacs and techniques required to establish cooling of proton/ion beams, for example, provides a mutually beneficial cross-fertilization between the TJNAF LERF and Nuclear Physics. The LERF vault has recently been configured to enable higher throughput of cryomodule testing for LCLS-II HE. In addition, the LERF is supporting an R&D program to develop an accelerator-based concept to make Cu-67, a potentially useful radioisotope for medical imaging and radiotherapy.

TJNAF is applying its accelerator technology to collaborate with four other national laboratories to realize the Linac Coherent Light Source II, at the Stanford Linear Accelerator Center (LCLS-II at SLAC). TJNAF was responsible for construction of half of the superconducting cryomodules as well as the two cryogenic refrigeration plants. The lab expects to contribute to the commissioning effort for the accelerator as well as the cryogenics plants in the next year. An LCLS-II upgrade, LCLS-II-HE, is also underway to double the energy of LCLS-II from 4 to 8 GeV and extend the X-ray energy limit from 5 keV to 12.8 keV. TJNAF will build 10 cryomodules for the LCLS-II-HE project.

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TJNAF has been selected to produce cryomodules for the Spallation Neutron Source Proton Power Upgrade (SNS PPU). The scope of the project is to build 7 new high beta cryomodules with 28 new SRF cavities to increase the SNS linac beam energy to 1.3 GeV. Vendor-provided cavities have started to arrive and are being qualified in our Vertical Test Area.

Cryogenics (funded by DOE SC – Nuclear Physics)

Over the last 25 years, TJNAF has developed a unique capability in large-scale cryogenic system design and operation that is a critical resource for the U.S. national laboratory complex. The TJNAF cryogenics group has been instrumental in the design of many construction projects requiring large-scale cryogenics: SLAC (LCLS-II), Michigan State University (FRIB), Oak Ridge National Lab (SNS), TJNAF (12 GeV Upgrade), and NASA (James Webb Space Telescope), as well as improving the cryogenic efficiency of existing systems (Brookhaven National Laboratory). In the process, many inventions have been patented, and one has been licensed by Linde (one of two companies that build cryogenic systems) for worldwide applications on new and existing cryogenic plants. This work has also resulted in many master's and Ph.D. theses, to ensure the continuity of this expertise in the coming decades.

The group has completed the design, specification, and procurement—and started the commissioning—of the helium refrigerators for LCLS-II. This work is based on the successful CHL2 design for the 12 GeV Upgrade and designs developed for FRIB. Significant CEBAF upgrades in progress include the installation of a replacement 2K cold box for CEBAF operations which was fabricated at TJNAF using the latest cold compressor technology. Installation and commissioning of this cold box is to be completed by July 2021. Work continues on the modification and installation of a surplus SSC refrigerator, ESR-2, to support future CEBAF end-station operations. Additionally, project work including procurement of equipment is underway to utilize funding received to upgrade the 2K capacity of the Cryogenic Test Facility that supports superconducting cavity and magnet testing at the Test Lab. The combination of ongoing operations of five refrigerators supporting the TJNAF experimental program, the upgrading of those refrigerators, and the work outside the lab has enabled the training of the next generation of cryogenic engineers in the newest technology as well as the details of plant operations supporting a dynamic experimental program.

Science and Technology Strategy for the Future/Major Initiatives

The TJNAF science strategy for the future involves pursuit of four major initiatives that advance key objectives in the field of Nuclear Physics and also position the lab to more broadly contribute to the programs in the Office of Science. These initiatives position TJNAF to diversify its scientific mission by building upon our foundation in nuclear physics research to pursue new research directions and facility capabilities, particularly in advanced computing.

Infrastructure

Overview of Site Facilities and Infrastructure

TJNAF is located on a 169-acre DOE-owned federal reservation within the City of Newport News in southeast Virginia. Adjacent to the federal reservation is the Virginia Associated Research Campus (VARC), a 5-acre parcel owned by the Commonwealth of Virginia and leased by SURA which sub-leases five acres to DOE for TJNAF use. Also adjacent is an 11-acre parcel owned by Newport News that contains the Applied Research Center (ARC) where JSA leases additional office and lab space. SURA owns 37 acres adjacent to TJNAF where it operates a 42-room Residence Facility at no cost to DOE.

TJNAF consists of 69 DOE-owned buildings comprising 882,990 square feet (SF) of office, shop, technical, and storage space. JSA leases additional office and lab space in the VARC (37,643 SF) and ARC (11,097 SF). JSA also leases two off-site storage warehouses (17,549 SF). Distribution of space by type is summarized in Table 4. There are currently no excess facilities and none are expected within the next 10 years. In addition to real property assets, 42 personal property shipping containers represent 12,920 SF of added storage.

TJNAF provides office and workspace for approximately 760 JSA contractor, JSA, and federal government employees plus 1,600 transient users and visiting scientists. Facility space is well utilized with a current asset utilization index of 99.6%. The condition of TJNAF facilities is generally good as summarized in the table below.

Type of Use	Total Usable Square Feet, Owned and Leased
Technical and Laboratory	258,768 (39%)
High Bay	150,198 (23%)
Office	101,420 (16%)
Storage	92,847 (14%)
Common	54,579 (8%)
TOTAL	657,812 (100%)

Table: Distribution of Usable Space by Type of Use

Condition		Mission-Unique Facilities		Non-Mission-Unique Facilities		Other Structures and Facilities	
		Number	SF	Number	SF	Number	SF
Rating	Adequate	36	339,976	30	353,596	35	N/A
	Substandard	0	0	7	249,069	4	N/A
	Inadequate	0	0	1	6,638	0	N/A
	TOTAL	36	339,976	38	609,303	39	N/A
Utilization	Underutilized	2	3,240	0	2,873	0	N/A
	Excess	0	0	0	0	0	N/A

Table: TJNAF Facility Rating and Utilization Assessment

TJNAF is entirely dependent on public utility service. JSA sources power from Dominion Energy at an average rate of $0.06/kWh and water from Newport News at an average rate of $3.69/HCF, and disposes of wastewater through the Hampton Roads Sanitary District at an average rate of $8.77/HCF. Utility service meets mission requirements although occasional, unplanned commercial-power outages periodically disrupt accelerator operation.

The TJNAF Land Use Plan is maintained on the TJNAF website and summarized in Enclosure 1. With the decision not to site the EIC at TJNAF, the Campus Plan and Land Use Plan have been updated to align with this decision. Additionally, a future High Performance Data Facility has been ideally located on the campus. The SURA-owned land, as well as Newport News-owned land reserved for TJNAF interests, still preserve expansion opportunities critical to the lab's strategic plan.

The SLI-funded CEBAF Renovation and Expansion (CRE) project received CD-1 in March 2020. The project includes the acquisition of the ARC, renovation of CEBAF Center, and a 22K SF building expansion—which will eliminate the VARC lease. The ARC acquisition process is anticipated to be concluded in FY 2021. An extension of the current 11,097 SF lease is in place until the acquisition is complete.

Campus Strategy

The S&T strategy described in Section 4 of this plan dictates the campus investment plan. Working with the Chief Research Officer, the facilities planning team reviews the capabilities of the current infrastructure against the S&T strategy to identify current and projected gaps. TJNAF then performs an analysis of alternatives (AOA) to select the optimum solutions to close the gaps between mission needs and infrastructure capability. The selection of solution and time phasing is driven by mission priority and constrained by the projected levels of indirect, GPP, and SLI program funding.

This plan reflects the heightened urgency to improve infrastructure reliability given the recent trend of increasingly disruptive failures impacting experimental schedules. Accelerator reliability is the product of the joint availability of all component systems (cavities, magnets, controls, infrastructure, and so forth). To meet the CEBAF 85% availability goal, the Accelerator Division has allocated to facilities infrastructure an availability requirement of >98.5%, which translates to <81 hours of total downtime over a 32-week experimental period. To accomplish this, Facilities Maintenance and Operations completed 6,162 preventative maintenance tasks and 2,001 corrective tasks in FY 2020.

The recent failure history suggests that continued substantial improvement in infrastructure reliability and high-power electronic equipment design is needed to reach this availability requirement. The impact of electrical transients to the operation of high-power electronic equipment remains the greatest cause of impact to accelerator operations and the area of major concentration. JSA continues to work with Dominion Energy to improve power quality including major maintenance of the substations feeding the lab (22, 33, and 40 MVA), removing trees near transmission lines, inspecting overhead lines, coordinating utility preventive maintenance (PM) tasks with accelerator downtimes, proactively monitoring line voltage variations within tariff limits, and meeting regularly to review power reliability. In 2020, Facilities Maintenance and Operations performed PM tasks on electrical distribution system components and multiple oil-filled transformers. Electrical safety and reliability upgrades were completed on the 40 MVA substation including a remote reset ground fault relay, upgraded controls for the automatic voltage regulators, and upgraded metering. Two transformers at the Central Helium Liquefier (CHL) were tested and de-gassed. Additionally, 33 of 55 1,000-watt high intensity discharge (HID) light fixtures in the experimental halls were replaced with 300-watt light emitting diode (LED) fixtures.

Belt-driven rack fans cooling the RF power supply racks have been in service since the original accelerator start-up and are failing at an increasing rate with parts obsolescence making it extremely difficult to maintain. An alternate design is being evaluated with plans for replacement in 2021.

A project was identified and started to increase CEBAF reliability and the cooling capacity of the linear accelerator (LINAC) service buildings as a result of increased accelerator operations during the warm summer months. The scope of the project increases chilled water capacity, improves air flow, reduces infiltration of unconditioned air, and increases air conditioning.

Replacement of accelerator fire detection and suppression systems was completed in FY 2020. This project replaced end-of-service-life components including all fire suppression, detection, and monitoring systems. A nitrogen-filled dry pipe system replaced the existing air-filled system, which will slow corrosion, improve the life of the system, and decrease maintenance costs.

Presented in the table below is the correlation between S&T mission requirements, required infrastructure capability, current shortfall in this capability, and optimum solution.

Core Capability (SC-X)	**Infrastructure Requirement**	**Current Shortfall**	**Optimum Solution and Need Date**
Accelerator Science and Technology (SC01)	Provide liquid helium to the Test Lab to enable the development, production, and testing of SRF components and cryomodules, both for use by TJNAF in CEBAF and projects for other labs.	The Cryogenics Test Facility (CTF) has experienced heavy utilization due to the CEBAF upgrade and BES multi-lab partnership projects. Approximately $5M of system components have reached end-of-life and others require upgrading to maintain adequate capacity for projected workload.	Complete the **CTF Upgrade.** Funding was provided in FY20 under the SLI-GPP program.
	Provide sufficient high bay, storage, and office space needed to design, produce and test SRF components and systems.	10,000 SF of high bay space in the Test Lab is unavailable for SRF needs due to occupation by Physics' large-scale assembly and testing activities. SRF office space needs in the Test Lab exceed available capacity. 10,000 SF of technical storage is leased in warehouse space remote from TJNAF. This introduces additional labor and time requirements to control and access this high-value material.	The **Thomas Jefferson Infrastructure Improvement (TJII)** project will construct a new 45,000 SF Test Lab High Bay Annex for Physics' large-scale assembly and testing activities, thus making existing Test Lab high bay space available for SRF. Physics engineering office space will be relocated to a modernized Experimental Equipment Lab (EEL) to ensure adequate space is available for SRF in the Technology and Engineering Development Facility (TEDF). A new 15-20,000 SF warehouse will relieve the demand for remote, off-site leased storage. Need date is immediate.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
	Low Energy Recirculator Facility (LERF) for R&D on electron guns, dedicated cryomodule testing for DOE Projects, and R&D for production of medical isotopes.	Mechanical systems are at end-of-service-life and electrical systems are at or past capacity. Finishes are well worn and need to be renewed.	The **LERF Renovation** will ensure the facility can meet its planned operational use. Need date is FY24.
Large Scale User Facilities/R&D Facilities/Advanced Instrumentation (SC16)	Central Helium Liquefier (CHL) capable of supplying CEBAF with 9400W of 2K cooling and 22 g/s of LHe at >96% reliability.	Two plants, CHL1 and 2, must operate to meet the 2K cooling requirements, but CHL1 is unable to meet the up-time requirements due to an aging cold box.	Complete the **CHL1 2K Cold Box Replacement**. Need is immediate and project is underway as an FY 2017 SLI-GPP project scheduled for completion in FY21.
	210 tons of cooling capacity are required in each of the two linac service buildings to support CEBAF operations.	Existing cooling system is 36% undersized for current loads. Shortfall is 75 tons in each linac.	The **LINAC Additional Cooling** project increases chilled water capacity, improves air flow, reduces infiltration of unconditioned air, and increases air conditioning. Need date is immediate.
	45,000 SF of environmentally controlled high bay and technical space to support SRF production, cryogenics fabrication, and equipment assembly and staging for four experimental halls operating at 34 weeks/year.	High bay space in the EEL, Test Lab, and TED buildings is heavily over-utilized. Overcrowding increases the safety risk to staff and visiting scientists. Off-site space is currently being leased to meet the demand.	The **TJII** project will construct a new 45,000 SF Test Lab High Bay Annex for Physics' large-scale assembly and testing activities. Need date is immediate.
Nuclear Physics (SC20)	End station refrigeration capable of supplying Halls A, B, and C with 4000W of 4K cooling and 40 g/s of LHe at >85% reliability.	Current End Station Refrigerator serving Halls A, B, and C only has 1500W of 4K cooling and 11 g/s of LHe, has been operating nearly continuously for 20 years and is near end-of-life.	Complete installation of the SSC Cold Box to activate the **End Station Refrigerator 2 (ESR2)**. This will close the capability gap and provide a long-term solution to meet the experiment plan. Need date is immediate. Project funding was provided in FY20.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
	Up to 210,000 SF of office and collaborative space that meets DOE high-performance, sustainable building standards to house staff, students, and visiting users.	CEBAF Center (127,000 SF) is overutilized and substandard due to aging mechanical systems that require immediate replacement. An additional 45,000 SF of office space is leased in adjacent buildings at disadvantageous rates.	The **CEBAF Center Renovation and Expansion (CRE),** including acquisition of the Applied Research Center (ARC), renovates CEBAF Center and provides an additional 144K SF of space. The project consolidates staff and vacates leased space. Need date is immediate. Initial project funding was received in FY20.
	The EEL provides 54,800 SF of technical and lab space for Physics, Engineering, and Facilities staff and is integral to our campus plan.	EEL has end-of-life mechanical systems and numerous code deficiencies. Office and technical space is insufficient, poorly distributed, and not integrated with the campus.	The **TJII** project fully renovates and modernizes the EEL facility to meet mission needs. Need date is immediate.
Support Facilities and Infrastructure (SC25)	Provide 100,000 SF of outside storage to accommodate large experimental assemblies, support structures, and equipment for future experiments and operations.	Current laydown space is scattered in multiple locations around site. Stored material in some of these sites is visible from off-site and creates an eyesore. Some 70,000 SF of existing laydown area will be lost due to future building construction.	The **Laydown Yard Expansion** roughly doubles an existing, centrally located storage area which is not visible from off-site. Consolidation will improve material management and provide an opportunity to eliminate unneeded material. Need date is immediate.
	To meet DOE sustainability goals for 2025, TJNAF must reduce potable water consumption by 36% relative to 2007 baseline.	Must reduce potable water consumption from current intensity of 63.5 gal/GSF to 41 gal/GSF.	The **Cooling Tower Water Reuse** project develops a 50M gal/year alternate water source for use in cooling towers by directing and treating water from off-site retention ponds. Need date is FY22.
	Relocate Facilities Maintenance and Operations functions	Functions are located in two substandard buildings (13 and 19) located in the administrative core of the campus. Critical spares are inefficiently scattered across the campus.	**The Integrated Maintenance and Logistics Center (IMLC) Phase 1** provides a fully integrated solution and relocates these functions to the lab’s service corridor. Need date is immediate.
	Relocate logistics functions.	TJNAF logistics functions are primarily located within high bay space	The **IMLC Phase 2** provides a fully integrated solution and relocates these

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
		within the EEL building, which is already oversubscribed and needed to support research and technical operations.	functions to the lab's service corridor. Need date is immediate.
	Suitable access roads and parking to meet safety and regulatory requirements.	Continued expansion of the TJNAF campus as outlined in this plan along with development of property immediately surrounding TJNAF requires expansion and alteration of campus access and parking to support vehicle loads, and maintain compliance with safety and regulatory requirements.	The **TJII** project provides site-wide road, parking, and sidewalk improvements, which rebuild existing roads and resolve impacts created by both on-site and adjacent off-site construction. Need date is immediate.
	Provide 1,900 gal/hr of chilled water to cool R&D equipment in the Test Lab, EEL, CEBAF Center, and Accelerator service buildings.	Existing Test Lab chillers are approaching the end of their service life and use refrigerant that will no longer be available after FY30.	The **TJII** project includes replacing the existing chillers with a new chiller to be installed in the Central Utility Plant (CUP). Need date is FY30.
	Suitable potable water distribution to reliably meet need for 120M gal/year use.	Portions of the water system exceed 50 years and have experienced severe corrosion. The site lacks a full water loop with isolation valves to allow for normal maintenance without severely affecting operations.	The **TJII** project replaces aging sections of piping and provides for completion of the site water distribution loop with adequate isolation valves for system operations and maintenance. Need date is FY25.
	Suitable sanitary sewer system to meet the service needs of the site.	Portions of the system have insufficient slope and have experienced breaks or surface water infiltration. The capacity is marginal to meet future needs.	The **TJII** project will correct existing deficiencies and add additional capacity to meet expected growth requirements. Need date is FY25.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
	Main entrance appropriate for a DOE national laboratory and adequate wayfinding signage to safely direct users and visitors.	The existing entrance does not reflect the scope and capabilities of the site or its important technology anchor role in the community.	The **Main Entrance and Site Signage** project will enhance the main entrance and provide needed wayfinding signage across the site. The site circulation plan will be impacted with the CRE project. Need date is FY25.
	Provide an isolated and secure facility to calibrate radiological instruments and house rad waste processing equipment and work in process.	Campus growth is encroaching on the existing calibration lab, creating a safety and security risk.	Construct a new **RadCon Calibration Lab and Waste Processing** work center in a more remote area adjacent to the Central Material Storage Area (CMSA). Need date is FY26.
	Relocate service entrance road to the TJNAF campus.	TJNAF service vehicle traffic flow and Facilities Maintenance and Operations functions do not support future growth of administrative, research, and technology portions of the TJNAF campus.	Construct a new **Service Entrance Road** to directly connect the TJNAF campus to a major public road, which will facilitate the future relocation of the facility maintenance and logistics functions. Need date is FY29 or sooner if practical.
Advanced Computer Science, Visualization, and Data (SC02) and Computer Science (SC10)	40,000 SF of data center space and administrative space for 100+ staff to grow core capabilities in computational science.	CEBAF Center's data center (6,000 SF) is at capacity, and insufficient administrative space exists in CEBAF Center to support the growth of Computational Sciences and Technology (CST).	Construct a new facility with a 40,000 SF data center and sufficient administrative space for 100-165 staff.

Table: Campus Strategy Reflecting Realistic Solutions to Address Infrastructure-Capability Shortfalls to Meet TJNAF S&T Strategic Objectives

The gaps identified above can be closed using a combination of SLI, SLI-GPP, and NP-GPP funding of $205M. In addition to providing essential capabilities for mission performance, these investments will eliminate $5M of deferred maintenance.

The primary focus of our facilities operations and maintenance program is to increase the mean time between failure of facility systems through accelerated replacement of end-of-life systems and adding redundancy for critical systems to eliminate downtime from single-point failures. Similarly, when failures occur, TJNAF will reduce the mean time to repair by making sure sufficient stock of critical spares is on hand to immediately restore operation, rather than accept lengthy downtimes to source replacements.

The most recent TJNAF Condition Index is 0.95. However, this could drop over time if Facilities Operations and Maintenance funding continues to be limited to 1.25% of replacement value. Modernization projects and construction of new facilities through SLI and GPP funding have enabled TJNAF to maintain a modest deferred maintenance value ($7.0M in FY20). Over the next decade, no significant increase in deferred maintenance is expected as JSA implements the capital spending plan.

Site Sustainability Plan Summary

TJNAF remains strongly committed to achieving targets established in the DOE Strategic Sustainability Performance Plan. TJNAF received a 2018 Federal Energy and Water Management Award in the Lab and Data Center category for energy and water cost savings, optimized energy and water use, and the use of advanced and distributed energy technologies under the Computer Center Modernization project achieving a power usage effectiveness (PUE) of 1.3. For FY 2020, all but three sustainability interim target goals were met: potable water intensity, renewable energy, and sustainable buildings (by building count).

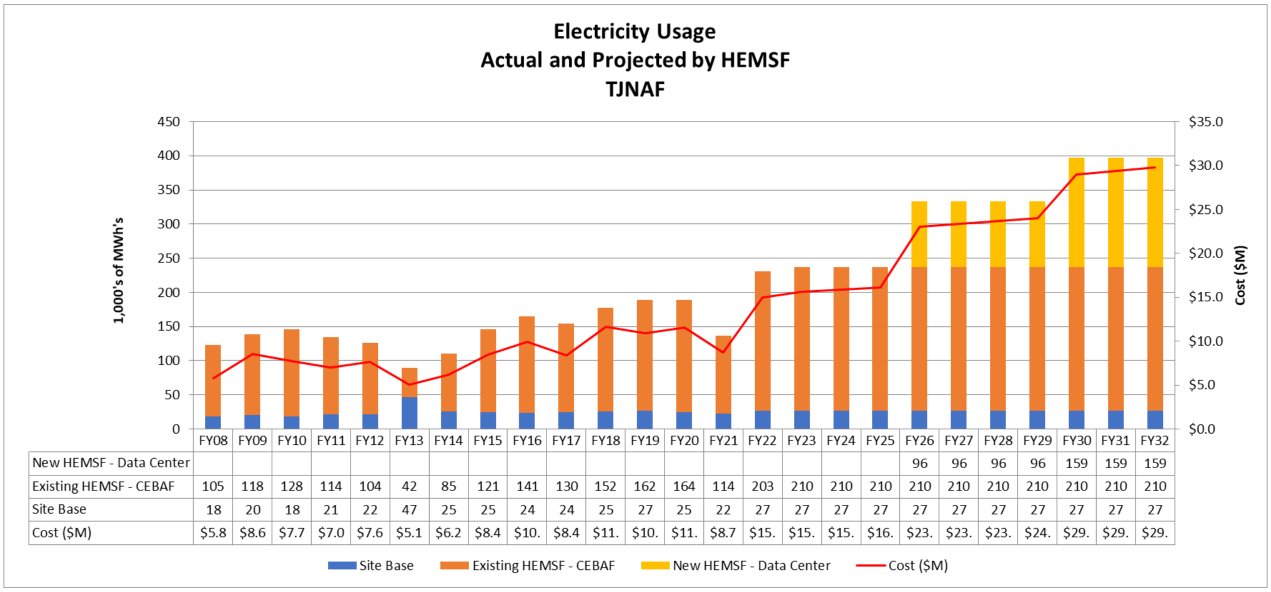
Achievement of the potable water intensity reduction goal of 36% relative to a FY 2007 baseline remains the most significant challenge due to the large amounts of water required for evaporative cooling of high energy mission-specific facilities. TJNAF has, however, identified strategies for implementation and integrated these into the Campus Plan. A project was completed in FY 2019 that reduces potable water consumption by 4M gal/yr (an annual savings of $60,000) by reusing discharge water from the Test Lab ultra-pure water system as a make-up water supply source for a nearby cooling tower. Additionally, funding has been requested to implement a storm water reuse project, which is projected to further reduce potable water consumption by up to 50 million gallons per year.

TJNAF has and continues to plan and implement clean and renewable energy technologies. Several facilities currently utilize geothermal heat pump systems that produce and consume approximately 5,306 MMBTU/yr of thermal energy. A renewable energy integration project identified in the Campus Plan is capable of providing 3 megawatts of solar energy with battery storage. Until funding is received and work is completed, however, renewable energy credits will be purchased annually to comply with interim goals in this category.

Due to operational risk, JSA decided against awarding a Utility Energy Service Contract (UESC) project totaling approximately $3.48M to address lighting, domestic water conservation, and mechanical upgrades. As an alternative, these elements are being implemented separately, either as part of operations and maintenance efforts or by incorporation into larger recapitalization projects. This approach is expected to reduce the risk while delivering the same or better outcome at a lower cost. These building-level energy and water reductions will contribute to additional facilities meeting the guiding principles for sustainable buildings.

Electricity Usage and Cost Projections

The figure below shows TJNAF’s historical and projected electricity usage and costs. Projections are based on scheduled operations for FY 2021 of 6.5 weeks and, for FY 2022, 34 weeks—with some limited portions at lower energy levels. From FY 2023 onward, 34 weeks of operations at the highest achievable beam energy are projected for each year. Additional projections related to a proposed new high-energy, mission-specific data center facility are also included in the projections from FY 2026 forward.



	FY08	FY09	FY10	FY11	FY12	FY13	FY14	FY15	FY16	FY17	FY18	FY19	FY20	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30	FY31	FY32
New HEMSF - Data Center																			96	96	96	96	159	159	159
Existing HEMSF - CEBAF	105	118	128	114	104	42	85	121	141	130	152	162	164	114	203	210	210	210	210	210	210	210	210	210	210
Site Base	18	20	18	21	22	47	25	25	24	24	25	27	25	22	27	27	27	27	27	27	27	27	27	27	27
Cost ($M)	$5.8	$8.6	$7.7	$7.0	$7.6	$5.1	$6.2	$8.4	$10.	$8.4	$11.	$10.	$11.	$8.7	$15.	$15.	$15.	$16.	$23.	$23.	$23.	$24.	$29.	$29.	$29.

Figure: Electricity Usage and Cost Projections

APPENDIX 1
SCIENCE AND ENERGY CORE CAPABILITIES

The Programs reporting to the Under Secretary for Science and the Under Secretary for Energy have together identified twenty four categories of core capabilities that comprise the scientific and technological foundation of its national laboratories. There are three criteria to define core capabilities. They must:

- Encompass a substantial combination of facilities and/or teams of people and/or equipment;
- Have a unique and/or world-leading component; and
- Be relevant to a discussion of DOE/NNSA/DHS missions.

Below is a table of the core capabilities that have been affirmed by DOE at each of the thirteen Science and Energy national laboratories. The following pages give a detailed definition of what each core capability encompasses.

Figure: Distribution of Core Capabilities across the Science Laboratories

	Core Capabilities	AMES	ANL	BNL	FNAL	LBNL	ORNL	PNNL	PPPL	SLAC	TJNAF
1	Accelerator Science and Technology		✓	✓	✓	✓	✓			✓	✓
2	Advanced Computer Science, Visualization, and Data		✓	✓	✓	✓	✓	✓		E	**NEW**
3	Applied Materials Science and Engineering	✓	✓	✓		✓	✓	✓			
4	Applied Mathematics		✓	✓		✓	✓	✓			
5	Biological and Bioprocess Engineering		✓			✓	✓	✓			
6	Biological Systems Science			✓		✓	✓	✓			
7	Chemical and Molecular Science	✓	✓	✓		✓	✓	✓	**NEW**	✓	
8	Chemical Engineering		✓	✓		✓	✓	✓			
9	Climate Change Science and Atmospheric Science		✓	✓		✓	✓	✓			
10	Computational Science		✓	✓		✓	✓	✓	E		
11	Condensed Matter Physics and Materials Science	✓	✓	✓		✓	✓	✓	E	✓	

	Core Capabilities	AMES	ANL	BNL	FNAL	LBNL	ORNL	PNNL	PPPL	SLAC	TJNAF
12	Cyber and Information Sciences		✓			✓	✓	✓			
13	Decision Science and Analysis		✓			✓	✓	✓			
14	Earth Systems Science and Engineering					✓	✓	✓			
15	Environmental Subsurface Science					✓	✓	✓			
16	Large Scale User Facilities/Advanced Instrumentation		✓	✓	✓	✓	✓	✓	✓	✓	✓
17	Mechanical Design and Engineering					✓	✓		✓		
18	Nuclear and Radio Chemistry		✓	✓		✓	✓	✓			
19	Nuclear Engineering		✓	E			✓	✓			
20	Nuclear Physics		✓	✓		✓	✓				✓
21	Particle Physics		✓	✓	✓	✓				✓	
22	Plasma and Fusion Energy Science					✓	✓		✓	✓	
23	Power Systems and Electrical Engineering			E		✓	✓	✓	✓		
24	Systems Engineering and Integration		✓	✓		✓	✓	✓	✓		

✓ = DOE Endorse Core Capability E = Emerging Core Capability NEW = Core Capability Proposed in 2021

1. **Accelerator Science and Technology:** The ability to conduct experimental, computational, and theoretical research on the physics of particle beams and to develop technologies to accelerate, characterize, and manipulate particle beams in accelerators and storage rings. The research seeks to achieve fundamental understanding beyond current accelerator and detector science and technologies to develop new concepts and systems for the design of advanced scientific user facilities.

2. **Advanced Computer Science, Visualization, and Data:** The ability to have a widely recognized role in advances in all applications in computational science and engineering. A core capability in these areas would involve expertise in areas such as programming languages, high-performance computing tools, peta- to exa-scale scientific data management and scientific visualization, distributed computing infrastructure, programming models for novel computer architectures, and automatic tuning for improving code performance, with unique and/or world-leading components in one or more of these areas. The capability requires access to (note: these resources do not need to be co-located) a high-end computational facility with the resources to test and develop new tools, libraries, languages, etc. In addition, linkages to application teams in computational science and/or engineering of interest to the Department of Energy and/or other Federal agencies would be beneficial to promptly address needs and requirements of those teams.

3. **Applied Materials Science & Engineering:** The ability to conduct theoretical, experimental, and computational research to understand and characterize materials with focus on the design, synthesis, scale-up, prediction and measurement of structure/property relationships, the role of defects in controlling properties, the performance of materials in hostile environments to include mechanical behavior and long-term environmental stability, and the large-scale production of new materials with specific properties. The strong linkages with molecular science, engineering, and environmental science provides a basis for the development of materials that improve the efficiency, economy, cost-effectiveness, environmental acceptability, and safety in energy generation, conversion, transmission, and end-use technologies and systems. Primary supporting disciplines and field include materials synthesis, characterization, and processing; chemical and electrochemistry, combinatorial chemistry, surface science, catalysis, analytical and molecular science; and computation science.

4. **Applied Mathematics:** The ability to support basic research in the development of the mathematical models, computational algorithms and analytical techniques needed to enable science and engineering-based solutions of national problems in energy, the environment and national security, often through the application of high-performance computing. Laboratory capabilities in this area would involve expertise in such areas as linear algebra and nonlinear solvers, discretization and meshing, multi-scale mathematics, discrete mathematics, optimization, complex systems, emergent phenomena, and applied analysis methods including but not limited to analysis of large-scale data, uncertainty quantification, and error analysis.

5. **Biological and Bioprocess Engineering:** Applies understanding of complex biological systems and phenomena to design, prototype, test and validate processes components, technologies and systems

relevant to (1) bioenergy production, (2) environmental contaminants processing, and (3) global carbon cycling and biosequestration. Primary supporting disciplines include chemical engineering, agricultural science, fermentation science, materials science and engineering, and systems science.

6. **Biological Systems Science:** The ability to address critical scientific questions in understanding complex biological systems via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and individuals with expertise in biological systems research and related disciplines to advance DOE missions in energy, climate, and the environment. This unique combination of tools and people is the foundation for research of scale and breadth unmatched by other facilities world-wide, for example, on research that employs systems and synthetic biology and computational modeling approaches enabled by genome sequencing and functional characterization of microbes, plants, and biological communities relevant to (1) bioenergy production, (2) carbon/nutrient cycling in terrestrial environments and (3) microbial biogeochemical controls on contaminant transport and biosequestration at DOE sites. Primary supporting disciplines include systems biology, plant biology, microbiology, biochemistry, biophysics and computational science.

7. **Chemical and Molecular Science:** The ability to conduct experimental, theoretical, and computational research to fundamentally understand chemical change and energy flow in molecular systems that provide a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Areas of research include atomic, molecular and optical sciences; gas-phase chemical physics; condensed phase and interfacial molecular science; solar photochemistry; photosynthetic systems; physical biosciences; catalysis science; separations and analytical science; actinide chemistry; and geosciences.

8. **Chemical Engineering:** The ability to conduct applied chemical research that spans multiple scales from the molecular to macroscopic and from picoseconds to years. Chemical engineering translates scientific discovery into transformational solutions for advanced energy systems and other U.S. needs related to environment, security, and national competitiveness. The strong linkages between molecular, biological, and materials sciences, engineering science, and separations, catalysis and other chemical conversions provide a basis for the development of chemical processes that improve the efficiency, economy, competitiveness, environmental acceptability, and safety in energy generation, conversion, and utilization. A core capability in chemical engineering would underpin R&D in various areas such as nanomanufacturing, process intensification, biomass utilization, radiochemical processing, dielectric materials, advanced conducting materials, high-efficiency clean combustion, and would generate innovative solutions in alternative energy systems, carbon management, energy-intensive industrial processing, nuclear fuel cycle development, and waste and environmental management.

9. **Climate Change Sciences and Atmospheric Science:** The ability to apply knowledge of atmospheric, oceanic, terrestrial, ecological, hydrological, and cryospheric processes, that combine with human activities and anthropogenic emissions, in order to understand and predict climate change and different patterns of meteorological conditions, with a particular focus on (1) understanding and describing the causes, impacts, and predictability of climate change via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and individuals with expertise in future climate change research and related disciplines. This unique combination of tools and people is the foundation for research of scale and breadth unmatched by other facilities, world-wide, for example, on (1)

atmospheric-process research and modeling, including clouds, aerosols, and the terrestrial carbon cycle; (2) climate change modeling at global to regional scales; (3) research on the effects of climate change on ecosystems; (4) integrated analyses of climate change, from causes to impacts changes, including impacts on energy production, use, and other human systems; (5) understanding and predicting future extreme weather as the climate evolves, that in turn introduces risk and vulnerability to energy and related infrastructures; (6) understanding the carbon cycle, with focus on the interdependence of a changing climate and terrestrial ecosystems, and (7) predict the influences of terrain and atmospheric processes and systems on the availability, behavior, and quality of energy resource and operations.

10. **Computational Science:** The ability to connect applied mathematics and computer science with research in scientific disciplines (e.g., biological sciences, chemistry, materials, physics, etc.). A core capability in this area involves expertise in applied mathematics, computer science and in scientific domains with a proven record of effectively and efficiently utilizing high performance computing resources to obtain significant results in areas of science and/or engineering of interest to the Department of Energy and/or other Federal agencies. The individual strengths in applied mathematics, computer science and in scientific domains in concert with the strength of the synergy between them is the critical element of this core capability.

11. **Condensed Matter Physics and Materials Science:** The ability to conduct experimental, theoretical, and computational research to fundamentally understand condensed matter physics and materials sciences that provide a basis for the development of materials that improve the efficiency, economy, environmental acceptability, and safety in energy generation, conversion, transmission, and utilization. Areas of research include experimental and theoretical condensed matter physics, x-ray and neutron scattering, electron and scanning probe microscopies, ultrafast materials science, physical and mechanical behavior of materials, radiation effects in materials, materials chemistry, and bimolecular materials.

12. **Cyber and Information Sciences:** The disciplines, technologies, and practices designed to protect, analyze, and disseminate information from electronic sources, including computer systems, computer networks, and sensor networks. A core competency in this area would involve recognized expertise in one or more of the following topics: cyber security, information assurance, information analytics, knowledge representation, and information theory, control systems design and engineering, embedded systems, reverse engineering, and advanced hacking techniques. This core competency would be applied to: the protection of information systems and data from theft or attack; the collection, classification, analysis, and sharing of disparate data; and the creation of knowledge from heterogeneous information sources; securing control systems integrated into critical infrastructure; and increasing security, reliability, and resilience of automated processes and systems.

13. **Decision Science and Analysis:** Derives knowledge and insights from measured and modeled data sets to further the understanding of and tradeoffs among resource and technology options, to identify and quantify the risks and impacts of current and emerging technologies on environmental systems, and to assess the impact of market dynamics, human behavior and regulations, policies or institutional practices on the development and uptake of technology. Primary supporting disciplines include engineering, environmental science, applied math, finance, business, social and political science, and market and behavioral economics.

This capability provides credible and objective information to support DOE and others to support strategic planning and program direction, policy formulation and implementation, efforts to remove market barriers to deployment and engagement with stakeholders.

14. **Earth Systems Science and Engineering:** The ability to understand environmental and ecological systems, processes, and interrelationships to predict, assess, and mitigate the impacts of past, current, and future energy production, transmission, distribution, and use on subsurface, terrestrial, coastal, and marine environments. Knowledge is used to develop technologies that minimize emissions and/or control technologies that protect these environments.

15. **Environmental Subsurface Science:** The ability to understand and predict the physical, chemical, and biological structure and function of subsurface environments to enable systems-level environmental prediction and decision support related to the sustainable development of subsurface resources, environmentally-responsible use of the subsurface for storage, and effective, mitigation of the impacts of environmental contamination from past nuclear weapons production and provide a scientific basis for the long-term stewardship of nuclear waste disposal via the integration of laboratory-specific research facilities, instrumentation and/or leadership-class computational systems, and multidisciplinary teams of individuals with expertise in environmental subsurface science and related disciplines in microbial ecology and biogeochemistry. This unique combination of tools and expertise is the foundation for research on (1) linking research across scales from the molecular to field scale, (2) integration of advanced computer models into the research and (3) multidisciplinary, iterative experimentation to understand and nutrient cycling and contaminant transport in complex subsurface environments. This ability can contribute to mitigating the impacts of environmental contamination from past nuclear weapons production and provide a scientific basis for the long-term stewardship of nuclear waste disposal, as well as understanding subsurface environments and their role in the functioning of terrestrial ecosystems.

16. **Large-Scale User Facilities/R&D Facilities/Advanced Instrumentation:** The ability to conceive, design, construct and operate leading-edge specialty research facilities available to universities, industry, and national laboratories customers to conduct groundbreaking research and development activities and/or 'at scale' testing and demonstration of technology. This includes the ability to manage effectively construction of $100 million or greater one-of-a-kind scientific facilities, and to host hundreds to thousands of U.S. and international users in addition to carrying out world-class research at the facility itself. The ability to conceive, design, build, operate and use first-in-class technical instruments intended for a particular research purpose, often requiring the material expertise of multiple scientific disciplines. Instrumentation that can be created by a small number of individuals or that would sit on a laboratory bench-top is not considered part of this core capability.

17. **Mechanical Design and Engineering:** Applies the principles of physics, mechanics, and materials science to analyze, design, test, validate, and enable operation of advanced engineered systems, machines and tools. Includes equipment used to move or extract energy bearing materials (e.g., oil, gas, coal) or from moving fluids (e.g., water, wind, steam), as well as equipment used to convert energy to useful services (e.g., mobility, home heating and cooling, robotics, imaging devices, etc.) or to manufacture products. Primary supporting disciplines include physics, materials science, aerospace engineering, mechanical engineering, chemical engineering, electrical engineering and computational science.

18. **Nuclear and Radio Chemistry:** The ability to use a broad range of facilities, instrumentation, equipment and, often, interdisciplinary teams that apply the knowledge, data, methods, and techniques of nuclear chemistry, mechanical engineering, chemical engineering to missions of the Departments of Energy and Homeland Security. The elements of this capability are often brought together in unique combinations with those of other disciplines to address high priority needs such as new and improved nuclear systems; radioisotope production and advanced instrumentation for nuclear medicine; development of methods and systems to assure nonproliferation and combat terrorism; and environmental studies, monitoring, and remediation.

19. **Nuclear Engineering:** The ability to use a broad range of facilities, instrumentation, equipment and, often, interdisciplinary teams that apply the knowledge, data, methods, and techniques of nuclear engineering, mechanical engineering, nuclear reactor physics, measurable science and risk assessment to missions of the Departments of Energy and Homeland Security. The elements of this capability are often brought together in unique combinations with those of other disciplines to address high priority needs such as new and improved energy sources and systems; advanced instrumentation for nuclear systems; accelerator science and technology; and development of methods and systems to assure nonproliferation and combat terrorism.

20. **Nuclear Physics:** The ability to carry out experimental and theoretical research to provide new insights and advance our knowledge on the nature of matter and energy. This includes the design, operation and analysis of experiments to establish the basic properties of hadrons, atomic nuclei, and other particles, and the development of models and theories to understand these properties and behaviors in terms of the fundamental forces of nature.

21. **Particle Physics:** The ability to carry out experimental and theoretical research to provide new insights and advance our knowledge on the nature of matter and energy, and the basic nature of space and time itself. This includes the design, operation and analysis of experiments to discover the elementary constituents of matter and energy and probe the interactions between them and the development of models and theories to understand their properties and behaviors.

22. **Plasma and Fusion Energy Sciences:** The ability to conduct world-leading plasma research that can range from low-temperature to high temperature/high pressure plasmas. This ability can be in operation of the state-of-the-art experimental fusion facilities to carry out world-leading research on the fundamental physics of plasmas, in theory and computations, which is critical to the full understanding of the plasma phenomena being studied or to enable technologies that allow experiments to reach and in many cases exceed their performance goals.

23. **Power Systems and Electrical Engineering:** Applies understanding of electromagnetic phenomena to design and engineer circuitry, electrical and electronic devices and equipment, sensors, instruments and control systems to address the efficiency and reliability of power transmission and distribution systems, and the interface of the grid with variable generation and modern loads. Primary supporting disciplines include electrical engineering, power systems engineering, computational science, and materials synthesis, characterization and processing.

24. **Systems Engineering and Integration:** The ability to solve problems holistically from the concept and design phase to ultimate deliverable and completion phase, by synthesizing multiple disciplines, and to develop and implement optimal solutions. The ability to develop solutions that address issues of national energy and environmental security. Areas of application of this capability include development of programs in energy supply, storage, transportation, and efficiency; and deployment of novel solutions to materials and sensor problems in fields of interest to the Department of Energy and/or the Department of Homeland Security.

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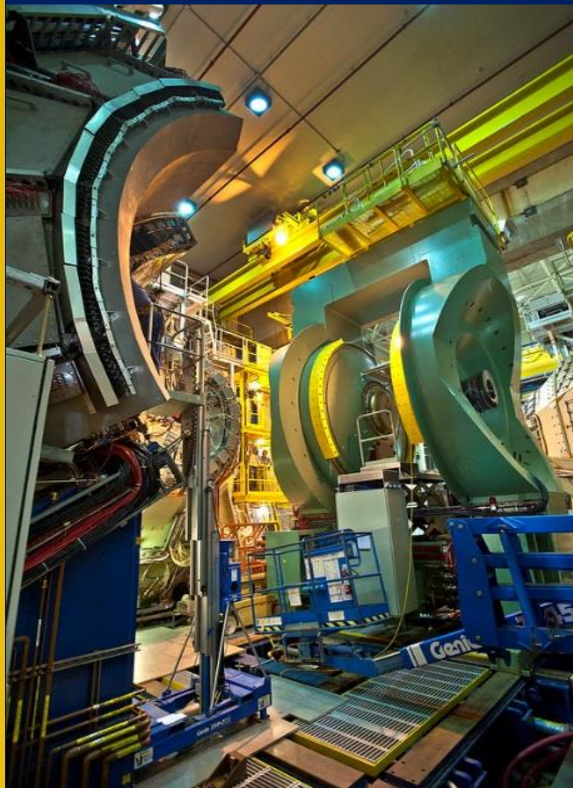

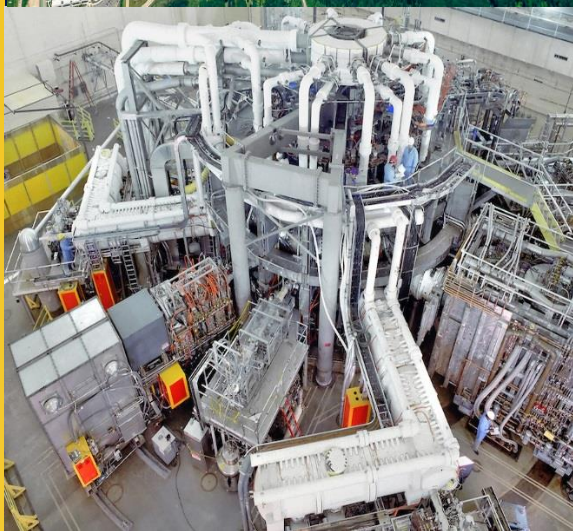

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