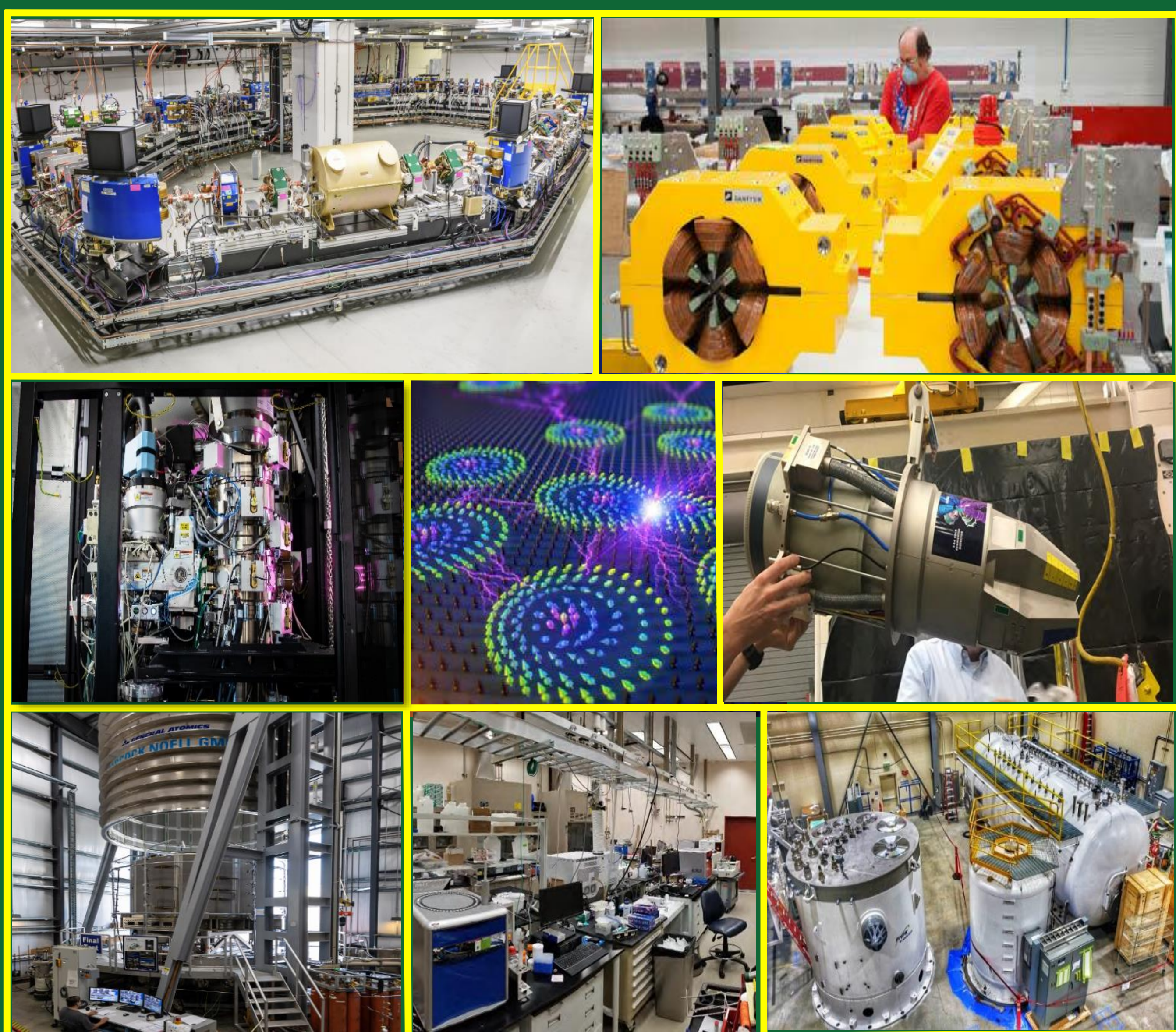
U.S. DEPARTMENT OF ENERGY

The U.S. Department of Energy's Ten-Year-Plans for the Office of Science National Laboratories FY 2020



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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 38,000 facility users and more than 7,400 visiting scientists in Fiscal Year (FY) 2019, 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 2020-2030.

[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

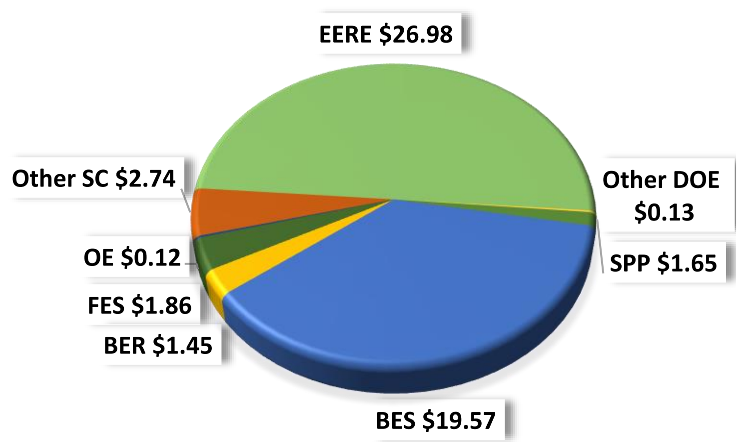
Location: Ames, IA
Type: Single-program Laboratory
Contractor: Iowa State University of Science and Technology
Site Office: Ames Site Office
Website: www.ameslab.gov

- **FY 2019 Lab Operating Costs:** $53.99 million
- **FY 2019 DOE/NNSA Costs:** $53.23 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $0.76 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 1.4%
- **FY 2019 DHS Costs:** $0 million

Physical Assets:
- 10 acres and 13 buildings
- 340,968 GSF in buildings
- Replacement Plant Value: $105 M
- 0 GSF in 0 Excess Facilities
- 0 GSF in 0 Leased Facilities

Human Capital:
- 303 Full Time Equivalent Employees (FTEs)
- 47 Joint Faculty
- 38 Postdoctoral Researchers
- 98 Graduate Student
- 88 Undergraduate Students
- 0 Facility Users
- 104 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



Mission and Overview

Ames Laboratory delivers critical materials solutions to the nation. For more than 73 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 recycling science, atomistic and molecular design and control for energy and chemical conversion; and novel synthesis to manufacturing, each with a particular focus on rare earth elements, alloys, and compounds. Building upon its 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, the 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 team project is developing new catalytic methods for upcycling hydrocarbon-based polymers and establish 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.

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.

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. 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. 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 Strategy for the Future

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, and national security. The challenges facing the country require the accelerated discovery, design, and implementation of new chemistry and materials that enable critical technologies. The design of such chemicals and materials must incorporate ways of managing critical resources at all stages of development to better reuse and recover materials, in order to efficiently convert end-of-life products into useful sources for further use. We seek a sustainable future for discovery, application, and recovery of materials and chemicals. To do this, we will accelerate the fundamental understanding, development, and implementation of new chemistry and materials capabilities to enable new technology. We will transform the way we do science for better predictions, more precise synthesis and chemical transformations, and for developing integrated environments that will advance new capabilities. We will enable enhanced reuse of chemicals and materials, by designing them for reuse, and by enabling new capabilities that efficiently transform them into useful products. Ultimately, our goals are to transform the way we do science and to create next-generation materials and chemistry to enable a more sustainable future.

Our vision is to lead the nation in translating foundational science for energy and chemical conversion into critical technology innovation. This is reflected in our strategy: *Today's fundamental science for tomorrow's critical chemistry and materials solutions*. Ames Laboratory will focus its priority research on the following strategic directions, each with a particular focus on rare earth elements, alloys, and compounds:

- *Discovery for a Sustainable Future – Critical Materials and Recycling Science.* Ames Lab will conduct basic and applied science to achieve a sustainable future through efficient separations, chemical transformations, and materials design and synthesis.

- *Making Every Atom Count – Atomistic and molecular design and control for energy and chemical conversion.* Ames Lab will master interfacial, atomic, and electronic phenomena to create transformative capabilities in directing chemical and material behavior.
- *Innovating for Science and Industry – Novel Synthesis to Manufacturing.* Ames Lab will develop the fundamental knowledge to control synthetic pathways and chemical transformations to precisely fabricate materials across length scales.

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 and engineering that will transform science and lead to technological breakthroughs.

We will 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: (1) applied materials science and engineering, (2) chemical and molecular science, and (3) 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 $105M.

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). These buildings were constructed 59 to 71 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 has 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 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. 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 Ames Laboratory for a Critical Materials and Supply Chain Research Facility (CMRF). The Laboratory envisions this facility will serve as an integrated platform that allows early stage research, from fundamental science through applied technology, development that spans the supply chain.

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

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.

Current Gaps

Through continued investment, we plan to fulfill our Strategic Plan objectives and goals to (1) provide facilities to support scientific objectives, (2) provide infrastructure that supports mission readiness, and (3) pursue opportunities for future scientific capabilities.

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. 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 $61.5M in facilities gaps, with more than 95% of the facility investments for the three older research buildings ($58.5M).

To address the needs of its aging facilities, the Laboratory recommends $3 million of capital funding be invested 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:

<u>Fire Alarm and Emergency Notification Systems:</u> These Lab-wide systems are at the end of their useful life, and the Laboratory is currently in the design phase for the complete replacement of the fire alarm system, funded with BES-GPP ($1.5M). Construction will be completed in FY 2021, 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.

<u>Building Envelopes:</u> 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. GPP funds are used when the investments lead to improvements, and overhead funds are used when the investments are focused on repairs. The next planned project will 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.

<u>Backup-Emergency Power & UPS Systems:</u> 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: 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 2017, the Laboratory renovated 16,500 square feet of this poor or fair condition space. Our capacity to renovate space is approximately 4,000 to 6,000 square feet per year. At the current pace, it will take the Laboratory approximately 16 to 25 years to renovate these spaces.

Helium Recovery: 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 Low-Temp Lab ($1M). Ames Laboratory is working closely with ISU to ensure the electrical infrastructure in Zaffarano Hall (ISU building) are sufficient to support a new Helium recovery 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 consolidating and updating two IT rooms, one in TASF and one 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. As an example, the exterior doors of the Laboratory are open throughout the day. 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.

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% 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% 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 2019, completing the window replacement in Spedding Hall, starting renovations to 5,000 square feet of space on the 3rd floor of Spedding Hall for DNP expansion and NMR consolidation, and awarding the construction contract to replace the main air handler in Metals Development. The Laboratory is in the midst of design for several projects, including: upgrading telecommunications infrastructure, helium recovery and recycling operations, fire alarm and emergency notification systems, and renovating a portion of the 2nd floor in Metals Development.

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. 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 $10.0M to $90.0M (target $30.0M). Ames Laboratory is currently working toward achieving CD-1 and starting the design effort for this project in FY 2021. 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 they will positively impact our mission. Ames Laboratory plans to fund maintenance and repair activities through overhead at 2.0% 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. The Laboratory is currently assessing how future investments will reduce DM.

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 is updating and modernizing approximately 5,000 square feet in Spedding Hall for Dynamic Nuclear Polarization (DNP) research expansion, and Nuclear Magnetic Resonance (NMR) research consolidation, and 3,000 square feet of research space in Metals Development.

Objective 2: Provide infrastructure that supports mission readiness. The Laboratory completed the replacement of the Spedding Hall windows in FY 2019. Design was completed and the construction subcontract was awarded for the replacement of the main HVAC air handler in Metals Development ($1.0M). Design is ongoing for the replacement of the fire alarm and emergency notification systems across the Laboratory ($1.5M).

The Laboratory requests $3.0M in GPP funding to continue the effort to update poor and fair condition spaces across the Laboratory. The Laboratory requests $3.0M in Safeguards and Security (S&S) funding in FY 2021 for access control upgrades in Spedding Hall and Metals Development. We request sustained funding of $1.0M per year (BES-GPP), and $2.0M per year (SLI-GPP) from FY 2021 to FY 2032 to focus on SLI and BES Mission Readiness Renovations.

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

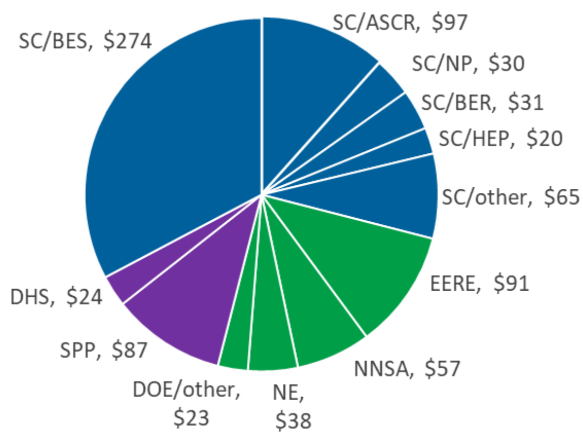
Location: Lemont, Illinois
Type: Multi-program Laboratory
Contractor: UChicago Argonne, LLC
Site Office: Argonne Site Office
Website: www.anl.gov

- **FY 2019 Lab Operating Costs:** $837 million
- **FY 2019 DOE/NNSA Costs:** $727 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $87 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 13%
- **FY 2019 DHS Costs:** $24 million

Physical Assets:
- 1,517 acres and 156 buildings
- 5.1 million GSF in buildings
- Replacement Plant Value: $3.9B
- 0.02 million GSF in 16 Excess Facilities
- 0.3 million GSF in Leased Facilities

Human Capital:
- 3,448 Full Time Equivalent Employees (FTEs)
- 379 Joint Faculty
- 317 Postdoctoral Researchers
- 224 Graduate Student
- 297 Undergraduate Students
- 8,035 Facility Users
- 809 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



Mission and Overview

Argonne National Laboratory accelerates science and technology to drive US prosperity and security. We are recognized internationally for an impactful legacy that continues today, most notably through:

- Seminal discoveries in fundamental science
- Innovations in energy technologies
- Leadership in scientific computing and analysis
- Excellence in scientific and operational stewardship of national user facilities

Our work advances understanding in the physical, biological, and environmental sciences and overcomes critical technological challenges in energy and national security. In doing so, we support the national and global goals of the US Department of Energy (DOE), other government agencies, and the private sector.

The five national user facilities that we steward propel breakthroughs by researchers from Argonne and hundreds of other institutions. The Argonne Leadership Computing Facility enables application of world-class supercomputers and artificial intelligence to research. Two facilities provide extraordinarily powerful tools to characterize the structure and function of materials: the Advanced Photon Source and Center for Nanoscale Materials. The Argonne Tandem Linear Accelerator System gives unmatched insights into low-energy nuclear physics, and the Atmospheric Radiation Measurement Facility's Southern Great Plains Site gathers data essential to understanding the earth's climate.

Based in the Chicago suburbs, Argonne is managed for DOE by UChicago Argonne, LLC. We have conducted joint research with the University of Chicago since our founding in 1946; current areas of collaboration include cosmological, computer, polymer, and quantum science. A second Argonne location in the City of Chicago facilitates collaboration with the area's leading research universities, partnerships with regional industries, and STEM outreach to urban communities.
Drawing on Argonne's broad capabilities, we have contributed to the COVID-19 response through DOE's National Virtual Biotechnology Laboratory. We are identifying paths to potential treatments and vaccines and modeling virus propagation, supported by partnerships with UChicago and others. This is but one example of our commitment to extend Argonne's legacy of unlocking scientific and technological frontiers to deliver economic growth and secure America's energy future and quality of life.

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 key 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 US prosperity and security.

Our multifaceted R&D portfolio enables our scientists and engineers to deliver groundbreaking discovery science and innovative solutions to critical challenges in energy, security, and infrastructure. Our collaborations with other research institutions and industry enrich our contributions to the nation.

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 in bringing medical advice and expertise to Argonne during the current pandemic; plans to transition to normal operations are being informed by advice from UChicago epidemiologists, and the university's medical center is providing support in testing Argonne employees for the COVID-19 virus.

Our core capabilities, listed below and summarized on the following pages, lie in basic research, early-stage applied R&D, and major facilities. The expertise of our scientists and engineers both supports, and is supported by, our suite of large-scale experimental facilities that also 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 Climate Research Facility's Southern Great Plains (ARM-SGP)
- 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.

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, stability and feedback systems, and 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 BNL, 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 currently 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 US 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.

Mission relevance and funding

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

Capability

Argonne is a leader in computer science, visualization, and data. 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 will continue to enhance and promote this capability and will build new capacity in these 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, cloud computing, and high-performance computing; this includes platforms to support the basic and applied sciences
- New 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
- New 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
- New 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 (an Argonne-led collaboration won the SCinet Technology Challenge at the Supercomputing 19 conference by demonstrating such real-time analysis)
- 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 machine learning 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 US
- 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 machine learning and deep learning models makes it easier for researchers to benefit from advances in those technologies
- Applied AI in response to COVID-19: we are building infrastructure to integrate AI and machine learning 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-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.

Mission relevance and funding

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

Capability

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 include materials characterization at the APS and CNM; computational science using the ALCF; Center for Molecular Engineering (CME) expertise; and one-of-a-kind facilities such as our DOE/EERE-funded Materials Engineering Research Facility (MERF). The MERF enables synthesis, process R&D and scale up of materials as well as fabrication/testing of components and devices.

The MERF's capabilities enable scientists and engineers to bridge the gap between bench-scale science and industrial implementation. 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, new 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 those materials 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 such as electrospinning, atomic layer deposition, and vapor deposition. We extend those technologies to a variety of high-performance applications, including solid-state batteries, fuel cell catalysts, radio-frequency energy harvesting, water treatment, advanced communication devices, and recently to antiviral filter media in support of COVID-19 response.

We also develop ultracapacitor materials for transportation applications and 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 the recovery and reconstruction/upcycling of specialized materials, an example of which is the DOE/EERE-VTO funded ReCell Center focused on recycling of lithium-ion batteries.

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, nanofiber magnets, high-performance lubricants, and improved nuclear energy fuels and materials. Ongoing work has shown promise for more-efficient nuclear fuel reprocessing, lighter-weight transportation alloys, advanced energy storage devices, and higher-performance superconducting materials for use in detectors, accelerators, and energy transmission. Argonne's extensive experience in storage materials research and development positions us to make significant contributions to DOE's Energy Storage Grand Challenge.

We are expanding the MERF to provide additional laboratory and collaborative space to enable additional materials manufacturing, synthesis, and processing capabilities for varied application domains and to enhance partnership opportunities. Over time, we plan to extend our manufacturing research and development capabilities to emerging and anticipated DOE priorities such as quantum systems and pandemic response/biosecurity.

Argonne's nuclear materials work focuses on verifying the safety of current light-water reactors and developing new materials to improve the economics and enhance the safety of advanced reactors. This research builds on our capability to design and develop materials for extreme conditions and our nuclear engineering capability.

The Argonne Collaborative Center for Energy Storage Science (ACCESS) is facilitating maturation of novel battery materials and their deployment to industry. Through the Advanced Materials for Energy-Water Systems (AMEWS) Energy Frontier Research Center and recently awarded Israel-US water research program - the Collaborative Water-Energy Research Center (CoWERC) - we develop materials technologies to solve global water challenges. We also partner with industry through Manufacturing USA institutes such as PowerAmerica and Reducing Embodied-energy and Decreasing Emissions (REMADE).

Mission relevance and funding

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 capability in condensed matter physics and materials science, with the goal of enhanced impact from moving those discoveries to market. It is aligned with the goals of the DOE Energy Materials Network (EMN) and supports many of the consortia, including Chemical Catalysis for Bioenergy (ChemCatBio) and Lightweight Materials (LightMat).

Current sponsors include ARPA-E, DOE/EERE, DOE/NE, DOE/NNSA, DOE/SC-BES, DOE/IA, DARPA, NRC, NSWC Crane (a US Navy short command), and a growing range of industrial partners who manufacture critical materials to enhance American competitiveness and strengthen national security.

Applied mathematics

Capability

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 machine learning for scientific applications
- Expanding our capabilities in machine learning, statistics, quantum algorithms, and other strategic areas
- Combining approaches – machine learning, 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:

- New 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
- New multimodal machine learning, statistical modeling, and algorithmic approaches to analyzing experimental, observational, and simulation data, including APS data and environmental observations
- Automated machine learning, 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 by multiple R&D 100 and ECRP awards and the naming of staff members as Fellows of the Society for Industrial and Applied Mathematics.

Mission relevance and funding

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 leverage our applied mathematics expertise.

Biological and bioprocess engineering

Capability

Argonne's approach to biological and bioprocess engineering combines synthetic biology and synthetic chemistry to create biomaterials with tuned functionalities. We determine the fundamental engineering mechanisms for biological energy capture and conversion, from the molecular to the unit-operation scale, and use the results to pioneer first-principles bioengineering approaches.

This capability draws on the CNM, the APS, and Argonne's biological, chemical and computational capabilities. CNM's tools for imaging and manipulating biomolecules, cells, and processes over multiple scales are used extensively for bioprocessing. We use multiple APS beamlines – including one dedicated to the DOE/SC-BER-funded Structural Biology Center – to determine the crystallographic structure of biological macromolecules and to characterize catalysts in thermochemical conversion processes; associated capabilities include bionanoprobe and micro-diffraction tools. Our Advanced Protein Characterization Facility can produce and characterize tens of thousands of unique proteins each year, including their biophysical and biochemical properties. Our computational expertise and resources have enabled us to be leaders in developing bioinformatic tools for the larger research community.

The proposed Sensing and Imaging at Argonne facility (SIA) would expand studies of protein-protein interactions, relevant to understanding viruses such as COVID-19. SIA also would enable nondestructive methods to study the dynamics of biologically driven processes using advanced sensors and computer vision. It further would provide space to further development of new quantum methods for advanced sensing to enable interaction-free imaging of biological systems.

Current research directions and investments focus on:

- *Synthetic biology for biosystems design.* We annotate and model microbial and microbiome systems (DOE Systems Biology Knowledgebase) to enable discovery of enzyme function, predictive design of strains and communities, and ecological understanding. We integrate this capability with our experimental expertise in protein characterization, structure-based design of proteins, engineering of microbial genomes, and use of biohybrid materials to visualize biological functions in cells and the environment. We are advancing this capability through internal investments, university collaborations, and strategic partnership projects. Engagement with UChicago and Northwestern University has centered on the impact of automated laboratories for biology.
- *Bioprocesses and biomanufacturing.* Our work emphasizes directed molecular evolution for natural and artificial photosynthetic systems, catalyst separation and reuse, bioreactor design and operation, and extraction and separation of biofuel candidates from bioreactors without disruption of bioprocesses. Sustainable plastic design combines efforts across Argonne in data science, artificial intelligence, environmental science, biology, and soft-matter and high-throughput chemistry. As the lead lab for the DOE/EERE-BETO Bioprocessing Separations Consortium, we have applied ion-adsorbent wafers to directly capture organic salts produced

during fermentation and we have developed and applied nanomaterials that can be used *in situ* in fermentations to selectively bind toxins or inhibitors and be reused more than 100 times.

Through recent advances in biological and bioprocess engineering, we have demonstrated the ability to predictively engineer microbes from the environment, microbes for biotechnology, energy-converting proteins with radically altered function, and enzymes to transform biomass. This creates a synthetic biology capability to develop designer microbes and communities for fundamental understanding of biological functions, biomanufacturing, novel polymer production-transformation, and energy-water research, and for linking with biohybrid research by our chemists and material scientists. We couple computational and experimental approaches to facilitate analyses, predictive modeling, and design of microorganisms and environmental microbiomes across scales.

Through the DOE-SC/BER KBase project, we integrate modeling and computational analysis − including metabolic modeling, cheminformatics, omics, and meta-omics − to support bioengineering efforts for microbes, plants, and microbial communities. We also contribute to the development of biomanufacturing technologies as part of the DOE/EERE-BETO Agile Biofoundry Project and we are a member of the Feedstock Conversion Interface Consortium initiated by that office. In addition, we are a leader in lifecycle and techno-economic analyses of bioenergy-related processes and analyses of the impacts of bioenergy system deployment on soil carbon, water footprint, water quality, and landscape design.

Mission relevance and funding

This capability supports the missions of DOE and other entities that seek to better understand plants, microbes, 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

Capability

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

Studies explore trends in chemistries across the periodic table, from hydrogen through the heavy elements, and includes expertise in gas phase, liquid phase, and solid-state chemistries. In support of the DOE/SC mission, these strengths deliver scientific advances relevant to catalysis, gas phase chemistry, electricity production from chemical energy, energy storage, geochemistry, heavy element separations, and solar and photosynthetic processes. Argonne has unique competencies in ultrafast characterization of reactions, thermochemical analysis, organometallic chemistry combined with heterogeneous catalysis, synthesis of unique physical and chemical environments, characterization of interfaces and interphases, heavy element separations, electronic structure and nuclear dynamics calculations, and modeling of interacting sequences of gas-phase reactions.

Computational resources and characterization tools available through 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 is expected to lead to a 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 elements chemistry and separations science are moving into newly constructed facilities, including new radiological facilities, in Argonne's recently opened Materials Design Laboratory. That move will advance a systems approach by fostering new interdisciplinary science within a state-of-the-art research complex that includes the Energy Sciences Building.

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.

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 expertise embodied in our core capabilities in chemical engineering and applied materials science.

Argonne's strategy advances an integrated, systems approach to the chemical and molecular sciences in concert with our chemical engineering and applied materials science and engineering core capabilities. We seek to unify the understanding of the periodic table, taking advantage of our expertise in the chemistry of the light elements, through the transition metals and on to the heavy elements. We seek to understand transient processes within molecules through our ultrafast chemistry and ion and electron transport expertise. Additionally, competing reactions are at the core of our strategy. Complex reaction 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 of complex environments will impact areas such as separations, catalysis, geochemistry, and photochemical processes. Finally, understanding interfaces in dimensions of x, y, z, and time is vital to our work within this core capability.

Recent investments will expand capabilities in polymer design and upcycling; 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, electrocatalytic, and electrochemical processes. To address the challenges and opportunities of predictive chemistries, we will further integrate our expertise in computational, theoretical, and data sciences 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* and *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.

Mission relevance and funding

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

Chemical engineering

Capability

Chemical engineering research at Argonne addresses the nation's energy and security challenges by building on and informing basic energy research while developing transformational technologies for electrochemical energy storage, biomass (including post-use carbon resources) conversion, chemical and light energy conversion, and water cleanup. 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.

Our success in applying our foundational knowledge in electro-, photo- and thermo- chemistry and catalysis from our core capability in chemical and molecular science, and in interfacial sciences expertise built from additional core capabilities, has led to global recognition for our lithium-ion (Li-ion) battery, solar conversion, combustion chemistry, and fuel-cell research. 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-VTO-funded ReCell Center. Our multidisciplinary efforts are developing advanced membranes, electrodes, and electrocatalysts that reduce the cost and improve the durability of fuel cells based on both solid-oxide and polymer-electrolyte membrane technologies. Recent work is investigating rail, marine, and aviation applications of fuel cells. Our gas-phase chemistry and chemical and material scale-up expertise are 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 are accelerating 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-HFTO ElectroCat research consortium, which we co-lead with Los Alamos National Laboratory. We also lead a thrust of the DOE/EERE-HFTO Fuel Cell Consortium for Performance and Durability (FC-PAD), applying our advanced characterization capabilities, including those at the APS, to study electrocatalysis. Other efforts are intended to reduce the costs to produce renewable liquid transportation fuels through advances in catalysis.

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, and techno-economic and life cycle analysis. Facilities include:

- *Cell Analysis, Modeling and Prototyping (CAMP) 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 (EADL)*. 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 (HTR) Laboratory*. This laboratory provides robotic tools and reactor systems for fast, automated, and parallel approaches to chemical synthesis and materials development, thereby accelerating discovery and optimization of materials for catalysis, energy storage, fuel cells, solar energy, and nanoscale chemistry.
- *Materials Engineering Research Facility (MERF)*. This facility allows researchers to explore the scale up of materials and chemical processes as we work with industry to move national laboratory discoveries and industry innovations to the marketplace. It is described in more detail under our applied materials science and engineering capability.

To meet increased needs, we recently completed a three-fold expansion of CAMP and currently are expanding MERF. DOE/EERE provides most of the funding for the five facilities described above.

Mission relevance and funding

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

Capability

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 mediating water, energy, and carbon exchanges 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 oversee operational activities across all Atmospheric Radiation Measurement (ARM) sites supported by DOE/SC-BER. We also 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. As part of ongoing improvements at the SGP site, we recently added ARM's tethered balloon system and are upgrading the guest instrument facility. We also will deploy open-source edge computing technology and use artificial intelligence and machine learning to allow instruments to dynamically adapt to current conditions.

We also provide the global scientific community with unique expertise and software for retrieving geophysical variables from atmospheric remote sensing instrumentation. Our Py-ART software for radar data is recognized internationally. Likewise, our tools for understanding tropical/equatorial convection and for working with time series are well recognized.

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. 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. We also have identified the root causes of poor representation of evapotranspiration in earth system models.

Argonne's efforts to advance earth science simulation emphasize the application of high-performance computing to develop robust predictive capabilities. We support the computational objectives of DOE's flagship Energy Exascale Earth System Model (E3SM) in addition to the data and analytical needs of other DOE R&D areas related to climate and atmospheric science.

We are developing models that we use in combination 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. We have used the APS to understand dust iron composition in aerosol samples. The APS Upgrade will vastly expand the capabilities of this technology for environmental science.

Argonne is an international leader in downscaling earth system modeling results to project possible future local climate conditions. Our 12-km-resolution climate projections for North America support quantitative analysis of risks to industrial infrastructure from future extreme weather. We are now developing even higher resolution, 4-km scale regional climate models. We also 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.

More broadly, our soil and biogeochemical scientists are developing a deep predictive understanding of soil responses to environmental change and perturbation, from the molecular to the regional scale. We collaborated with the broader scientific community to provide novel synthesis of regional carbon dioxide fluxes from arctic and boreal soils, and we have produced the first high-resolution, spatially explicit estimate of permafrost-region soil organic carbon stocks. 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 pioneering rapid mid-infrared spectroscopy technique enables researchers to quickly assess the degradation state of organic matter in those soils. This information is vital to predicting future carbon emissions from soils in high-latitude regions. We are also developing novel sensor technology to monitor soil moisture, a critical variable in both soil and atmospheric processes.

Mission relevance and funding

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

Capability

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 varied domain expertise. 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. 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 machine learning.
- 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 Large Synoptic Survey Telescope.
- 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 new multi-laboratory partnership under the auspices of the High Energy Physics Center for Computational Excellence, which works to employ leadership computing resources for simulation and data analysis for high energy physics experiments

Mission relevance and funding

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

Capability

Argonne's internationally recognized condensed matter physics and materials science research predicts, designs, and creates new materials and advances understanding of their behavior. Areas of recognized accomplishment include magnetic, superconducting, ferroelectric and topological materials; quantum metamaterials; correlated oxides; polymers and active soft matter; and electro-chemical 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 APS, CNM, and ALCF capabilities into our work.

Our programmatic strategy rests on understanding and exploiting the science of defects and interfaces as expressed 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. We support these core themes with crosscutting and enabling strategies: precision synthesis, *in situ* and *operando* coherent x-ray and electron studies coupled to modeling and simulation, and artificial intelligence (AI) and data-driven science approaches. We add expertise in soft matter and in semiconductor- and superconductor-based QIS platforms through joint staff appointments between UChicago and Argonne's Center for Molecular Engineering.

Collaboration is a key element of our strategy. Argonne leads the Midwest Integrated Center for Computational Materials, a collaborative effort with UChicago and four additional universities. Argonne's research benefits greatly from close interactions between this core capability and the Laboratory's core capability in chemical and molecular science, particularly in the areas of molecular design and synthesis, electrochemistry, and the role of interfaces. Our core materials science reinforces the work of the Argonne-led Joint Center for Energy Storage Research and plays a principal role in materials-focused Energy Research Frontier Centers. We also play a key role in the Center for Predictive Simulation of Functional Materials at Oak Ridge National Laboratory.

Expertise and capabilities unique to our portfolio position us to deliver scientific breakthroughs We shape new understanding through materials discovery, exploring novel systems in bulk and thin-film form and advancing materials platform discovery in QIS. We are innovating *in situ* characterization approaches – including coherent diffraction and three-dimensional pair-distribution analysis of diffuse x-ray and neutron scattering – to reveal static and dynamic behavior of electrons and ions through their fingerprints in local atomic structure. Argonne's new Materials Design Laboratory is providing state-of-the-art infrastructure for quantum, magnetic, superconducting, and scattering science programs. Our work has had recent impact at frontier areas of science including (1) coherent control of defect behavior in silicon carbide, (2) self-assembly of chiral liquid crystals to sculpt macroscopic crystals, and (3) determination of the electronic structure in low-dimensional nickelates to shine light on the origins of high temperature superconductivity.

Looking forward we will expand on this last success, linking multiple Argonne programs to create and explore a new class of nickel-based superconductors. Building on a recently launched program that applies machine learning to understand quantum order, we plan new fundamental research at the materials frontier that links QIS, artificial intelligence, and data science. In QIS, we will develop new qubit platforms based on designer defects. We will also investigate novel phenomena such as topological behavior in new quantum materials and bridge from quantum materials to microelectronics science.

Preparing for Argonne's AI- and data-centric Aurora exascale computer in the ALCF, we will explore exascale approaches to materials design, including first-principles, simulation-based prediction of synthetic pathways for inorganic solids. This focus on synthesis science will extend to thin-film deposition through design of interfaces and interfacial chemistries tailored to control materials defects. Our explorations of defect science will encompass both hard and soft matter, emphasizing the creation and control of topological defects.

We also will expand our synchrotron-based efforts in ultrafast science. 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 in part on applications in soft matter. Looking ahead, we will propose scientific programs and expertise to shape the planned Sensing and Imaging at Argonne building (see Sec. 6.2), including the extension of coherent imaging frameworks to electron probes.

Mission relevance and funding

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

Capability

Through our cyber and information sciences programs, we protect, analyze, and disseminate information from computer systems and other electronic sources to defend our nation from cyberattacks. Our analytical tools support critical national missions. This work supports 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. Internally, our cyber and information sciences activities leverage Argonne's fundamental sciences, advanced computing and engineering capabilities, including the APS, ALCF, and Laboratory Computing Resource Center. Our external partners include researchers from universities, other national laboratories, and the private sector.

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, machine learning for intrusion detection, and other technologies to improve national security
- Share cyber threat information using real-time, machine-to-machine methods in support of the DOE enterprise, and the energy sector using the Cyber Fed Model, which Argonne runs as DOE's primary system for sharing cyber threat information related to the Cybersecurity Information Sharing Act of 2015
- Design tools and testbeds for evaluating 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
- Inform government and private-sector entities of potential cyber vulnerabilities through the DHS Regional Resiliency Assessment Program using custom developed cyber methodologies
- Apply cutting-edge research and development to design systems supporting power grid operations that are 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 collegiate CyberForce Competition™ to increase students' understanding of cyber-physical vulnerabilities and consequences
- 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 using information retrieval methods that employ natural language processing and machine learning to better understand proliferation patterns in support of US 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 UAV (unmanned aerial vehicles) and birds
- Integrate cutting-edge research into network optimization models for analysis of military transportation, disaster response and recovery, and supply chains

Facilities that support this capability include enterprise data centers that host a multi-agency secure private cloud and state-of-the-art facilities for analyzing vehicle cybersecurity. We currently are investing resources to integrate high-performance computing and dependency modeling as it applies to the cybersecurity mission space.

Mission relevance and funding

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

Capability

Argonne is recognized for developing and applying novel decision science and analysis approaches to address pressing national, cross-border, and global challenges. These approaches include agent-based modeling, complex adaptive system modeling, system dynamics, and complex network analyses. We are an international leader in the development of high-performance computing software tools (Repast, EMEWS, and PLASMO), including their use in extreme-scale agent-based modeling applications. This capability, linked with our cyber, information science, and systems engineering capabilities, positions us to deliver impactful solutions to complex problems that require multidisciplinary solutions.

Argonne demonstrated many aspects of this core capability during the US response to COVID-19. For example, our researchers updated our Resilience Analysis and Planning Tool in order to inform emergency managers about vulnerable populations and supported the City of Chicago with the CityCOVID agent-based model to forecast virus propagation and the effect of mitigations.

To address uncertainty, rapidly changing environments, and imperfect/incomplete data, we approach problems as dynamic and interrelated systems. Combining dynamic models with traditional deterministic methods enables analytic outputs that better inform decision makers.

Argonne has applied leadership computing capabilities to the analysis of social and behavioral systems, from predictive modeling of the spread of infectious disease or information in urban areas to the effectiveness of interventions to mitigate disease spread. 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, exascale systems, and machine learning.

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

- Analyze infrastructure assets and systems to inform government and private-sector decisions related to emergency preparedness planning, mitigation investments, and disaster response and recovery operations, with emphasis on the energy, water/wastewater, transportation, and communications sectors
- Apply decision science principles and techniques to create a framework for evaluating the relative criticality of specific infrastructure assets to overall system operations and performance
- Assess the complex interactions of infrastructure dependencies and interdependencies in local, regional, national, and international systems to identify potential cascading and escalating failures and inform resilience-enhancement decisions
- Extend decision science capabilities to address emerging problems involving energy-water interdependence and urban sciences

- 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 national stockpile of critical materials that support national security and advanced energy technologies
- Develop and deploy a human-in-the-loop, machine-learning-based threat assessment process for federal security personnel that enhances overall understanding of facility-level threats and vulnerabilities and optimizes countermeasure recommendations
- Apply our expanded Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) life-cycle-analysis model to inform decisions about new technologies and concepts within initiatives such as the DOE/EERE-FCTO H2@Scale program and GREET for Buildings.

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, spreads through social networks. We are collaborating with UChicago researchers in several of these areas.

Mission relevance and funding

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

Capability

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 across nearly the entire DOE/SC portfolio.

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*, *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 30 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. ALCF also hosts the Joint Laboratory for System Evaluation, which gives our staff and collaborators access to the latest production and prototype computing resources, and operates Cooley (a Cray Xeon cluster), which is used for data analysis. In 2021, the ALCF will deploy DOE's first exascale system, Aurora (an Intel/Cray 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)

Funded by DOE/SC-BES, the CNM 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 APS include a hard x-ray nanoprobe and a synchrotron x-ray scanning tunneling microscope. We are working with DOE to continue to upgrade CNM instrumentation to enable the Center's users to continue to make groundbreaking discoveries. A multi-laboratory Major Items of Equipment proposal to DOE/SC-BES for Nanoscale Science Research Centers Recapitalization has identified opportunities to greatly strengthen this capability.

Mission relevance and funding

The ALCF, APS, and CNM have supported critical research as part of DOE's response to the COVID-19 crisis. The ALCF has supported modeling aimed at identifying potential treatments and forecasting virus propagation. The APS has given structural biologists extraordinary access to characterize COVID-19 proteins, targeted at developing therapeutics. The CNM has supported work to alleviate supply-chain gaps for personal protective equipment and to understand how common fabrics perform in home-made masks.

On an ongoing basis, this capability supports the DOE-SC mission to operate scientific user facilities that provide the highly advanced research tools needed to address the world's greatest challenges in science and technology. Our facilities are sponsored by DOE/SC-ASCR, -BER, -BES, and -NP. Support for specific capabilities also is provided by DOE/NNSA, DOE/OE, NIH, NSF, and industry.

Nuclear and radio chemistry

Capability

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 future nuclear energy systems
- Production and chemical separation of radioisotopes essential to groundbreaking medical and national security technologies
- Structure-property relationships foundational to actinide chemistry and solvent extraction across a broad spectrum of energy-related areas, from nuclear fuel and materials separations to radioisotope production
- Correlations that underpin effective syntheses of transuranic materials and drive actinide/fission-product separations
- Technical bases for 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: a low-energy electron linear accelerator and a chemical separations system for radioisotope production and isolation
- Radiological laboratories that enable development and testing of advanced electrochemical and aqueous processes, to support development of innovative nuclear fuel cycle and safeguards technologies

We apply these capabilities, including the use of artificial intelligence and machine learning, to actinide science that produces novel approaches to the synthesis, characterization, and modeling of transuranic complexes and their properties. Our work uses these purpose-built radiological facilities to extend understanding of the pure and applied chemistry of these artificially made elements. We target predictive bonding and energetics models, within the context of 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 research and development 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 and chemical purification methods to facilitate domestic molybdenum -99 production without the use of weapons-usable materials.

We have used our isotope production expertise to develop the Low-Energy Accelerator Facility (LEAF) and our radioisotope separations capability to produce theranostic medical isotopes. 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 National Isotope Development Center 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. These two radioisotopes 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.

Mission relevance and funding

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

Capability

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.
- Make leading contributions to development of the Versatile Test Reactor and other vital components of the national infrastructure for nuclear energy
- Increase fundamental understanding of nuclear energy materials, processes and systems, thereby enhancing the scientific basis for their safe use and efficient regulation
- Develop and validate advanced, mechanistic modeling and simulation capabilities to better predict the performance characteristics and safety behavior of nuclear energy systems, leveraging Argonne's broader capabilities in artificial intelligence, machine learning, 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
- Advance DOE/SC goals for isotope production and research

Mission relevance and funding

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

Capability

Argonne is a global leader 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 high-purity beams of radioactive isotopes from the californium rare isotope breeder upgrade (CARIBU), stable beams at energies up to 20MeV/nucleon, and state-of-the-art instruments such as the helical orbital spectrometer. The recent addition of the 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; production techniques for medical radioisotopes in collaboration with Argonne's radiochemists; and atom trap trace analysis for geophysics, oceanography, and national security applications. Our one-of-a-kind national center for radio-krypton dating commenced operations in FY19. Argonne's accelerator research and development group supports ATLAS, but our expertise and facilities for cavity processing and fabrication are 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. In FY19, this support included the design and fabrication of the bunch-lengthening system for the APS Upgrade as well as the half-wave cryomodule for Fermilab's Proton Improvement Plan II project.

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 proposed Electron Ion Collider (EIC), our goal is to make major contributions to the science program and the design and simulation of the detector and accelerator. Our detector research is aimed at bolometers and time projection chambers in support of neutrinoless double beta decay, silicon detectors, microchannel-plate photomultiplier photosensors for the ring-imaging Cherenkov detectors for the EIC, and superconducting nanowire detectors. In quantum science, our physicists will build on our strengths in atom trapping, quantum sensors, and quantum algorithms for nuclear physics to build a strategy, working with our materials and computing scientists and the Chicago Quantum Exchange.

Mission relevance and funding

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

Particle physics

Capability

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

The study of the Higgs boson, discovered in 2012, as a tool for new physics is at the center of our experimental program at the Large Hadron Collider (LHC) at CERN in Switzerland. A focused analysis program studying jets with heavy quarks is significantly advancing understanding of the role that the

Higgs boson plays in nature. We are heavily involved in the design and construction of a new pixel detector, development of state-of-the-art trigger hardware and software, and creation of meta-databases and new input/output frameworks that will enable full exploration of LHC data.

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 new experimental searches that attempt to answer a number of open questions.

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 the most accurate, large-volume perspective on the dynamic evolution of the universe that is currently available. Our particle physicists, in collaboration with Argonne's computing researchers and staff from other DOE laboratories, play a leadership role 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; they generate synthetic sky maps that enable current construction projects to exercise their data analysis pipelines and provide comparisons with actual observations to give, for example, new insights into the dark sector of the universe. Our goal is to provide advanced statistical tools to the cosmology community 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 cosmic microwave background (CMB) radiation and have taken a leading role in proposing a fourth-generation CMB 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, in collaborations via the Chicago Quantum Exchange. We continue to transfer to industry our pioneering large-area photodetectors with picosecond timing resolution.

We also play key roles in construction of Fermilab's muon-to-electron-conversion experiment, following our completion of 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 in high-accelerating-gradient 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.

Mission relevance and funding

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 and integration

Capability

We bring together multiple engineering disciplines to integrate science discoveries into practical technological solutions that strengthen the US energy, environmental, and security portfolio and enhance the nation's economic competitiveness. We develop experimental facilities and analytical tools to advance understanding of urban environments, communications, transportation, critical infrastructure, and other large-scale systems. Our work also draws on our capabilities in decision science and analysis.

We develop systems engineering methods, processes and tools and apply them to understand complex systems. Our systems engineering research allows us to:

- Assess dynamic transportation system changes at scale to understand new mobility technologies, connectivity and automation, user decisions, and business model evolutions. We do this through POLARIS, a broad, high-fidelity transportation modeling platform. This tool enables scenario analyses that provides knowledge and outcomes for planning practitioners, industry and governing agencies.
- Evaluate emerging technologies such as electric aviation and unmanned and robotic mobility.
- Compare millions of propulsion and vehicle technologies to quantify fuel economy benefits with simulation tools such as Autonomie, supplemented with experimental validation at our Advanced Mobility Technology Laboratory (AMTL). To enhance our support for the DOE/EERE-VTO Energy Efficient Mobility Systems Program, we have upgraded the AMTL infrastructure, which will enable more accurate and reproducible testing results.
- Study engine combustion and fuels as a complex system to gain larger efficiency and emissions benefits with experimental and predictive combustion phenomena modeling.
- Use the EV-Smart Grid Interoperability Center to conduct research to facilitate interoperability between electric vehicles and their charging infrastructure, leading to smart - grid integration, grid resilience, and full infrastructure interoperability. A component of this work is enabled by discoveries in our science programs, such as concepts for advanced batteries.
- Develop analytical and modeling tools, including advanced computational algorithms, to drive engineering improvements in our nation's electrical infrastructure in partnership with industry, as part of the DOE Grid Modernization Laboratory Consortium.
- Develop systems engineering methods to help overcome security, risk, resiliency, and interdependency challenges facing lifeline infrastructures. We have created tools for infrastructure analyses, design, experimentation, and computation that enable us to model the interdependencies of key systems, such as electricity and natural gas, to identify opportunities to strengthen infrastructure.

Advanced computing at the ALCF 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. In these research areas, we consistently apply machine learning and artificial intelligence for computational efficiency and enhanced throughput.

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.

With DOE/EERE support, we use our system engineering competence to boost US manufacturing job creation through our ongoing collaborations with industrial partners, the European Commission, and the United States – China Clean Energy Research Center's Clean Vehicles Consortium.

Mission relevance and funding

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 partnership sponsors include DOD, DOS, DOT, NERC, NGA, and companies such as Exelon, Ford, and General Motors.

Science Strategy for the Future / Major Initiatives

Our 30-year vision for Argonne's role as a DOE national laboratory derives from our commitment to accelerating science and technology to drive US prosperity and security. In our vision for the future, Argonne is a global leader in:

- Advancing fundamental understanding of the phenomena and matter that make up our world
- Creating rich predictions and visualizations of phenomena and states of matter through advanced experimental characterization and computational science
- Building on discovery science to develop impactful energy-related technologies that enable sustainable prosperity and security

We will realize this vision through our broad portfolio of core research programs, our renewed user facilities, and our continued focus on critical national and global challenges.

Our eight strategic initiatives are intended to enhance our current core capabilities, establish new Argonne strengths, and extend our impact in the world:

- Argonne's two flagship major initiatives – *Hard X-ray Sciences and Future Computing* – will transform the characterization and computation capabilities available to users of the Advanced Photon Source (APS) and Argonne Leadership Computing Facility (ALCF). These initiatives will drive advances in science and technology across Argonne's core programs and research initiatives, made possible by the APS upgrade, the Aurora exascale computer, and future artificial-intelligence-oriented computing systems.
- Two major initiatives – *The Universe as Our Laboratory and Argonne Quantum Initiative* – will deepen and broaden our expertise in selected aspects of physics, materials science, and computer science that are relevant to key national and international priorities in discovery science. These efforts seek to produce insights into and long-standing mysteries in physics and fundamental quantum science.
- Two initiatives are designed to directly support US prosperity and security. *The Manufacturing Science and Engineering* major initiative will enhance our ability to accelerate the scale-up of complex materials and chemical processes to benefit US industry. The *Crisis Response* emerging initiative seeks to establish sustained readiness to quickly mobilize to help combat future biological crises like the COVID-19 pandemic.
- Two emerging initiatives – *Science Innovations for a Circular Economy and Accelerator-based Radioisotope Discovery* – will build on and develop Argonne science, engineering, and computing capabilities that are well aligned with DOE priorities for increasing the re-use of manufactured materials and producing medical isotopes.

We will pursue our initiatives through both internal and sponsor investment and by using regional, national, and international activities and partnerships. Through UChicago Argonne, LLC, UChicago will continue to support Argonne's vision through seed funding of new research directions under the Joint Task Force Initiative (JTFI), sponsorship of leadership development programs, peer reviews, and intellectual collaborations that open up new opportunities to meet national research needs. Partnerships with additional universities, other national laboratories, and industry will remain integral to our core programs and our initiatives. Our strategy is expected to have national and global impact and to contribute to the vitality of the Chicago region.

Infrastructure

Site Facilities and Infrastructure

Argonne's main site in Lemont, Illinois, a suburb of Chicago, is overseen by DOE/SC. The average age of Argonne-operated facilities and infrastructure is 55 years, with 61% of the assets being more than 50 years old. Our facilities are roughly 90% occupied. Tables 6.1 and 6.2 summarize the attributes of Argonne's facilities and utilities. In addition to buildings operated by Argonne, the site 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 about 330,000 sq ft.

In FY20, Argonne entered into two new leases. We leased 100,800 sq ft of multi-use space in Lemont in support of the APS-U project. To establish a physical presence in the city of Chicago, we also leased approximately 20,000 sq ft from UChicago to provide research and collaboration space in the city of Chicago, near the university campus.

We reduce operational risks by focusing investments on inadequate support infrastructure and utilities, which account for most of Argonne's deferred maintenance. We identify these risk-reduction measures within our ten-year site modernization plan – entitled Facility and Infrastructure Strategic Investment Plan, which aligns with the Annual Laboratory Plan and details our intended facility operations funding portfolio.

Table 6.1 Facility and utility assets summary

Mission dependency/condition	Replacement plant value ($ million) (a)	Deferred maintenance ($ million)	Gross square footage (ft^2)	*Average utilization (%) (b)*
Mission critical				
Adequate	1053.2	28.4	1,710,095	*97.2*
Inadequate	34.0	2.1	14,511	*65.0*
Substandard	1593.2	46.6	2,368,662	*93.2*
Mission dependent, not critical				
Adequate	109.7	3.3	359,733	*90.9*
Inadequate	0.3	- -	1,957	*100.0*
Substandard	237.4	20.2	577,458	*85.9*
Not mission dependent				
Adequate	4.2	- -	4,907	*100.0*
Inadequate	0.5	- -	2,640	*50.0*
Substandard	19.2	0.1	48,373	*9.1*
Excess	11.6	0.1	23,893	- -
Total	3,063.1	100.8	5,112,229	- -

(a) Table values include building and utility assets but exclude accelerator assets. With accelerator assets included, the total replacement value would be $3.9 billion.

(b) For any given mission dependency/condition, the average utilization percentage is calculated by dividing the total square feet of space actively used by the total square feet of usable space in that dependency/condition category.

Table 6.2 Utility condition summary (linear feet)

Utility	Adequate	Substandard	Inadequate
Domestic water	7,298	106,012	10,845
Cooling/chilled water	16,110	32,029	2,158
Canal water	2,275	33,745	1,720
Laboratory water	-	20,155	169.1
Sanitary/laboratory sewer	44,748	91,828	13,792
Storm sewer	97,917	12,006	8,423
Natural gas	41,648	1,469	-
Steam/condensate	40,648	10,658	3,391
Overhead/underground electric	307,371	4,023	-
Total	558,015	311,925	40,498
Percentage	*48%*	*27%*	*3%*

Campus Strategy

Ten-year modernization plan

Our vision for the future is driven by a foundational goal of resilient facilities and infrastructure to enable mission readiness both during regular operations and under off-normal circumstances. The ten-year modernization plan establishes a roadmap for achieving this vision, with investments that position Argonne to anticipate, avoid, prepare for, adapt, withstand, respond to, and recover from events that affect our facilities and infrastructure. We have seen the positive impact of our infrastructure planning during the COVID-19 pandemic, as we smoothly transitioned to minimum safe operations and continued construction projects without interruption.

Our campus strategy incorporates resilience planning by establishing site-specific performance goals for our infrastructure portfolio and mitigating event-recovery and performance gaps with planned investments. We are investing in artificial intelligence (AI) and machine-learning to drive resilience by optimizing and automating utility, facility, and maintenance operations. This investment will help Argonne reduce deferred maintenance by making the most effective use of limited resources for maintenance. Execution of the ten-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.

Four main principles guide our campus strategy to assure mission readiness:

- *Support the Laboratory's science strategy*. Argonne continues to commit internal resources and communicate needs for external funding to establish an executable plan for supporting immediate and future infrastructure investments required for future programs and major initiatives.
- *Construct replacement facilities and complete targeted renovations.* We renovate and modernize existing facilities to meet current and future scientific needs while reducing deferred maintenance, improving asset condition, and increasing utilization rates. These efforts apply overhead investment to enable re-use of facilities that, although obsolete due to age, retain positive structural and space characteristics that support modern scientific research.
- *Repair and modernize support infrastructure.* We use a rigorous process, informed by AI, to assess site facility and infrastructure conditions to prioritize and implement repairs and upgrades to meet capacity, reliability, redundancy, and resilience goals. The goal of our planned investments is to reduce our identified deferred maintenance backlog to achieve DOE's goal for "adequate" condition of all infrastructure.

- *Eliminate legacy waste and excess facilities*. Removal of legacy waste and excess facilities is consistent with the DOE/SC goal of maximizing asset utilization and eliminating inadequate-condition facilities. It also supports complex-wide DOE requirements for overall footprint reductions via space banking and reduction in yearly operations and maintenance costs. We are aggressively consolidating radiological facilities and reducing inventories of radiological materials, while preserving the capability to perform mission-important activities. Execution of the excess facilities strategy in the identified period is critical to our long-term deferred maintenance reduction and facility utilization strategy. We will continue to work in close coordination with DOE/SC and DOE/EM.

As we improve facilities and site support infrastructure under these four principles, we will benefit from shorter event-recovery times, greater preservation of system functionality, and more-efficient, automated operations using AI and machine learning.

Key near-term investments to achieve Argonne's infrastructure strategy

Despite steady investments in infrastructure, Argonne carried $85 million in deferred maintenance (DM) costs in FY18 and $101 million in FY19; deferred maintenance is projected to remain level or slightly increase in FY20. In FY19, we extensively evaluated DM and created a comprehensive ten-year strategy to significantly reduce it. Significant, large-scale investments are crucial to Argonne's strategy for greatly reducing or altogether eliminating current and future DM, as outlined below.

Figure 6.1 summarizes the effect of Argonne's proposed investments on DM, while Figure 6.2 shows the locations of the proposed investments. Tables 6.3 and 6.4 detail the facility investment plan.

Electrical capacity distribution capability ($60 million SLI)

An upgrade to Argonne's high-voltage power supply is required to support projected load increases associated with scientific growth and provide a fully redundant power supply to all site research programs, facilities, and systems. Argonne today receives power from a single location that has original 1960 equipment and installations.

This condition increases the risk of an external power outage affecting the site and mission-critical programs, including the Advanced Photon Source (APS), Center for Nanoscale Materials (CNM), Argonne Leadership Computing Facility (ALCF), and Argonne Tandem Linear Accelerator System (ATLAS). The power upgrade also will provide additional capacity to support increases in electrical usage associated with exascale computing efforts expected in the FY21 timeframe and beyond.

This investment is considered enabling infrastructure; however, it directly addresses risks associated with the following core capabilities: accelerator science and technology; advanced computer science, visualization and data; chemical and molecular science; condensed matter physics and materials science; and nuclear physics.

Argonne utility upgrade ($215 million SLI)

The Argonne utility upgrade (AU2) project replaces, repairs, and upgrades several critical utility systems – chilled water, domestic water, steam/condensate, and sewer – to reduce operational risks, eliminate deferred maintenance, and reduce the risk of unplanned service outages. Argonne's main support facilities and utility distribution infrastructure are original to the site: much of the equipment has reached the end of life and parts are becoming unavailable as emergency repairs increase. This condition poses a severe threat to the goal of a resilient laboratory.

Upgrades to Argonne's central chilled-water capacity and distribution will enable integration of isolated buildings into the main system, reducing operating and maintenance costs while decommissioning aging satellite plants and their associated failing equipment. Chilled water provides cooling for equipment processes and is critical to the operation of several national scientific user facilities on Argonne's main site.

Repairs and replacements will address deteriorated and failed portions of steam and condensate distribution piping. The project also will replace an obsolete, unsupported control system for the steam plant. Loss of steam distribution would result in a loss of space heating in site buildings and would prevent the APS from maintaining the precise temperature and humidity control needed for facility operations. All repair or replacement work under this project will incorporate facility and utility meter replacements, control hardware, and software upgrades into the various infrastructure systems.

Building on internal investment, we will first develop machine-learning algorithms to automate system optimization for operations and maintenance to help achieve performance goals for site resilience. AI-enabled operations for infrastructure will then be accelerated through investments under the AU2 project. Utility system controls and metering infrastructure upgrades will be interconnected through existing software applications to collect data, establish system baselines, and enable remote system control. Investing in these capabilities during the project is crucial to accommodate AI-enabled operations and our vision of a resilient laboratory.

The Argonne utility upgrade project incorporates multiple investments required to assure that three mission-critical facilities – APS, CNM, and the Advanced Protein Characterization Facility (APCF) – can continue to function as 24/7 scientific user facilities. Investments specific to this part of the campus, the 400 Area, include electrical and mechanical systems modernization to support reliable and continuous operations; these investments are considered enabling infrastructure. These investments also directly address risks associated with the following core capabilities: accelerator science and technology; advanced computer science, visualization and data; biological and bioprocess engineering; chemical and molecular science; condensed matter physics and materials science; nuclear physics; and large-scale user facilities/advanced instrumentation.

Repair and modernize support infrastructure: facilities and site work ($77.6 million GPP-SLI)

Argonne is proposing multiple projects that focus on overall site conditions and high concentrations of deferred maintenance. These projects include large-scale building renovations, roof replacements, road and parking surface repairs, and elevator replacements.

Large-scale building renovations will address aging interior infrastructure, including plumbing, heating and cooling, mechanical and electrical systems, and space refurbishments. These modernization projects will accelerate AI-enabled operations by providing metering and controls hardware and software upgrades and taking advantage of existing operational efficiency software to optimize building operations and maintenance. Our ten-year plan includes deploying this software, combined with deep-dive assessments of building systems, to Argonne's top 40 energy-consuming buildings under the Smart Labs initiative (see Sec. 6.4).

The average age of our facility roofing is 35 years, which is far beyond the expected service life. The rate of roof failures and leaks continues to increase each year and is beyond what internal budgets can address. Leaks and water infiltration pose a major risk to our operations as shutdowns of facilities during repairs, or damage to scientific equipment, can impact research programs.

Due to weather conditions in the Chicago area, more than 25% of our site's existing paved-surface conditions are in inadequate condition and require investments for rehabilitation. Inadequate pavement conditions for pedestrians and vehicles increase the probability of injuries and damage to vehicles and the equipment they transport.

Because of their age, passenger elevators in numerous buildings frequently malfunction and stop. These elevators are 24 to 59 years old and will be replaced to provide reliable and modern equipment.

Alternative financing approaches

Argonne continues to investigate alternative financing approaches to achieving the site's facilities modernization strategy. Through partnerships with the State of Illinois, Argonne has constructed several facilities, most recently the APCF. To address future growth in energy storage and materials synthesis scale-up, we have proposed the Energy Innovation Center and Materials Scale-up Laboratory. As noted in Sec. 6.1, we have begun to expand Argonne's presence in Chicago. This longer-term strategy began with the current lease in a building on Harper Court and will expand to future long-term development in the area.

Site Sustainability Plan Summary

Argonne's site sustainability program, which is an integral part of our campus strategy, leads efforts to meet DOE goals under Executive Order 13834: *Efficient Federal Operations*. In FY19, we formalized our Smart Labs initiative, which improves facility and utility performance and safety while achieving DOE's sustainability performance goals. Our approach applies retro-commissioning and *Guiding Principles for Sustainable Federal Buildings** to modernize buildings and sustain system performance using operational efficiency software (Energy-AnalytiX by Iconics). The Smart Labs initiative supports our first phase of AI-enabled operations for infrastructure. In FY19, we began implementing Energy-AnalytiX in Buildings 200 and 401. The software uses analytic tools to identify facility system improvements and predict maintenance needs. Next steps include developing machine-learning algorithms to use our data to automate system optimization and maintenance efforts.

We continue to use energy savings performance contracts to improve efficiency and resilience of facilities and utility systems. In FY19, we completed our first two contracts, which saved Argonne $20,620,690 over their life. To improve energy resilience, in FY19 we developed a plan for on-site investments in solar photovoltaics; it identifies 20 sites that could generate 53,600 MWh of solar energy annually or 70% of Argonne's base site electricity load. Next steps are to incorporate solar photovoltaics investments into the ten-year modernization plan, with a focus on meeting our performance goals for emergency power and energy resilience.

We have documented 19.8% of Argonne's buildings as meeting the CEQ guiding principles, exceeding the 15% DOE goal. Table 6.9 and Figure 6.3 summarize sustainability projects and electricity use; the projected increase in electricity use is due primarily to anticipated exascale computing systems.

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 2019 Lab Operating Costs:** $587.5 million
- **FY 2019 DOE/NNSA Costs:** $528.9 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $57.4 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 10%
- **FY 2019 DHS Costs:** $1.2 million

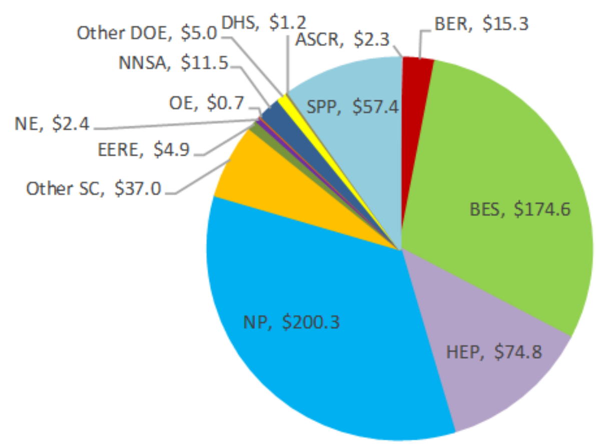
Physical Assets:

- 5,322 acres and 314 buildings
- 4.83 million GSF in buildings
- Replacement Plant Value: $5.8 B
- 159,912 GSF in 27 Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:

- 2,421 Full Time Equivalent Employees (FTEs)
- 139 Joint Faculty
- 159 Postdoctoral Researchers
- 200 Graduate Student
- 286 Undergraduate Students
- 3,555 Facility Users
- 1,523 Visiting Scientists

FY 2019 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 produces transformative science and advanced technologies, and does it safely, securely, and environmentally responsibly, with the cooperation and involvement of local, state, and international scientific 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. The Relativistic Heavy Ion Collider complex, the National Synchrotron Light

Source II, the Center for Functional Nanomaterials, and the Accelerator Test Facility serve over 3500 scientists/year.

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

Core Capabilities

Fifteen core technical capabilities underpin all activities at Brookhaven National Laboratory. 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 and environmental science 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 transformational science and technology that is relevant to the DOE/Department of Homeland Security (DHS) missions. All together, they make BNL unique. This year, BNL was assigned two new core capabilities in Computational Science and Applied Mathematics that were previously "emerging."

Accelerator Science and Technology

Summary: BNL has long-standing expertise in accelerator science 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), and looks forward to hosting a high-energy, high-luminosity polarized Electron-Ion Collider (EIC). Among the nowadays widely-used technologies developed at BNL are the strong-focusing principle and the Chasman-Greene lattice, which were transformational developments for modern accelerators and synchrotron light source facilities, respectively. With the construction of NSLS-II, the Laboratory adopted recent advances in accelerator technology to achieve unprecedented brightness. Similarly, the EIC at BNL will combine many recent innovations in collider technology and push them beyond the current state of the art to achieve unprecedented performance parameters.

Since 2015, NSLS-II has provided reliable, stable, and intense beams of synchrotron radiation to the user community. Major advances in reliability were accomplished by implementing improvements that targeted major machine subsystems. Over the past few years, the facility added 20 new insertion devices, with several narrow-gap in-vacuum undulators and increased the operating current to 400 mA, recently achieving 500 mA in beam studies. The storage ring emittance of 800 pm rad remains one of the smallest among operating light sources. NSLS-II is making important contributions to the Advanced Photon Source and Advanced Light Source Upgrade projects that will deliver unprecedented brightness. Core strengths of NSLS-II include expertise in physics of light sources, collective effects and novel ring lattices, designs of permanent magnet undulators and front-ends, RF, advanced control systems, and high-performance beam diagnostics. The wealth of knowledge accumulated at NSLS-II from early designs to today's operations lays a solid foundation for a future NSLS-II upgrade in approximately 2030.

BNL continues to aggressively extend the physics reach of RHIC. An order-of-magnitude additional improvement in RHIC luminosity for heavy ion collisions, now reaching nearly 50 times design luminosity in Au+Au collisions, was delivered by 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. Bunched-beam electron cooling was demonstrated for the first time and is being employed to reach higher luminosity at beam energies far below the original design goal. Together these advances enable the ongoing multi-year high statistics beam energy scan that is executing the most comprehensive search ever for a Critical Point in the phase diagram of quark-gluon matter. This past year, in collaboration with Cornell University, BNL scientists demonstrated, for the first time, multi-turn acceleration and energy recovery of an electron beam using a single permanent magnet recirculation loop. Core strengths in hadron cooling, superconducting radiofrequency (SRF), energy recovery linac (ERL) technology, and high-brightness electron storage rings are the foundation of the future EIC at BNL, which will enable the most detailed exploration of the fundamental constituents of matter in the history of science. 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).

BNL's Superconducting Magnet Division (SMD) played a central role in the early development of superconducting magnets for high-energy colliders, thus enabling RHIC construction. The excellent performance of the SMD-supplied ring magnets directly contributed to the success of the RHIC physics program. SMD 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. SMD 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 SMD to develop magnets based on high-temperature superconductors led to the fabrication, presently underway, of a very high field solenoid magnet to aid in the search for axionic dark matter, potentially one of the missing pieces in our understanding of the structure of the universe. SMD provides diverse capabilities that support all of BNL's accelerator facilities and that are essential for the construction of an EIC.

The Accelerator Test Facility (ATF) is the flagship user facility of the DOE Accelerator Stewardship Program in the Office of High Energy Physics (HEP). 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.

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, and engagement with the joint BNL-Stony Brook University (SBU) Center for Accelerator Science and Education (CASE). Roughly ten Ph.D. students conduct accelerator research at BNL under the auspices of CASE.

The Office of Nuclear Physics (NP), the Office of Basic Energy Sciences (BES), and HEP, as well as SBU, New York State Energy Research & Development Authority (NYSERDA), and Laboratory Discretionary Funds are the primary sources of funding for the ongoing AST efforts.

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), US Lattice Quantum Chromodynamics (USQCD), 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 180 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 ROBUST, and the Scientific Discovery through Advanced Computing (SciDAC) Institute for Computer Science and Data-RAPIDS). 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 Office of Biological and Environmental Research (BER), BES, HEP, the Offices of Electricity (OE) and 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), 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 ASCR PanDa for ATLAS. The impact of this technology was demonstrated as part of the COVID-19 response in Argonne National Laboratory drug discovery pipelines, which were accelerated by an order of magnitude through RADICAL. 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 ECP CODAR projects.

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

Summary: 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, and fundamental studies of charge and discharge mechanisms and the associated material-structure evolution.

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 has become an important player in grid modernization for efficient and resilient electricity distribution systems with high penetration of renewables with a focus on the challenges of New York State and the Northeast. BNL is a member of the DOE Grid Modernization Laboratory Consortium and plays a key role in several of its projects. BNL also supports New York State’s efforts to restructure its electricity markets under the “Reforming the Energy Vision (REV)” initiative.

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 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.

Biological Systems Science

Summary: 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 integrates computational and experimental platforms to generate and test hypotheses using approaches that include molecular biology, biochemistry, structural biology, and imaging. Ultimately this work lays the foundation for desired manipulations of growth rates, biomass accumulation, resistance to stresses, and the accumulation of desired feedstocks for bioenergy and bioproducts in organisms relevant to BER. This program is synergistic with programs in physical biosciences (funded by BES, Section 3.5).

BNL's Quantitative Plant Science Initiative (QPSI), addresses the grand challenge of "enabling predictive biology." A key goal is accelerating the discovery of gene and protein function. The initial focus of QPSI is on genes that contribute to micronutrient resilience that will underlie the biodesign of high yield, 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 also makes use of the world-leading analytical capabilities at NSLS-II, computational capabilities in CSI, and those within the CFN, to probe molecular structure and dynamics at unprecedented spatial and temporal resolutions. 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 capability is an integral part of the BNL biological systems program. BNL researchers contribute to the KBase development team (led by Argonne, Lawrence Berkeley, and Oak Ridge National Laboratories).

NSLS-II continues to expand its science program for molecular characterization and imaging, with the support of the National Institutes of Health (NIH) and BER. 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 newly commissioned cryo-EM capability complements the world-leading performance of the X-ray diffraction and scattering programs. A laboratory building for the cryo-EM was constructed, and support for operations obtained through BER. The unique combination of spatial, chemical, and molecular imaging capabilities of NSLS-II will be further enhanced by cryo-electron tomography. New capabilities will enable examination of rhizosphere and plants under realistic conditions. All the developments will be supported through targeted training and dissemination.

Funding comes from BER. BNL also contributes to two Bioenergy Research Centers, i.e., the Center for Advanced Bioenergy and Bioproducts Innovation and the Joint Bioenergy Institute and three Biosystem Design projects (led by Berkeley, Cold Spring Harbor Lab, and the University of Illinois). Collaborations are also supported by Joint Genome Institute Community Science Programs, the Environmental Molecular Sciences Laboratory's user program, the Facilities Integrating Collaborations for User Science (known as 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

Summary: 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 exploits 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 15 years of operation and is in its second 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 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 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

Summary: 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. Scale-up of some materials is underway with industry partners.

These programs are funded by BES, the EERE Hydrogen and Fuel-cells Technologies program, and through Strategic Partnership Projects and CRADA efforts with industrial partners.

Climate Change Sciences and Atmospheric Science

Summary: BNL's atmospheric and terrestrial ecosystem science efforts aim to develop process-level insight into the role of aerosols, clouds, and ecosystems in a changing climate. 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. 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.

BNL scientists study fine-scale processes that have a global impact on climate. A dedicated effort to build fundamental physical understanding and scale 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 and modeling at fine scales that will bring these two components, required for improving climate predictability, together. As computing resources grow and models achieve higher resolution, observations must also push current resolution boundaries. BNL staff are well-poised to bring new measurement technologies, 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, explicit simulations of the atmosphere 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. BNL has also established a mobile remote-sensing platform to support research in off-shore wind resource characterization, urban system studies, and national security applications.

Funding comes from BER and Laboratory Discretionary Funds.

Condensed Matter Physics and Materials Science

Summary: 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 oxide molecular beam epitaxy, angle-resolved photoemission, and spectroscopic imaging scanning tunneling microscopy), is fully operational and had a productive past year, with seven papers published. 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). The first experiments focused on the universality of the phase diagrams of high T_C superconducting cuprate families.

The OASIS effort has undergone a change in leadership in the past year. BNL hired a new lead scientist for its STM leg who is playing a key role in guiding the scientific direction of OASIS. OASIS will continue to study superconducting cuprates but will expand to include two dimensional (2D) materials and heterostructures that can support topological excitations.

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 (UED). In operation is the BNL MeV UED facility, 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 (UEM), 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.

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. With an eye towards QIS, in the past year the expertise in 2D materials was strengthened with the hire of a staff theorist in addition to the lead scientist for the STM effort mentioned above.

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

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

Summary: As a key part of its mission, BNL develops and operates user facilities that exceed the funding and expertise available at individual institutions. In FY 2019, 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 and generated 227 peer-reviewed publications in 2019.

NSLS-II is completing its fifth year as a User Facility, having hosted over 1700 unique users in FY 2019. Twenty-eight beamlines are in service, with 27 in General User operations. NSLS-II is operating at 400 mA, with 98.2% reliability year-to-date. NSLS-II has strong R&D programs in nano-focusing optics and nano-precision engineering and a strong partnership with the CFN, running four endstations 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 becoming 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.

The CFN maintained a high level of productivity and impact in 2019, by assisting 593 external users and contributing to research resulting in 333 peer-reviewed publications, both the highest ever in a single year. The strengths of the CFN's comprehensive portfolio of nanoscience capabilities are tools for creating nanomaterials through assembly of nanoscale components, and instruments for high-resolution studies of nanomaterials in working environments using electron, X-ray, and photon probes. This year, the CFN added: an in situ atomic force microscope for real-time nanoscale studies of surfaces in controlled gas atmospheres or liquid environments; a new detector for the aberration-corrected X-ray photoelectron emission microscope (at the NSLS-II Electron Spectro-Microscopy beamline) with improved signal to noise and time-resolution; and a hyperspectral dark field imaging 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. Forward 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 and bring participants in the LHC heavy ion program back as users of RHIC.

BNL will host a new user facility, the Electron-Ion Collider, that builds on the RHIC user facility. It would 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. This facility is unique in terms of the breadth of advance accelerator and laser experiments that it supports.

BNL also makes important contributions to international facilities – the LHC, and such future facilities as a Long Baseline Neutrino Facility (LBNF)/DUNE and the Rubin Observatory, which is under construction. This core capability (CC) is strongly tied to CC 1, 11, 12, and 13.

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.

Data collected from the Long Island Solar Farm at BNL has led to the creation of one of the largest data sets for a utility-scale solar plant 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.

BNL's Instrumentation Division provides cutting-edge support for the Lab's major scientific user facilities and national security applications through its development of state-of-the-art detectors, electronics, and optical and laser systems. Major contributions have been made to instruments and experiments at BNL and other accelerator- and reactor-based facilities worldwide. The Division supports such efforts from concept through construction and 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 for measuring synchrotron beamline optics. 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 diamond detectors for advanced synchrotron radiation imaging at NSLS-II and for novel applications in proton and ion beam therapy.

The major sources of funding are: BES, NP, HEP, BER, the National Aeronautics and Space Administration (NASA), New York State, NIH, and Laboratory Discretionary Funds.

Nuclear & Radio Chemistry

Summary: 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. This year, the tri-Lab collaboration submitted a drug master file on accelerator-produced Ac-225 to enable its use in clinical trials. 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 one of the two Nuclear and Radiochemistry summer schools 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 supports NNSA Defense Nuclear Nonproliferation efforts.

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

Summary: 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 Scientific Data and Computing Center (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 more 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 Jefferson Lab 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 (CC 1), while enhancement of the RHIC detector capabilities benefits from the support of the BNL Physics Department and the Instrumentation Division (CC 9). 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. In 2016, 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 four and a half million data retrievals from the NNDC websites.

Support is provided by NP as well as New York State, RIKEN, and Laboratory Discretionary Funds.

Particle Physics

Summary: 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); hosting computing facilities for the BELLE II experiment at KEK; and construction and data collection from the Rubin Observatory cosmological survey.

These roles are enhanced by BNL high energy physics theory efforts and by BNL's international leadership in critical detector and advanced accelerator research and development, including superconducting magnets, for the next-generation collider 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 RACF and the Particle and Nuclear Physics Software group. BNL's software and computing capability have also been applied to the Belle II experiment since 2017. Particle physics software and computing development for both experiment and theory benefit strongly from synergies with RHIC facilities funded by DOE 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 has constructed the CCD sensors for the Rubin Observatory camera, which is in commissioning and will become a premier tool for the exploration of cosmic 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 participated strongly in the Basic Research Needs workshop organized by DOE in December 2019.

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 leads the world in X-ray brightness and in FY 2019, five years after the start of operations, hosted over 1700 researchers and operated 28 beamlines. 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.

Another example is the RHIC accelerator complex, the largest accelerator and only collider complex in the Americas. The cutting-edge technologies developed at BNL and employed at the complex include high-intensity ion sources, a high-power proton target for medical isotope production, rapid cycling synchrotrons, advanced stochastic and electron beam cooling techniques, and two superconducting accelerators to produce high luminosity heavy ion and polarized proton collisions.

A third example is BNL's development of noble liquid detectors from concept, through demonstration, to implementation in major particle physics experiments (D0 at FNAL and ATLAS at LHC), with continuing R&D aimed at developing the very large LAr TPCs that form DUNE. The cold electronics developed at BNL for LAr TPCs in MicroBooNE, SBND, and ProtoDUNE have been used in research and development of various modifications of TPCs, including LArIAT at FNAL and ARGONTUBE at the University of Bern.

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.

Computational Science (New)

Computational science, both numerical modeling and data analytics, is essential to enabling advanced scientific discovery at BNL's facilities - RHIC, EIC, and the BLIP (NP); 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 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 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, BER Predictive Genomics project, BES efforts for Dynamics and Control of Magnetic and Charge Order in Complex Oxides and GENESIS, 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 and facilities such as NSLS-II, cryo-EM, and CFN, BNL co-designs new experimental capabilities that integrate advanced imaging technologies with high powered edge computing devices and streaming ML and AI.

CSI is developing a growing research program at the intersection of Quantum Information Science, Applied Math, and High Energy Physics. In the context of entanglement of purification and holography, BNL researchers aim to gain a deeper understanding of bulk spacetime. Progress was made towards a proof of the holographic entanglement of purification conjecture, used entanglement of purification to design a better holographic tensor network, studied the connection between multi-boundary wormholes and entanglement of purification, and generalized entanglement of purification and reflected entropies to multipartite and conditional forms. Plans for the future include: designing novel quantum algorithms in the Noisy Intermediate-Scale Quantum (NISQ) era for finding ground states of classically inaccessible spin chains and strengthening the black hole information paradox by using the Hayden-Preskill process for extracting information from Hawking radiation. BNL is also developing the basic building blocks needed for HEP simulation on near term quantum computers. New quantum algorithms were created for finite temperature simulations and early universe cosmology on NISQ systems. This is complemented by a growing Quantum ML (QML) research program that is bringing novel machine ML approaches to QIS systems. The goals of this program are to optimize the operation of those systems and to develop new QML algorithms to solve challenging problems in HEP. This is supported by an HEP project entitled “Quantum Convolutional Neural Networks for High Energy Physics Data Analysis” in collaboration with the DUNE and ATLAS experiments.

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

Applied Math (New)

As a premier experimental physics research institution, BNL’s mathematics research traditionally has focused on areas distinctly relevant to HEP, NP, synchrotron (BES), and accelerator physics. In the 1970s, Brookhaven scientist Michael Creutz pioneered the first numerical simulations of quantum field theory that paved the way for the huge success of applying lattice QCD methods to predicting 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 focused on rebuilding a distinct applied math research program aligned with the changing needs of the BNL science directorates and DOE. After carefully considering 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.

Newer activities include inverse problems in the context of accelerator physics, RHIC, and the EIC and Applied math for QIS.

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 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.

In addition, CSI is cultivating a program at the intersection of applied mathematics and QIS, investigating what potential mappings exist between subclasses of graphs and quantum states. BNL found a relationship between hypergraphs and stabilizer quantum states and is examining if directed graphs can represent the entropies of all quantum states. BNL is developing a first implementation of non-Abelian braiding statistics, which would provide the basis for superior topological quantum error correcting codes. A blueprint for demonstrating the fundamental braiding properties of the Fibonacci code was also developed. BNL investigates approaches that could enable quantum computers to efficiently perform floating point operations, a critical capability toward scientific computing on such systems. Potential "testbed" targets include linear algebra problems and computational fluid dynamics. In initial work, BNL has completed the design of a simple quantum adder and multiplier.

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

Summary: These core capabilities, along with BNL's proven expertise in large science project management, will enable the Lab to deliver its mission and customer focus, to perform a complementary role in the DOE laboratory system, and to pursue its vision to deliver discovery science and transformative technology that power and secure our nation's future.

Science Strategy for the Future/Major Initiatives

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, an inclusive, diverse, and equitable environment, and a focus on renewed infrastructure.

The Laboratory's high-level science and technology priorities for the coming decade focus in several broad areas:

- Advancing fundamental research in nuclear and particle physics to gain a deeper understanding of matter, energy, space, and time, including completing the mission of the Relativistic Heavy Ion Collider (RHIC) and constructing a next-generation nuclear science facility, the Electron-Ion Collider (EIC). BNL also anticipates playing a leading role in global particle physics experiments.
- Developing and applying photon sciences and advanced materials research to energy, biological, environmental, and national security problems of critical importance to the nation. This requires building out the beamlines at National Synchrotron Light Source II (NSLS-II) over the next

decade, recapitalizing instrumentation at the Center for Functional Nanomaterials (CFN), and preparing for the NSLS-II upgrade. Key focus areas will include quantum materials for applications in scalable quantum qubits and energy storage materials for large-scale grid integration.
- Developing new techniques for manipulating, analyzing, and storing large data sets, using artificial intelligence (AI) and machine learning (ML) for applications across many fields, including quantum information science toward a quantum internet.
- Developing accelerator science and technology with broad applications: from operating transformational facilities for fundamental science to isotope production and national security.
- Applications of these strengths, particularly across disciplines, to new opportunities (and national challenges, e.g., the COVID crisis) as they arise.

A key element of Brookhaven's strategy is to position the Lab's major user facilities (RHIC and its transition to the EIC, NSLS-II, the CFN, and the Accelerator Test Facility [ATF]) as well as the Computational Science Initiative (CSI) for continued leadership roles as they evolve. BNL will also establish a regional bulkhead, Discovery Park, that can serve as a driver to regional, national, and international partnership and outreach.

Infrastructure

Overview of Site Facilities and Infrastructure

BNL's scientific vision is structured around the achievement of seven initiatives as described in Section 4. Two additional operational initiatives: a renewed research campus and safe, secure, and efficient operations 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 2019, there were 2421 staff on site in 315 buildings totaling 4,815,924 square feet (sf) and 9,878 sf of real property trailers. All real property is owned by the DOE Office of Science (SC) except for FIMS Asset ST0705, Reactor Stack, which remains under the Office of Environmental Management (EM). BNL does not lease any facilities and the average age of all non-excess buildings is 46 years with sixty-one buildings (720,186 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 conditions and utilization statistics can be found in Appendix A.

The CFR project eliminated 156,205 sf of underutilized space in FY 2019. In addition, ~31,000 sf of underutilized space was declared excess and in FY 2020 an additional 10,133 sf will be declared excess. 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 2019, there were 27 excess buildings, comprising 159,912 sf, and 20 buildings totaling 318,468 sf in Standby status

Subject to availability of funds, EM will remain responsible for the decontamination and decommissioning (D&D) of the additional excess facilities, including Building 491 (Brookhaven Medical Research Reactor [BMRR]), Building 650 (Hot Laundry), Building 701 (Brookhaven Graphite Research Reactor [BGRR) and Building 750 (High Flux Beam Reactor) 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. EM is funding the removal of EM OSF asset ST0705 (Reactor Stack) and SC asset Building 650 in FY 2020.

The BNL Land Use Plan, being updated in 2020, 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. In addition, the Laboratory's world-class 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. Support the growing population of scientific users through an innovative concept called "Discovery Park"

Ensure renewed critical infrastructure and buildings are resilient against severe climate and weather.

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). In addition, Other Infrastructure Projects (OIP), which include alterations and non-capitalized betterments support the Lab's strategy.

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 National Synchrotron Light Source) for which construction began in FY 2019.

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, currently an SLI-funded project, will fulfill three key mission needs by providing efficient science user and visitor processing capability, provide collaboration and conference space for the research community, and provide modern, efficient office space to enable operational efficiencies through staff colocation 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 buildings associated with the 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 buildouts.

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 safety of facilities, 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, it is estimated that ~250,000 sf of net excess space will be eliminated, the majority of which is WW-II-era buildings. However, an additional 200,000 sf could be eliminated with the assistance of direct funds

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.

In FY 2019 as part of the continuing consolidation planning to right size the campus, one building (19,593 sf) and two modular buildings (2,989 sf) were demolished. At the end of FY 2019, there were 27 excess buildings totaling 159,912 sf, and two real property trailers totaling 1,158 sf. In addition, a small portion of the former NSLS accelerator remains to be cleaned-up and the HFBR, BGRR, and BMRR, await EM funds for demolition.

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 very tight 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 their useful life. The project also contains 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 expected to be completed in FY 2022.

The aging 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 – 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. Design of the Federal component and development of the ground lease for the first-privately financed facility are underway with planned initial occupancy in the FY 2022/FY 2023 timeframe.

Element 5 – 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 1.2% of Replacement Plant Value for 2019 for non-excess and non-OSF 3000 assets. Key to BNL's strategy is to continue to consolidate out of those assets not worth maintaining, followed by cold and dark and ultimately by their demolition. Space consolidation, such as the ongoing efforts in FY 2020, will be enabled by renovation and alteration of underutilized buildings and through new proposed buildings, such as the SUSC as part of the Discovery Park development 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.

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 BNL 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. The scope of the project includes select revitalization of the building envelope, HVAC and other building systems, interior finishes, and building configuration as required for performing its new mission. The project received Critical Decision-0 (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 May 2019, and construction has commenced. The CD-4 completion date is September 2023.
- **Science and User Support Center (SUSC)** (TPC Estimate Range $72M - $96M, 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 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.
- **Critical Utilities Rehabilitation Project (CURP)** (TPC Estimated Range $70-$95M, 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 dating back to 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 is required to 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 2026 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 service dating back to WW-II. 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 Central Chilled Water Plant; 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 utility plant key 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 110,000 sf of buildings, trailers, and OSF assets. The project will co-locate maintenance and operation resources that are dispersed in 13 buildings and 19 trailers, located in five dispersed 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 enhance operations by centralizing the control areas for the computerized maintenance management and building management control systems. Due to co-location, shared facilities, more effective staffing and supervision, and energy efficiency, there will be an increase in operational efficiency.
- **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.

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 request), Electrical Distribution ($9.0M, FY 2022 request) and Roofing ($8.8M, FY 2024 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 funding for the D&D of Building 650 is anticipated in FY 2020.

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 ~$4.8M in 2019 (25% of the project's budget) and are forecast at ~$4.8M (29%) in 2020. Changes to IGPP rules, as described in Chapter 24 of the DOE Financial Handbook, were incorporated into BNL's indirect planning process.

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 programsDefer 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 funded development of housing and 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 comprised of the SUSC, private housing, and potential education outreach space, was designed to create a small mixed-use user community (Upton Square) that will become a user housing community, an entry portal, 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 99% of the originally estimated annual energy and green-house gas savings. Based on the success of this project, BNL and the Brookhaven Site Office are developing a second UESC project and expect a contract to be awarded in FY 2021.

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. As of FY 2019, nearly 20% of BNL's footprint is comprised of HPSBs and more are on the way, including the SUSC.

As has been the case for many years, one of the goals, energy intensity reduction, continues to be challenging and the Lab's historical success in lowering its energy intensity by nearly 60% partially accounts for this. Regardless, BNL continues to maximize the use of UESCs. The combination of the one completed in 2015 and the second that is under development is estimated to lower BNL's energy intensity by over 5%. The use of UESCs is a major component of BNL'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) as new buildings are constructed for the EIC and RHIC operations cease.

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 2019 Lab Operating Costs:** $491.64 million
- **FY 2019 DOE/NNSA Costs:** $490.12 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $1.51 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 0.3%

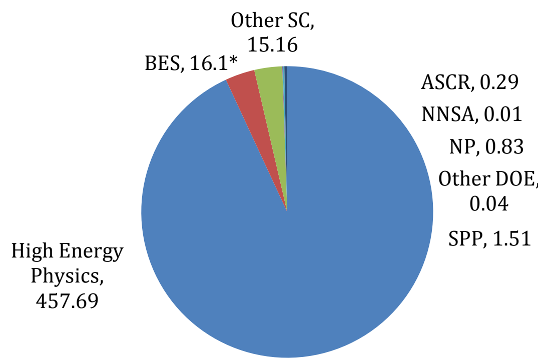
Physical Assets:

- 6,800 acres and 365 buildings
- 2.4 million GSF in buildings
- Replacement Plant Value: $2.44 B
- 28,913 GSF in 10 Excess Facilities
- 22,155 GSF in Leased Facilities

Human Capital:

- 1,810 Full Time Equivalent Employees (FTEs)
- 22 Joint Faculty
- 95 Postdoctoral Researchers
- 30 Graduate Student
- 65 Undergraduate Students
- 3,725 Facility Users
- 27 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



*BES number reflects funding of $15.537M provided by SLAC for LCLS-II work

Mission and Overview

Fermilab's mission is to be the frontier laboratory for particle physics discovery. Thousands of scientists, engineers, technicians, and university-based users 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 a laboratory that looks into 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, is for Fermilab to be the worldwide leader in accelerator-based discovery neutrino science, which will be 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), will be 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 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 LCLS-II 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 three 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. Fermilab's emerging initiative in quantum information science has already produced high-impact results in quantum computing and sensing and has fostered collaborations with 20 universities, multiple laboratories, and for the first time has developed a burgeoning partnership with industry giants: IBM, AT&T, Google, Lockheed, and the leading quantum startup Rigetti Computing.

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. Through the Joint Task Force Initiative (JTFI), UChicago and Argonne National Laboratory bring considerable operational and intellectual assets to create a partnership for forefront research.

Core Capabilities

Fermilab has unique and powerful infrastructure essential to the advancement of discovery in particle physics, including the nation's only accelerator complex dedicated to particle physics and 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; by its expertise and facilities for computing; and by 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 (HEP) 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** and is primarily funded by the DOE Office of High Energy Physics (DOE/HEP).

Particle Physics

Particle physics is the heart of the laboratory's science mission and 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 and Precision 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 that are studying neutrinos over both short and long distances, allowing the Fermilab 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 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 will begin operating this year, and the Short-Baseline Near Detector (SBND) that will follow in 2022. 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 is 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 success of the project by providing unique expertise. The project was successfully completed ahead of schedule and under budget.

A skilled and talented workforce of scientists, engineers, and technicians leverages Fermilab’s accelerator and detector R&D programs 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 the current understanding of the laws of physics by testing predictions to the highest accuracy and searching for phenomena that are either extremely rare or forbidden by current theories. Deviations from expectations are a possible indication 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 with delivery of the world’s most intense muon beam to the Mu2e experiment in 2023.

The Muon g-2 experiment will precisely measure a property of muons called the anomalous magnetic moment and investigate hints from previous experiments that the muon’s magnetic moment may be different from what was predicted by the Standard Model of particle physics. If true, this could be an indication of new physics with far-reaching implications. 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 leads the Dark Energy Survey (DES), is a key partner in several world-leading cosmic science experiments and contributes to R&D efforts toward new dark energy, dark matter, and cosmic microwave background (CMB) experiments. Fermilab researchers built the DES camera and are currently leading the science collaboration for the Dark Energy Survey (DES). Fermilab is working with other DOE laboratories to build three new large cosmic survey projects (DESI, Rubin Observatory, CMB-S4). The laboratory is engaged in world-leading searches for particle dark matter, fulfilling major responsibilities for the construction and operation of second-generation experiments (ADMX and SuperCDMS SNOLAB), while ramping down responsibilities on LUX-ZEPLIN (LZ). Fermilab plays an important role, together with other laboratories and the University of Chicago, 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 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 (see figure). Fermilab scientists have 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 the operation of the Rubin Observatory Legacy Survey of Space and Time (LSST). 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 (DESC). 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 efforts in cosmic science. 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, and recently the DOE has 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 facility, in collaboration with Northwestern University, for the characterization and calibration of cryogenic solid-state detectors with sensitivity to sub-GeV dark matter (NEXUS). 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 possible wave-like, ultra-low mass bosonic dark matter, including the QCD axion. While current generation experiments are limited by the standard quantum limit in readout noise, future experiments probing higher 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 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. Over the next 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 Outreach and the Lederman Science Center support students and faculty in STEM education and the DOE WDTS mission.

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. Together, these supported more than 3,700 users in FY 2019. 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 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 Booster neutrino beam and the high-energy NuMI beam) that enable the physics programs of the NOvA and MicroBooNE experiments. The Booster neutrino beam will deliver neutrinos to all three detectors of the Short-Baseline Neutrino program: MicroBooNE (already operating), ICARUS (starting 2020) and the Short-Baseline Near Detector (SBND, starting 2020). 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 that enables detector R&D tests with high-energy hadron beams and is used by more than 200 international researchers annually. The Irradiation Test Area (ITA) was taken from construction to being ready for commissioning between December 2019 and April 2020.

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 Large Hadron Collider (LHC) in Geneva, Switzerland. Fermilab also leads the HL-LHC CMS Upgrades, 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 upgrades to the CMS detector. 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 and 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 in 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 specific analysis projects. A number of new ideas leading to CMS and phenomenology publications originated through these close interactions.

Advanced Instrumentation

An experienced and talented workforce at Fermilab 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 recommendations of the 2015 HEPAP Accelerator R&D sub-panel: 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 University of Chicago. 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 upgrades to the complex 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 and is needed as the next step to achieving a beam power of more than 2 MW for LBNF/DUNE and beyond. Results from accelerator R&D at Fermilab 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 around $2x10^{17}$ protons per hour from the proton source to support the Short-Baseline Neutrino program and the Muon g-2 experiment.

High-Power Target Stations

Fermilab operates three high-power target stations: the 700+ kW NuMI beam (to be upgraded to 1 MW); the Booster Neutrino Beam; 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 the LBNF and DUNE projects. 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. Fermilab also executes a high-power targetry (HPT) R&D program directed at the challenges of future multi-MW target facilities. The laboratory leads the international RaDIATE collaboration researching new radiation- and thermal-shock-compatible materials and technologies. To ensure Fermilab's core competency in targets evolves to sufficiently support multi-MW operation, the HPT R&D program is launching a targetry materials science and technology initiative to create the needed infrastructure (expertise, equipment, and facilities).

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, is 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, its 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 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, 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 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 Accelerator Science and Technology section.

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: Quantum chromodynamics (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 the country's particle physics and accelerator laboratory, Fermilab is moving forward with new experiments, new 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. Serving as an effective host laboratory for the Long-Baseline Neutrino Facility (LBNF) and Deep Underground Neutrino Experiment (DUNE), powered by megawatt beams from an upgraded and modernized accelerator complex made possible by the Proton Improvement Plan II (PIP-II) project; solidifying existing and attracting new international engagements; and advancing accelerator and quantum science and technology are major initiatives in the coming years.

Fermilab's scientific vision builds on six main 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
- Be at the forefront of large-scale data analytics
- Become a national center for quantum science and technology

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) program. The Fermilab Accelerator Complex is DOE/SC's national science user facility at the laboratory. Fermilab employees include scientists and engineers from around the world who work together with the international user community to use the laboratory's scientific infrastructure for their research. The laboratory's infrastructure is evolving to support the significant requirements of the international LBNF, DUNE, and PIP-II projects and planned R&D program.

All real property at Fermilab in Batavia, Illinois is used and owned by DOE. Much of the real property dates from the 1960s and 1970s. In addition, DOE has a 22,155 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 2019, there were no new leases, renewed leases, leased disposals, gifts or third party financed projects. There are plans in development for a future hostel supported by third party financed projects in the early 2020s. The total Replacement Plant Value (RPV) for conventional facilities is $1.24B. The total RPV including programmatic accelerator and tunnel assets (OSF 3000) is $2.44B. Property use is predominantly comprised of R&D and administrative areas. Other land is preserved for future science by maintaining it as restored prairie, tilled agriculture, or woodland.

Fermilab is providing 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 added project office space in a leased area and is working in concert with SDSTA to improve infrastructure and construct underground detectors and support systems for LBNF and DUNE.

The Fermilab Campus Master Plan is being reevaluated in FY 2020 to ensure it supports the implementation of the laboratory's strategic plan and major initiatives. Executing the plan requires investment in demolitions to reduce the laboratory's excess facility operating burden. In FY 2019, overhead funds were used to complete demolitions totaling 5,014 GSF. Three trailers (1,362 GSF) were also archived in the DOE Facility Information Management Systems (FIMS). In FY 2019 Fermilab added one building to FIMS. There are currently no demolitions scheduled in FY 2020. Future demolitions will be included in strategic laboratory budgeting and project proposals to ensure a continued reduction in operating burden and risk.

The Laboratory Operations Board (LOB) infrastructure assessment in FY 2014 helped establish Fermilab's foundational strategy for facilities. In FY 2019, Fermilab revised its process to identify and prioritize current and future infrastructure needs. The process created an integrated prioritized list of infrastructure project needs that will be executed as funding becomes available. This integrated list of more than 125 infrastructure projects includes projects that directly support and/or enhance either: the laboratory's scientific mission; the reliability of lifeline infrastructure such as water, sewer, and electrical distribution systems; the modernization of laboratory workspaces; or security of the laboratory. Potential funding sources for each infrastructure project are also identified.

During FY 2019, the laboratory also made progress in implementing several new initiatives including:

- Advancing Fermilab's pilot program to centralize facility management
- Establishing a $314M Utilities Infrastructure Project (UIP) that builds on the success of the $36M Utilities Upgrade Project completed in 2018
- 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

Types and Conditions of Facilities

A detailed reassessment of all facilities and structures has resulted in an overall increase of substandard and inadequate classifications. If the UIP was fully funded, the four OSF projects reported as inadequate would be rectified. The evaluation and utilization of existing facilities, along with deferred and annual maintenance costs, are shown in the table below that was generated from FIMS data.

	Structures				Utilization				Maintenance	
Types of Facility (Usage Codes)	**Adequate**	**Inadequate**	**Substandard**	**Total**	**90-100%**	**75-89%**	**50-74%**	**0-49%**	**Deferred**	**Annual**
Laboratory/Experiment Buidlings (711, 721, 723)	20	9	3	32	32	--	--	--	$287,141	$2,166,250
Accelerator (785, 3221)	50	4	--	54	54	--	--	--	$2,017,142	$2,148,986
Office Buidlings (101)	16	17	11	47	43	1	--	3	$2,774,202	$2,323,308
Operations Buildings (291, 297, 551, 561, 591, 601, 611, 614, 621, 641, 642, 693, 694, 6271, 6719, 7009)	29	13	9	51	51	--	--	--	$4,868,367	4514512
Storage Buildings (400, 401, 410, 4020, 4010, 4171, 4500, 4221)	87	36	11	141	118	6	6	11	$292,164	$703,658
Residential Buildings (300,691)	61	1	1	63	62	--	--	1	$228,078	$509,178
Other Building types (234,294, 295, 298, 644, 801, 2449, 2909)	21	--	3	24	17	6	--	--	$71,821	$190,590
Utility Infrastructure (508, 525, 531, 595, 5171, 5569, 5789, 5906, 6919, 7261, 8129, 8131, 8171, 8329, 8549, 8561, 8629, 8719, 8929, 8939, 8949, 8979)	13	4	8	25	25	--	--	--	$22,080,806	$2,703,233
Roads and Walkways (1129, 1168, 1729, 1739, 1749, 1769, 1789)	6	--	4	10	10	--	--	--	$4,512,824	$445,773
Culverts, Dams, Fences (2429,2629,2819,2619)	4	--	--	4	4	--	--	--	$208,546	$123,836
Total	**307**	**84**	**50**	**451**	**416**	**13**	**6**	**15**	**$37,341,091**	**$15,829,324**

The table indicates that, of the 416 structures operating at or near 100% utilization, 109 are inadequate or substandard. Office buildings (FIMS-101) are nearly all utilized at 100% despite being in a degraded condition. Of the 47 office buildings on site, 28 of them are either inadequate (17) or substandard (11) with $2.8M in deferred maintenance. Laboratory and experimental spaces (711, 721, 723) have $0.3M deferred maintenance and 12 of 32 buildings in inadequate (9) or substandard (3) condition. The accelerator complex buildings (785, 3221) are proportionally better with only 4 of 54 inadequate but have a balance of $2M in deferred maintenance. The laboratory's infrastructure priorities align with these needs, targeting utilities and systems (CUB, UIP, ACORN), laboratory and office spaces (IERC, CAST, Wilson Hall), and general supporting infrastructure (sanitary sewer improvements).

As the laboratory completes the condition assessment of site infrastructure initiated in FY 2019 and implements centralized facility management beyond the pilot program, the level of substandard and inadequate facilities is expected to grow for two reasons. First, the detailed facilities and infrastructure assessments will likely lead to increases in substandard and inadequate levels due to a new understanding of extent of condition that goes beyond fault and repair history. Secondly, centralizing facility management will increase management efficiency and provide more accurate facility investment planning and reporting. These centralized facility management planning and reporting mechanisms are consistent with the Safeguards & Security Program and are inherently reliant on the Design Basis Threat (DBT) and Science and Technology (S&T) Policy requirements. The current Science and Technology (S&T) Matrix review process is a fluid practice and allows for the future scalability of S&T implementation needs.

Campus Strategy

The laboratory is focusing on three campus infrastructure objectives: improving sustainment and resiliency of existing assets; recapitalizing or dispositioning overaged, obsolete, and severely deteriorated components of the laboratory's infrastructure; and constructing new infrastructure to close identified infrastructure gaps. Fermilab's infrastructure planning and investment strategy addresses these three objectives and ensures Fermilab will continue to provide modern, world-class facilities for scientific research.

Planning infrastructure improvements is a core function of the laboratory's Campus and Facility Planning Board which identifies, coordinates, prioritizes, and communicates facilities projects to support future/major initiatives identified in Section 4. The following infrastructure gaps carry the risk of impacting one or more core capabilities. This planning process has developed solutions which will close infrastructure gaps as noted in the following table:

Infrastructure Gaps by Core Capability and Mission Objective

	Core Capability						
Infrastructure Gap	Accel. Science & Technology	Advanced Computer Science	Particle Physics	Large Scale User Facilities	**Core Capability Risk**	**Impact if not closed & when**	**Proposed Solutions (with lab ranking)**
Target and Horn Production Facility	x		x	x	Global leadership in neutrino science	Challenge to meet beam delivery expectations for planned R&D and the inability to meet DUNE schedule in FY22 if not started in FY21	Target Systems Integration Building (TSIB) expansion (1)
Beam Operating Infrastructure	x		x	x	Effect timely operation of the beamline with the new LINAC	Required to operate beamline when PIP-II is complete, estimated in FY25, requires start in FY21	Accelerator Controls & Infrastructure Support (ACORN) (2) Main injector cooling pond/cooling tower upgrade (14) Cross gallery modernization (19) MI vertical buss penetration revitalization (22) Transfer gallery 2nd floor renovation (26) Main injector sump line (29) MI-60 renovation (31) Upgrade return ICW line or PIP-II (33)
Underground Utilities	x	x	x	x	Sitewide risk from various systems, including industrial cooling, domestic water, and sewer, etc.	Limited capability or shutdown of areas as they are affected	Centralized Utility Building Upgrade (3) Core campus water Improvement (4) Sanitary System Improvements (5,6) Sitewide domestic water renovation (32) Sitewide electrical distribution substations (36,38) *The Utility Infrastructure Project (UIP), if fully executed, will address most of the underground utility gaps*
Building Structural Reliability	x	x	x	x	Degraded capability takes an increasing toll on operations. An incident would have a major impact on all operations	Degradation will continue until mitigated	Wilson Hall Envelope, Windows, and Utilities Projects (7,8,9) Sitewide demolition program (20) Revitalize Proton Assembly Building (23) Meson detector building roof (30) Modernize the daycare facility (39) Heavy Assembly Building 2nd floor buildout (40)

Safety and Security Infrastructure	x	x	x	x	Areas below standard thresholds for safety and security	Operating at increased risk of incident	2nd road to Neutrino Campus (10) S&T Matrix Security Projects (11) Pine Street entrance & guard house (16) Radiation Waste Storage facility (27) Sitewide indoor & outdoor lighting upgrades (37,38)
Production Facilities	x		x	x	Cryomodule and component production rate	Inability to meet demand of major 413 projects, including PIP-II	Technology Campus Industrial Buildings Revitalization (12) Consolidated Fabrication Facilities (13) Technology Campus ICB-A buildout, IB2 addition, and Industrial center gateway (18,19,22)
Quantum Science & Technology Facilities		x	x	x	Lack of available facilities for burgeoning requirement	Lost opportunities on the forefront of quantum science	Build up experimental space for FQI (15)

The Center for Accelerator Science and Technology (CAST) building and Integrated Engineering Research Center (IERC) projects will help to fill gaps. Many of the gaps identified in the table above include features associated with centralized space for scientists, engineers, and supporting staff. The current lack of a modern, efficient, centralized space for accelerator scientists and key mission support staff reflects an infrastructure gap. The CAST is envisioned as a mission-driven improvement that will transform the laboratory's core capability of accelerator science and technology in support of the P5 Plan. Executing the plan requires new or modernized laboratory space, offices, and collaborative work environments for accelerator operations, R&D, and training the next generation of accelerator scientists and engineers. Similarly, the IERC project, currently under construction, will further address the current lack of a modern, efficient, centralized space for collaborating staff in the laboratory's central campus by providing state-of-the-art spaces for the engineering and research communities. For example, in the near term, IERC will provide space for assembling, testing, and characterizing prototype particle detectors for DUNE in laboratory space that without IERC would not be available at Fermilab.

Sustainment

Fermilab is targeting investment improvements for sustainment of site infrastructure. Over the last three years the laboratory's annual maintenance and repair (M&R) spending has fallen consistently below DOE's recommended two to four percent of the laboratory's overall Replacement Plant Value (RPV) which is today's cost to replace an asset. The laboratory is working to adjust future financial plans to achieve the recommended two to four percent M&R spending level.

In FY 2020, Fermilab began updating the facility condition assessments that will, over time, provide a more accurate measure of facility condition. Combined with existing facility maintenance and repair records, the assessment data will be used to balance resources and improve risk-based planning and investing.

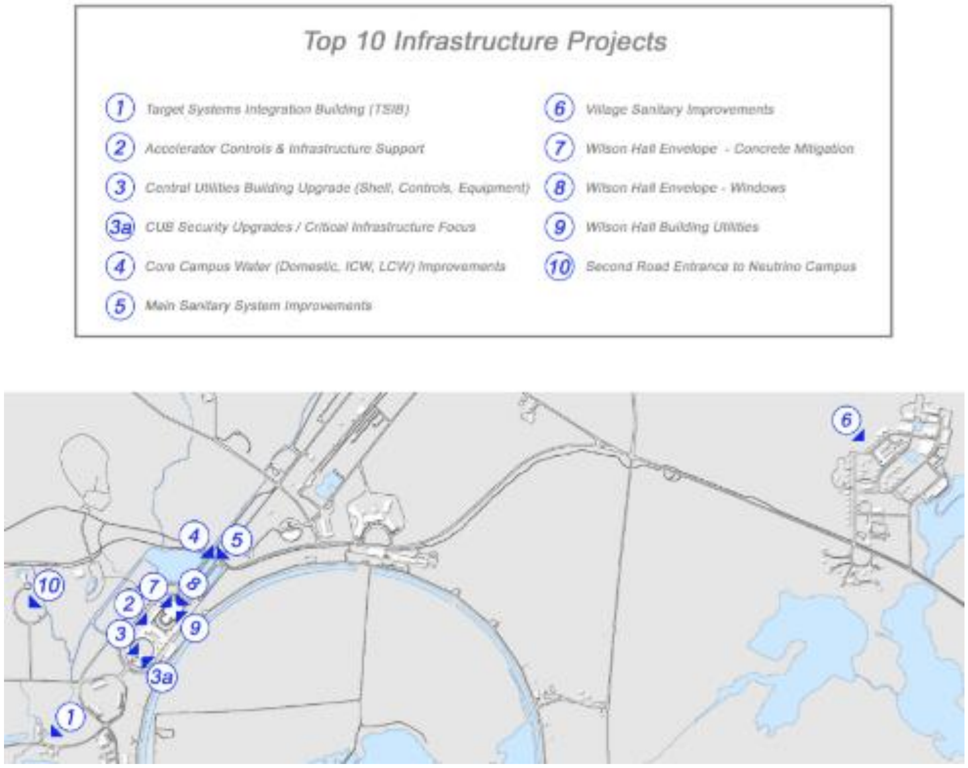
Finally, the laboratory continued to execute a pilot centralized facility management program with plans to roll out lab-wide in FY 2021. The program will adopt best practices, share resources, drive consistency, achieve efficiencies of scale, enable a lab-wide risk-based investment strategy, and enable more accurate facility investment planning and reporting. The success of the centralized facility management program is the integration of systems, personnel, and equipment. The enhanced technology use of safety and security monitoring devices by a central facility will tie critical infrastructure needs to the real time alarm, video, and access control data that is collected by the Fermilab Security Operations Center.

Recapitalization and New Construction

Fermilab has built a 10-year strategy to achieve the objectives of recapitalizing or dispositioning overaged, obsolete, and severely deteriorated aspects of the laboratory's infrastructure, and constructing new infrastructure to close identified infrastructure gaps. The strategy is comprised of 120+ prioritized infrastructure projects that directly support and/or enhance either: the laboratory's scientific *mission*; the *reliability* of lifeline infrastructure such as water, sewer, and electrical distribution systems; the *modernization* of laboratory workspaces; or *security* of the laboratory. Potential funding sources for each infrastructure project have also been identified. The current prioritized Top 10 List of infrastructure needs is shown below.

Project ID	Project Elements	Cost ($M)	Start By FY	IWG Score (value between 0-12)	CFPB Rank	Director's Rank	Quad Chart Owner
20AD041	Target Systems Integration Building (TSIB)	10.0	22	11	10	1	AD
20AD011	Accelerator Controls & Infrastructure Support	140.0	20	12	1	2	AD
20FE021	Central Utilities Building Upgrade (shell, controls, equipment)	90.0	20	11	2	3	FE
20FE02C	CUB Security Upgrades / Critical Infrastructure Focus	0.75	20	11		3a	ESH
20FE01A	Core Campus Water (Domestic, ICW, LCW) Improvements	5.0	24	12	3	4	FE
20FE04B	Main Sanitary System Improvements	9.0	21	10	4	5	FE
20FE04A	Village Sanitary Improvements	3.5	20	9	5	6	FE
20FE10B	Wilson Hall Envelope - Concrete Mitigation	10.0	20	7	6	7	FE
20FE10C	Wilson Hall Envelope - Windows	30.0	20	7	7	8	FE
20FE10E	Wilson Hall Building Utilities	18.0	21	7	8	9	FE
20FE08D	2nd road entrance to neutrino campus	3.0	20	11	9	10	FE

A map showing the locations of the top ten infrastructure projects is provided below.



Laboratory infrastructure projects and goals have been influenced by several initiatives that were identified and instituted in FY 2019 including: the centralization of facility management, strengthening the strategic assessment of the condition of facilities, establishing a Utilities Infrastructure Project (UIP), and maturing facilities processes and procedures to extend facility lifecycles and improve resiliency. Specifically, the laboratory is targeting resiliency when planning infrastructure projects. The intent is to add redundancy and flexibility where feasible to improve uptime and reduce frequency of emergency repairs. This would be accomplished with a combination of additional redundant interconnects and intelligent control features that would prioritize critical functions when support systems were under duress.

Site Sustainability Plan Summary

In FY 2019, the laboratory continued to execute a sustainability strategy anchored by the Fermilab Site Sustainability Plan and the Fermilab Campus Master Plan. These plans identify sustainability as a core laboratory value and list specific initiatives to improve sustainability performance in future years. In FY 2019, Fermilab committed significant resources to plan for capital facility and infrastructure improvements which will have lasting site sustainability performance impacts. Two major infrastructure projects valued at more than $700M were proposed to DOE; the Fermilab Utilities Improvement Project reached CD-0 in FY 2019 and aims to recapitalize vital infrastructure at the heart of Fermilab's core campus. A second set of projects will continue to be developed to revitalize Fermilab's core campus, including replacing sitewide accelerator controls and related infrastructure, renovating Wilson Hall, and modernizing and streamlining processes associated with Fermilab's Technology Campus.

Fermilab continued to evaluate existing buildings for potential candidacy as High Performance Sustainable Buildings (HPSB). Fermilab currently has eight buildings that meet HPSB requirements for buildings larger than 10,000 GSF (13.5 percent of total eligible). An additional seven facilities are projected to reach HPSB status contingent on DOE approvals and funding over the next several years.

As a result of the IERC construction, initiatives are in planning and underway to improve parking in the vicinity of Wilson Hall. The IERC requires conversion of some parking areas into construction or staging areas. Recent events associated with containment of the COVID-19 virus have significantly increased the level of telecommuting by laboratory staff, and sustainment of somewhat expanded telecommuting may create opportunities for the laboratory to reduce the demand for parking and dedicated office space for individuals and also contribute to a reduction of the laboratory's carbon footprint.

Examples of sustainability progress that support Fermilab's ability to deliver on its mission in the past year include:

- A new facility was completed in FY 2019; the Industrial Center Building Addition includes a high-bay space and adjacent workspaces and achieved HPSB status.
- Fermilab completed a "cold and dark" exercise for a former industrial Central Helium Liquefier facility. This exercise eliminated the energy wasted by heating, cooling, and lighting an unused facility. It also formalized a process to prepare significant industrial buildings for excess.
- A revitalized Campus and Facility Planning Board developed a new process to identify and prioritize capital infrastructure improvement needs. The prioritization process includes consideration for energy and cost savings.
- Fermilab established a new partnership with the natural gas utility provider to conduct audits of several site buildings and identify energy conservation measures.
- For the tenth consecutive year, Fermilab's Grid Computing Center was awarded Energy Star status.
- The Fermilab bicycle sharing program was fully implemented in FY 2019 with additional bicycle rack locations installed. Two bicycle fix-it stations were also installed in FY 2019 that provide bicycle commuters with a means to make minor repairs while cycling on-site.
- The Utilities Infrastructure Project is developing scope that would monitor and react to changing weather patterns, automatically transfer power in response to abrupt changes, and remain scalable for future growth to strengthen the resiliency of the site's critical infrastructure.

LAWRENCE BERKELEY NATIONAL LABORATORY

Lab-at-a-Glance

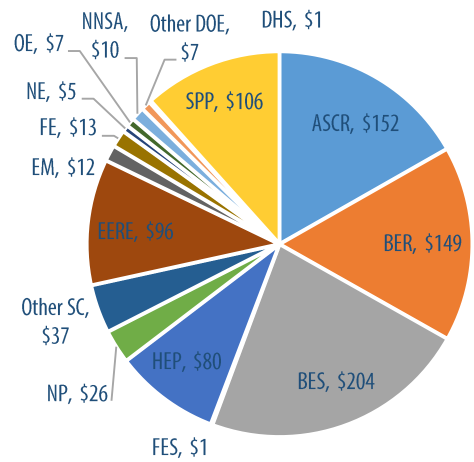
Location: Berkeley, California
Type: Multi-program Laboratory
Contractor: University of California
Site Office: Bay Area Site Office
Website: www.lbl.gov

- **FY 2019 Lab Operating Costs:** $907.07 million
- **FY 2019 DOE/NNSA Costs:** $800 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $105.68 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 11.7%
- **FY 2019 DHS Costs:** $1.40 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 2019 Costs by Funding Source ($M)



Mission and Overview

Established in 1931, Lawrence Berkeley National Laboratory (Berkeley Lab) plays 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 developing technologies needed to address national challenges such as energy resilience and sustainability, health, environmental quality, and economic competitiveness.

Berkeley Lab specializes in integrative science and technology, taking advantage of our world-renowned expertise in materials, chemistry, physics, biology, environmental science, mathematics, and computing. We advance the frontiers of science and technology through three approaches: advanced instruments and user facilities, large team science, and core research programs led by outstanding investigators. These three approaches are closely integrated to the benefit of DOE's entire research mission.

Berkeley Lab's mission, to bring science solutions to the world, runs deep within the organization. Our five national user facilities provide nearly 14,000 researchers with capabilities in high-performance computing and data science, chemical sciences, materials synthesis and characterization, and genomic science. The Lab's scientific strength is built upon its breadth of basic and applied science and its emphasis on collaboration with the national scientific community. We have robust partnerships with other national laboratories on a wide range of projects from subatomic physics to quantum information, biomanufacturing, environmental biology, and innovative energy technologies.

Berkeley Lab's close relationship with the University of California brings the 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 find innovative ways to use 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 Berkeley Lab's 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, Berkeley 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. ALS researchers 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 FY19 the ALS had 2,170 users (1,725 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 ~$67 million.

The Molecular Foundry provides communities of users worldwide – 1,346 in FY19 (1,011 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 13 years ago, the Foundry's reputation as a world-leading center attracts expert scientists from around the globe to do cutting edge research. In FY19, the Foundry received user proposals from 33 states and 27 countries, and published 388 peer-reviewed publications, 31% of which were in high impact journals. 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.

The ***DOE Joint Genome Institute (JGI)*** is a national user facility carrying out projects of central relevance to DOE missions in alternative energy, 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 a strategic focus on functional genomics that includes a growing DNA design and synthesis program. It has over 1,900 capability users and over 8,500 active data users per year; its FY19 budget of ~$71 million is funded primarily by BER. In FY18, the JGI developed a strategic vision for integrative and collaborative genome science. The recently-released plan lays out JGI's 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.

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. With the broadest workload of any computing facility, NERSC also has a responsibility to transition the DOE SC user community to exascale-era platforms. This transition began with NERSC's current premier system, "Cori" (NERSC-8) which uses an energy efficient many-core architecture. The Perlmutter (NERSC-9) system, which is scheduled to be available to users in FY21, will continue the transition by introducing GPUs to the broad SC user community. In 2015, NERSC launched the NERSC Exascale Science Application Program (NESAP) that helped achieve an average of 3x speedup on a portfolio of over 20 DOE SC applications. NESAP has now changed its focus in order to help application teams accelerate codes to run efficiently on Perlmutter. In less than a year, NESAP has enabled six key SC applications to achieve a speedup of more than 16X using GPUs on a NERSC development system, compared to performance on NERSC's Edison (NERSC-7) system. One example is a 25X speedup on the tomographic reconstruction code Tomopy used by researchers at the ALS and at Argonne's Advanced Photon Source. A growing part of NERSC's workload derives from the data analysis requirements of DOE SC's experimental and observational facilities such as light sources, telescopes, accelerators, sequencers and sensors and supporting these new requirements has been a key focus at 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 machine learning and deep learning frameworks to take advantage of HPC scale resources. The Perlmutter system will be the first NERSC system to be designed from the start with large scale simulation and data analysis in mind and will build on many of the capabilities deployed and developed for the Cori system. NERSC's scientific impact is enormous: more than 2,000 scientific publications cite NERSC each year. In 2019 alone, its current systems, Cori and Edison (which was retired n May 2019) provided more than eight billion computational hours to researchers. NERSC's FY19 funding was $105 million, provided by ASCR.

The Energy Sciences Network (ESnet) is the Office of Science'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 world's 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 FY19, ESnet completed a successful design review for ESnet6, a strategic facility project to upgrade its network to meet the increasing data needs of science. In addition, after successful execution of CD-1/3A in FY19, it executed on its 3A Long Lead Procurement (LLP) and prepared and achieved CD-2/3. ESnet is revamping its requirements review process across the SC program offices. ESnet's FY19 funding was ~$84M (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 the determination of 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 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 lab partner for the DOE Energy Innovation Hub devoted to the development of new photoelectrochemical approaches to fuel production, the Joint Center for Artificial Photosynthesis (JCAP).

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.

Other program components provide the capability to translate fundamental research in catalysis, chemical kinetics, combustion science, hydrodynamics and nanomaterials into solutions to technological challenges in energy storage and subsurface energy. 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, focusing on the development of 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 fossil energy, biofuels, and carbon capture and storage.

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, Berkeley Lab is 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, Berkeley Lab has 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. Berkeley 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. Berkeley Lab 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, Berkeley 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 Joint Center for Energy Storage Research (JCESR) 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. The Lab is a key partner of this hub, which is led by ANL.

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. Two LDRD projects are addressing materials sciences challenged relevant to energy-efficient microelectronics as part of the Lab-wide initiative in this area.

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. Berkeley Lab's geoscience 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. Researchers in this group 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 processes using acoustic and electromagnetic methods. In partnership with the ALS, Berkeley Lab 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 geoscience researchers to discover the molecular-scale mechanisms of fluid-rock processes and translate molecular- and nano-scale insights to larger-scale models and capabilities. Historically, three fundamental geoscience programs at Berkeley Lab have been funded by the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division—in geochemistry, isotope geochemistry, and geophysics. These groups are now integrated and working to develop a flagship geosciences group that will be unique in the United States. This exciting effort will catalyze collaborations among the disciplines and the expertise needed for rigorously understanding how coupled processes change the properties of rock-fluid systems in response to stress and reactive fluids and solutes. The capabilities that are united in the new geoscience group include molecular simulation methods; dielectric–to–X-ray spectroscopies for aqueous solvation, ion transport, and reaction; stable isotope probes of mineral reactions; methods for imaging fracture creation and evolution across scales; laboratory mechanical measurements; and the geochemical and geophysics theory and simulation required for data interpretation and new model development. While the geoscience program is becoming integrated, all CSGB program leads at Berkeley Lab are working together to develop a unified vision, and to promote synergy and knowledge transfer across the Chemical Sciences, Geosciences, and Biosciences groups.

Translation of fundamental knowledge to increasingly accurate subsurface models is a cross-cutting goal and one that ultimately requires the use of high-performance computing. Berkeley Lab leads the only two subsurface exascale application projects in the complex. The subsurface 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 EQSIM project will leverage emerging DOE exascale computers to increase the accuracy of assessments of earthquake hazard and risk by simulating for the first time, in a fully coupled approach, the regional-scale effects of strong ground motion on critical infrastructure response. The ability to understand the regional distribution of ground motions and resulting infrastructure risk is essential to the design of spatially distributed infrastructure such as energy transmission and transportation systems.

The Lab's applied subsurface portfolio is supported by EERE-Geothermal, FE Clean Coal, FE Oil & Gas, NE Spent Fuel and Waste Disposition, and by several significant SPPs. 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. Unlike other scientific fields where the bulk of the research can be explored in the laboratory, 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, Berkeley Lab has developed and is conducting significant research at several field-based subsurface energy test facilities. For example, Berkeley Lab's 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. This year, Berkeley Lab also initiated the Community Geothermal project focused on integrating low temperature geothermal energy and subsurface energy storage techniques directly with the needs of communities and the built environment.

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 hydrocarbon recovery. Berkeley Lab continues to be instrumental in understanding relevant processes in gas production from gas hydrate, and in developing tools for assessment of production methods from hydrate resources. Berkeley Lab also participates in field-based research at the new Eagle Ford Unconventional Testbed in Texas and leads a collaborative multi-national lab modeling and laboratory project evaluating shale stimulation that occurred in the Hydraulic Fracturing Test Site in the Permian Basin in Texas. The Lab's FE Clean Coal research focuses on enabling an effective transition to a clean energy future. Key aspects include pairing fossil energy use with carbon sequestration at scale, evaluating carbon sequestration risks through DOE's National Risk Assessment Partnership (NRAP) program, and developing advanced monitoring and accounting solutions and testing them at various demonstration sites such as the Decatur project in Illinois, and at the Aquistore site in Canada, or the Otway site in Australia. 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. LBNL is also assisting 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 developing machine learning techniques to interpret and manipulate reservoirs in real time. Currently, the emphasis of SMART is on CO_2 sequestration, but future emphasis will also include oil and gas applications. Finally, through NE research, Berkeley Lab is developing advanced approaches to enable safe long-term geologic disposal of nuclear waste and concomitant environmental protection.

Complementary to the DOE-supported research at Berkeley Lab are several significant new projects awarded by the California Energy Commission, including new approaches to monitor and evaluate risks associated with natural gas storage (such as the risks to natural gas pipelines arising from land subsidence or seismicity), development of tomographic imaging methods for geothermal reservoirs, evaluation of the feasibility of flexible geothermal energy production, and the development of networked observational systems to quantify methane fluxes from energy infrastructure using aircraft, towers, and intensive ground-based sensors.

Berkeley Lab's 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 and work with the DOE, the State of California, local governments, and local stakeholders on a number of critical infrastructure challenges. In a major effort supported by the 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 with tight coupling to new computational models for predicting the nonlinear response 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, with widespread applicability to the vast DOE enterprise and DOE sites, and spin-off applications to other sectors (e.g., energy, water, transportation). For example, a new project supported by DOE's Office of Energy uses these advanced simulation capabilities to assess hazard 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 utilizes unused telecom fiber optics cables, referred to as "dark fiber," to achieve spatially unparalleled acoustic sensing and ambient noise tomography in urban settings, and another focuses on upgrading hundreds of thousands of its smart electric and gas meter components in homes to include an acceleration measurement capability. Lab scientists have also developed and experimentally-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 technologies and tools can impact a wide range of infrastructure systems such as 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. Berkeley Lab's growing suite of fabricated ecosystem platforms is enabling new environmental biology research with unprecedented ability to predictably and reproducibly establish, monitor, and perturb laboratory ecosystems at multiple scales.

Biological and Bioprocess Engineering. Berkeley Lab's strengths in biological systems science are complemented by its unique capabilities for biological and bioprocess engineering to translate fundamental science discoveries to use-inspired solutions for energy and environment. The Lab has 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, and NERSC, and projects like ENIGMA, the Lab can develop the new technologies and processes needed to create renewable fuels and chemicals, remove environmental contaminants, and support biosequestration of carbon.

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, and demonstrated 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. 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 FY20, the ABPDU signed its 50th contract for process development with the mycelium leather company, Mycoworks. 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 national laboratory system; 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 continuously 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 FY20 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. The JGI offers a suite of capabilities that are unique in their ability and scale to advance energy and environmental science. Having evolved beyond a production sequencing facility, the JGI now 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 resources at LBNL IT 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 IT would enable JGI to meet this gap. To further address scientific productivity as well as organizational resilience, JGI is exploring the development of a distributed software and hardware infrastructure that will include hardware at non-Berkeley Lab sites, as well as the commercial cloud. 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.

The DOE Systems Biology Knowledgebase (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. The goals of this partnership are to 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, JGI and KBase have worked closely over the past year to develop systems within KBase, and hosted at NERSC, that allow users to import JGI public data sets, as well as JGI tools and pipelines. JGI and KBase have built working prototypes for both genome and gene homology services, and will focus on beta testing these products with their joint user community in FY19. JGI and KBase have accelerated efforts to integrate JGI tools into KBase and have now integrated the JGI metagenome assembly pipeline and metagenome binning tools into KBase. Access to JGI data in KBase has been simplified, and high-value datasets like Phytozome and Mycocosm have been imported into KBase. Further datasets are under consideration for importation.

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 their practice of hosting joint outreach activities and booths and holding 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 nascent National Microbiome Data Collaborative also provides critical support through leveraging existing resources, unique capabilities, and expertise across our four DOE 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 Pilot (27-month pilot, July 2019 - September 2021) has established a collaborative framework for coordinated integration of multi-omics data generated at the flagship DOE User Facilities, the JGI and PNNL's Environmental Molecular Sciences Laboratory (EMSL). The NMDC focuses on developing 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 high-performance computing systems, in particular NERSC, to provide an unparalleled integration of multi-omics data for DOE mission-relevant environmental microbiome research.

ENIGMA (Ecosystems and Networks Integrated with Genes and Molecular Assemblies) is the multi-institutional Berkeley Lab-led BER-funded SFA that advances understanding of microbial biology and the impact of microbes on their ecosystems. By linking environmental microbial field studies to powerful meta-functional genomic and genetics tools, the identity and diversity of microbes along gradients of geochemical parameters are being understood, enabling predictions of how environmental perturbations may affect microbial community structure and their ecosystems. ENIGMA's computation efforts are aimed at integrating diverse, complex, large datasets for studies of dynamic modular microbial architectures across scales, from single cells to full community assemblages.

A collaborative, coordinated, and integrated mission-driven SFA, mCAFES (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. The project targets molecular mechanisms governing carbon and nutrient transformation in soil, with a focus on microbial metabolic networks, and seeks to understand 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, giving researchers the ability 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, mCAFES and TEAMS (Trial Ecosystems Advancement for Microbiome Science). EcoPODs, currently being developed at Berkeley Lab, are enclosed environments of several meters cubed 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 system beyond UC Berkeley. For example, the JBEI partners include UC Davis, UC Santa Barbara, UC San Diego, and the UC Agriculture and Natural Resources in addition to UC Berkeley. The JGI and UC Merced partnered to establish the Genomics Distinguished Graduate Internship Program. In February 2020, 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 researchers at UC San Diego 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 2018, a new DOE-BER ECRP project was awarded that focused on advancing knowledge of plant cell walls, to enhance deconstruction and conversion into fuels and other bioproducts by microbial fermentation. This project builds upon research carried out in BER-CESD and connects climate relevant plant volatile emissions to biochemical roadblocks of biomass deconstruction, seeking to understand and manipulate these cell walls. The project will not only provide important knowledge on the physiology and ecology of plants but will also allow the generation of engineered bioenergy crops such as poplar for sustainable production of biofuels and bioproducts, addressing BER's goal of developing renewable bioenergy resources.

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 mechanistic understanding of and data-modeling tools to predict watershed hydrobiogeochemical function from genome to watershed scales, including process coupling occurring across bedrock through canopy and terrestrial through aquatic interfaces, and along significant environmental gradients. 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. As soil-microbe-interactions play a key role in water and biogeochemical cycling, the Watershed SFA is an anchor tenant of BioEPIC and prototype components of the new BioEPIC platform technologies, such as the EcoSENSE SMARTSoils testbed, are being developed to enable the Watershed SFA goals in sensing-data-model integration for hydrobiogeochemistry. Lab scientists co-led a DOE-BER community workshop that crossed government agencies and multiple stakeholder groups with common challenges in understanding complex watershed systems across local to continental scales. The workshop report maps out a strategy for Open Watershed Science by Design.

To improve prediction of future watershed function, a range of HPC and AI approaches are being developing, which includes a first-of-a-kind scale-adaptive modeling approach to simulate hydrological and biogeochemical dynamics using variable and dynamic resolution and testing a new 'functional zone' approach to predicting aggregated watershed exports. Adaptive mesh refinement and other physics-based simulation capabilities are being developed for watersheds through the multi-institutional Interoperable Design of Extreme-Scale Application Software (IDEAS) and ExaSheds projects, both funded by BER. The new ExaShed effort is making advances in hybrid physics and machine learned based approaches so as to dramatically improve our watershed system modeling capacity. The new 4D Digital Watershed sensing and numerical capabilities are being used to discover and predict how watersheds and their subsystems respond to variations in both the amount of snowpack and the timing of snowmelt, as well as the interplay among weather, water supplies, biogeochemistry, and energy resources. A new BER ECRP is investigating the impacts of streamflow disturbances such as floods and droughts on water quality using data-driven methods that include a data integration tool built for the Watershed Function SFA (BASIN-3D) and several machine learning techniques for classification and prediction.

Expertise and capabilities associated with monitoring and predicting hydrobiogeochemical watershed dynamics developed through BER-CESD 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 support from ARPA-E's "ROOTS" program, we are developing new root imaging and modeling approaches that may lead to a new paradigm for remote field phenotyping of plant roots and other applications. A new ARPA-E award has been made to the lab to develop machine learning approach for accurate carbon accounting during bioenergy feedstock productions. The Lab is using advanced methods to quantify the potential of the subsurface for storing water during dry years, and for manipulating agriculture sites for co-benefits to crop yield and soil health. With EM support, Berkeley Lab is developing a new paradigm of long-term monitoring of DOE's legacy contaminated sites, using the Savannah River Site as a testbed. The aim is to take advantage of the recent advances in *in situ* sensors and machine learning approaches for developing cost effective monitoring and early warning systems, as well as HPC capabilities for reactive transport modeling for predicting the future efficacy of proposed long-term strategies. The Lab also collaborates with the Japanese Atomic Energy Agency (JAEA) and other institutions on advanced modeling and data analytics important to support Fukushima's remediation and rehabilitation effort. In particular, the developed multiscale data integration software BDARM (Bayesian Data Assimilation for Radiation Monitoring) has been released as an open source software and adopted by JAEA for the standard method for radiation dose rate mapping based on a variety of radiation survey datasets. In a first attempt to take a watershed perspective toward understanding fire-water linkages, DOE-BER developed capabilities are being used and extended through UC 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 monitoring fire-water challenges. LDRD investments are extending BER-developed insights about coupled biological-environmental-climate systems to advance machine learning and systems approaches for predicting the onset of harmful algae blooms and to advance approaches to estimate subsurface biogeochenmical 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 and atmospheric science. The Lab continues to make major advances in the theory governing how atmospheric convection, one of the fundamental processes governing the equilibrium of Earth's climate, will respond to further warming of the environment. The Lab has complemented this work with novel observations of how the terrestrial ecosystem serves as a critical carbon sink, and how elevated concentrations of greenhouse gases are leading to measurable increases in the atmospheric greenhouse effect. Lab scientists 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 will produce new understanding and improved predictions of belowground biogeochemistry in the soil-plant-microbial system and the role of soils in global change. The Lab leads NGEE-Tropics, focused on a predictive understanding of how tropical forest carbon balance and climate system feedbacks will respond to changing environmental drivers. NGEE-Tropics is utilizing airborne measurements before and after Hurricane Maria in Puerto Rico to quantify hurricane impacts on tropical forests, and has established collaborations with the U.S. Forest Service, NASA, LTER, CZO, University of Puerto Rico, and other university and research partners to further investigate forest impacts. The Lab is advancing a representative, process-rich tropical forest ecosystem model (Functionally Assembled Terrestrial Ecosystem Simulator (FATES)), which allows representation of physiology, growth, competition, and mortality of individual plants at scales tractable for global simulations, and thus allows a mechanistic and trait-based approach to vegetation dynamics and climate impacts on ecosystems within the DOE E3SM climate model. The Lab is 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. 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. In 2019, the team developed a distributed temperature system and electrical-resistance tomography that have provided unparalleled insights about permafrost variability; measured CO2, CH4, 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 & CH_4 fluxes; and forecast that fire and 21st century climate will double deciduous plant productivity in high-latitude regions.

Three BER ECRP projects are emblematic of Berkeley Lab's efforts to scale from microbial mechanisms to ecosystem processes. Two ECRP awardees in the Earth and Environmental Sciences Area are focused on global change impacts on soil microbiomes and their consequences for global biogeochemical cycles and atmospheric feedbacks. One awardee 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. A second BSSD ECRP awardee focuses 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 in the Biological System Science core competency, a third project focuses on advancing knowledge of plant cell wall chemical compositions, 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 BER-CESD and connects climate relevant plant volatile emissions to biochemical roadblocks of biomass deconstruction.

Berkeley Lab also leads the AmeriFlux Management Project, which measures ecosystem-atmosphere fluxes of carbon, water and energy that enable scientific and modeling advances from a network of sites maintained by partnering institutions and supported by instrumentation from the GMF. As of December 2019, the number of registered sites increased by 85 to 475, including the addition of 31 NSF National Ecological Observatory Network (NEON) sites added under a new DOE-NSF MOU. Since the beginning of phase 2 of the project in the fall of 2015, Berkeley Lab's AmeriFlux sites data were downloaded more than 114,000 times by more than 2,800 scientists from around the world, and the community of registered users grew to 6,600 members. More than 600 publications utilized AmeriFlux data in the 2019, including 10 in *Nature* journals. The AmeriFlux Management Project is currently renewed through 2020, with a significant post-award augmentation for Data Management. A renewal proposal for fiscal period 2021-2025 will be submitted to DOE in March 2020.

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, Berkeley has developed and operated the ARM Carbon Project and ARM Aerosol Observing System Infrastructure to conduct precise and accurate measurement of trace gases, contribute to multi-agency validation of satellite-based column CO_2 estimates, and 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 publication, 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 50-m 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 lifecycles—critical information for developing cloud schemes for the next generation of weather models. A recent announcement of the SAIL ARM mobile facility at the East River, Colorado, site opens the opportunity to transform observation and prediction of water cycles in complex yet critically important mountainous watersheds from the atmosphere through bedrock and to receiving waters.

Berkeley Lab is a major contributor to DOE's flagship Earth system modeling project, by 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. In order 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, allowing for future projections of US-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. The Lab is now further enhancing the treatment of terrestrial ecological processes for future release in E3SM v2 by developing enhanced fire-ecosystem modeling, land-use land-cover change in FATES which will interact with E3SM's IAM component (i.e., GCAM), and experiment 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 2019, the Lab quantified atmospheric and oceanic drivers of co-occurring hydroclimate extremes in the western U.S. by producing high-resolution large-ensemble climate model simulations and novel gridded datasets of observed precipitation extremes. 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 datas.

BER is the primary sponsor of the research in the environmental subsurface science and climate change and atmospheric science core capabilities. Others include DOE ARPA-A, AMO, EM, SBIR; University of California; California Agencies, and other SPP. 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 advanced computer science, visualization and data. 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 of significance is our work on high performance parallel I/O 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, among other sources.

The design and deployment of a highly usable, energy-efficient exascale system presents research challenges in programming languages, system software, and tools. Berkeley Lab is a world leader in programming languages and compilers for parallel machines and utilizes this experience in the design of programming models for future systems. On the Summit HPC system, the Lab's Exascale Global-Address Space Networking (GASNet-EX) communication layer show operations achieving the same or higher bandwidth than MPI for all transfer sizes, with the difference in remote-memory access performance being particularly pronounced for small messages. In addition, GASNet-EX and UPC++, which are parts of the ECP Software Technologies portfolio, are used in the ECP application MetaHipMer extreme scale genome co-assembler, and recent re-engineering of k-mer analysis to use these tools improved performance up to 5x over previous MPI on NERSC Cori. We have started two complementary efforts, QCSearch and QFAST, to optimize quantum circuits for different qubit connectivities and gate sets.

While ASCR's main focus – and ours – is on exascale technology, we have also begun to explore extreme heterogeneity, specialized architectures for edge-computing, possible new digital devices, and alternative computing paradigms such as quantum computing to address the anticipated end of transistor density scaling. For digital computing, we have focused on application-specific accelerators, and tools to model extremely heterogeneous systems allowing exploration of large complex architectural design spaces. Additionally, we have begun to explore edge-computing by designing low-power processors that can be placed on the same silicon as, or very near, a detector, offering functionality such as real-time data reduction. For quantum computing, our architecture work has focused on the design of a RISC-V based instruction-set architecture for a classical processor enabling fast and flexible control of a quantum processor.

Berkeley Lab is one of the primary developers of new capabilities in high performance parallel I/O and data-intensive visualization and analysis. Key developments include new features in the SENSEI *in-situ* visualization and analysis infrastructure, where the visualization algorithms run concurrently with simulations; more scalable algorithms to deal with increasingly larger datasets and with more complex architectures; and the ability to visualize more complex datatypes such as graphs that are evolving in time. By using innovative machine learning algorithms that exploit features such as topological invariants, lab researchers have developed sophisticated segmentation and classification pipelines for micro-CT experiments, and tools for scientific image retrieval based on pictorial similarity. Our focus on scientific data standards in the areas of neurodata and many others, provides a modern, flexible software infrastructure for extensible standardization of scientific data. 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.

The Lab is a pioneer in scalable workflow solutions for scientific data, including meta-data generation, management, curation, quality-assurance, distribution, usability, and analysis. For example, 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 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. In the related Carbon Capture Simulation for Industry Impact (CCSI2) project, Berkeley Lab was a significant contributor to the open-sourced CCSI Toolkit. 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 troubleshooting and performance-analysis tools for complex, distributed applications, such as the PERFormance Service Oriented Network monitoring ARchitecture (perfSONAR) application, which 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 also exploring 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. 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 – proactively finding performance issues by developing a nano-second precision packet telemetry system leveraging FPGAs, programmable data planes, and an innovative software processing infrastructure. We are also participating in FABRIC (whatisfabric.net), targeting 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.

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.

Applied Mathematics. Berkeley Lab has world-leading capabilities for developing mathematical models, algorithms, tools and software for high-performance computing. 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 ground-breaking research on modeling and simulation of complex physical processes, bringing the power of predictive simulation to a broad range of science areas, the invention of new mathematics to tackle the challenges of transforming experimental data from DOE's scientific user facilities into understanding, 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 details, 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 terrestrial combustion processes, to ice-sheet formation and retreat, to nuclear flames in supernovae. Adaptive Mesh Refinement techniques pioneered at the Lab are globally recognized as a key enabling technology, and Berkeley's Exascale AMR Co-Design Center has publicly released AMReX, a GPU-accelerated software framework leveraging exascale computers that supports ECP and SciDAC scientific simulation codes for combustion, astrophysics, cosmology, accelerator technology and multi-phase flow.

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 a Monte Carlo radiation transfer code that enables the study of the underlying dynamics of supernovae by calculating model spectra. Additionally, by migrating the MAESTRO astrophysical code to use the AMReX software framework, scientists can now perform detailed high-resolution long-time dynamics simulations of low Mach number astrophysical flows that were previously intractable. Recent work that has added AMReX mesh refinement capability to the WarpX code has now enabled the simulation of 3D global pulsar magnetospheres from first-principles while also capturing small-scale kinetic effects such as magnetic reconnection.

In collaboration with New York University and San Jose State University, Berkeley Lab has also made significant strides in the development of methodology for simulating the dynamics of physical systems at microscopic and mesoscopic scales. This fluctuating hydrodynamics (FHD) technique has allowed researchers to model the transpiration of gas through a nanoporous membrane and to study the effect of thermal fluctuations in microscale flows of room temperature ionic liquids. They have also developed a new FHD immersed boundary technique that allows efficient simulation of electrolytes and charged molecules at sub-Debye length scales and at lower concentrations than previously possible, laying the foundation for the studying the operation of cellular ion-channels, solute transport through filtering membranes and layer behavior in fuel cells and batteries.

Berkeley Lab mathematicians, in collaboration with plasma physicists at PPPL, have developed the first fully conservative, adaptive finite element discretization of the Landau collision integral, which is the gold standard for integrating many-body dynamics into Vlasov's equation, the standard phase space model for fusion plasmas. This has been implemented in code optimized for the KNL processors on NERSC's Cori HPC system.

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. The 2016 BESAC Facility Upgrade Assessment cited CAMERA as "highly effective" in enabling researchers to analyze light source data. For example, the new multi-tiered iterative phasing (M-TIP) algorithm developed at Berkeley Lab was used in a collaboration with SLAC, the European XFEL, and the Max-Planck Institute, enabling the first ever reconstructions of three virus structures (rice dwarf virus, PR772 bacteriophage and the PBCV-1 virus) from the angular correlations of single-particle LCLS fluctuation X-ray (FXS) scattering data from the LCLS at SLAC. M-TIP is now a key component of the ExaFEL ECP project where it is being scaled to Exascale architectures for real-time FXS analysis at the LCLS. CAMERA scientists have also invented a mathematical approach for driving autonomous X-ray scattering experiments. By capitalizing on mathematical optimization methods, their algorithm automatically chooses the next, most appropriate experimental parameters from a large, high-dimensional landscape of possibilities. This capability is currently being used on beam-lines at NSLS-II where it has already increased beamline utilization from 20% to 80% with a six-fold decrease in the number of experiments required to achieve the same results. It is also currently being incorporated into the Berkeley Synchrotron Infrared Structural Biology Imaging Program at the ALS.

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. Lab scientists have recently added multi-GPU acceleration to the STRUMPACK sparse direct multifrontal solver, which will directly translate into speedup for application codes relying on sparse direct solvers on emerging Exascale-class supercomputers. In addition, recent advances have resulted in a parallel and scalable spectral nested-dissection code for sparse matrix fill-reducing ordering which rely on efficient multi-level Lanczos eigensolvers. This code provides much improved parallel scalability over state-of-the-art load-balancing libraries such as ParMETIS/PTScotch.

The accuracy of most machine learning algorithms critically relies on training datasets being large, which in turn requires new methods of solving the underpinning linear algebra problems. Berkeley Lab's fast linear solvers in STRUMPACK fulfill the requirements. Employing various hierarchical low-rank formats, nearly linear complexity is achieved in both memory and flop count. Combined with distributed-memory code, larger Kernel Ridge Regression problems can be solved for a variety of supervised learning problems with unprecedented speed.

A new fast iterative eigenvalue solver capable of computing interior eigenvalues of Heisenberg spin ½ models with more than 28 spins has been developed which will enable EFRC researchers to study localization and thermalization properties of quantum materials that depend on the interplay between many-body interaction and disorder. The previous record was for 26 spins. Additionally, a new parallel implementation of shift-invert and polynomial filtering-based spectrum slicing algorithm based on density-of-state estimation and K-means clustering for computing eigenvalues of symmetric matrices has enabled large-scale Kohn-Sham DFT-based electronic structure calculation for materials design.

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 the RAPIDS, where we provide senior leadership and which leverage our Applied Math and Advanced Computer Science, Visualization and Data core capabilities. Furthermore, the Lab plays key roles in in 12 Application Development subprojects in the Exascale Computing Project supporting computational science development for exascale systems across many disciplines. LBNL researchers, using applications commenced under SciDAC and enhanced through the ECP have theoretically predicted a new channel for Type Ia Supernovae, composed of sub-Chandrasekhar mass white dwarfs that explode via a helium detonation on their surface, and confirmed their existence in observational data. Similarly, researchers have demonstrated extreme-scale performance for the large scale material science code *BerkeleyGW* on hybrid GPU-CPU leadership HPC systems, enabling the simulation of the electronic excited state properties in prototype solid-state qubits at unprecedented scale and accuracy.

The Lab is deeply involved in the DOE-HEP and NSF project CMB-S4, and has funded the development of TOAST, a scalable HPC software framework for CMB simulation and analysis pipelines, that been extended to support ground-based CMB instruments and observations, re-packaged to support user-developers and to facilitate optimization on next-generation HPC systems, and scaled up to simulate and reduce currently up to 10% of the entire CMB-S4 data volume.

A multidisciplinary team working on early noisy quantum computing hardware has used error-correction, encoding logical qubits with multiple physical qubits, and new approaches to reducing readout noise to improve the performance of a variational quantum eigensolver algorithm applied to computational chemistry simulations.

The Computational Biosciences Group continues to bring together experts from our core capabilities of Computational Science, Applied Mathematics, Advanced Computer Science, Visualization and Data, and Biological Systems Science with a focus on coupling data analytics and statistical machine-learning with simulations to understand the dynamics and multi-scale nature of many biological problems. For example, we have created a templating process for computed tomography (CT) brain images, leveraging diffeomorphic mapping algorithms, which makes it possible to analyze and compare 3D brain scans across a large population, enabling the determination of brain injury.

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 enabling privacy-preserving analysis of and machine learning model training without exposing raw data, the ability to leverage hardware trusted execution environments and encrypted memory to isolate high-performance computing from cyberattack. Ongoing, current, and future work 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 maleficence 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 solar inverters or grid-attached storage.

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 in 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.

ASCR, the CEDS program in CESER office, and NSF are the primary supporters of this Core Capability, with additional previous support from OE, OCIO, NNSA, NSF, and DoD. Significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners such as the DoD 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, computer networks and 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 and dark matter and developing technologies for 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 software and computation 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, 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 construction of 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-3 in February 2017 and the construction of the apparatus is nearing completion. The experiment will begin operations in 2020. Berkeley Lab plays many leading roles in LZ, including the Project Director, Project Manager, Operations Director, and as of 2019 the LZ Collaboration Spokesperson. 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.

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 Fall 2020. 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 including 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 recently completed a Mock Data challenge. 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 led to the selection of this technology for the baseline design, a leadership role in the ND, and a DOE ECRP in 2018. The Lepton Flavor group is also finishing up 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 successfully leveraged resources at NERSC and the Lab’s Computing Research Division for HEP and incorporated machine learning 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 successfully 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.

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. The Particle Data Group provides a unique service to the international physics community through its compilation and analysis of data on particle properties.

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 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 and CD-3A in 2018.

A core capability within Nuclear Science is Berkeley Lab's 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. The next generation of 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 at the Lab, 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.

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). Berkeley Lab scientist Barbara Jacak received one of the inaugural DOE Distinguished Scientist Fellow Awards in 2019 in recognition of her leadership in the discovery and characterization of the QGP.

Berkeley Lab has 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.

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 Berkeley Lab. CUORE is also taking production data at Gran Sasso in Europe, and the Lab has a strong lead role. 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 recently 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. 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 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.

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 LHC Accelerator-Research-Program (LARP), as well as 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-2/CD-3b, enabling baselining of cost and schedule as well as the procurement of critical long lead items. 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 Petawatt BELLA laser is used for research in support of the SC-HEP mission, including reaching 10 GeV from a sub-meter-scale accelerator, and staging of two independently powered 5 GeV 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, and kBELLA, which 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. Berkeley Lab's 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 Berkeley Accelerator Controls and Instrumentation Program brings together decades of deep expertise in electron and ion acceleration, innovative RF structure design and engineering, advanced 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 Fermilab, BACI plays a leading role in technology development in LLRF controls for the PIP-II accelerator complex.

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 an emerging core capability in Plasma and Fusion Energy Science. 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 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 are used to support the needs of ALS-U, LCLS-II. Core capabilities in superconducting magnet technology are being applied to future fusion reactors. Topics of interest include development of advanced materials such as RECBO-based cable and novel quench detection methods for protection of HTS fusion magnets. We are part of LaserNetUS with high power lasers in the BELLA Center and are hosting users to conduct experiments in discovery plasma science and high energy density science.

Applied Science and Energy Technology

Applied Materials Science and Engineering. Berkeley Lab's research emphasizes the design and synthesis of advanced materials for energy, information technology, structural, and other applications in a wide range of physical environments. This capability develops 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.

Berkeley Lab has 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 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 are responsible for the injector, undulators, and 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 compressed-air energy storage. The research in large-scale subsurface energy storage encompasses numerical simulations of coupled processes in the porous reservoir.

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. The Lab-wide **strategic initiatives** explore new scientific directions that can leverage our unique capabilities in science and technology 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 modernizing traffic circulation, site access, and security infrastructure. This section provides an overview of existing infrastructure, and integrates approved, planned, and envisioned investments from DOE, alternative sources, as well as from Berkeley Lab, to comprise our 10-year infrastructure strategy. The strategy strives 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 85 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 at http://www.lbl.gov/community/planning/ldrp/.

The main campus structures consist of about 1.7 million gross square feet (gsf) of DOE-owned buildings (1.68 million gsf) and trailers (.018 million gsf). The Figure 1 summarizes the overall asset condition of mission unique/non-mission unique facilities, as reported in the Facilities Information Management System (FIMS) at the close of FY19.

There are 244,974 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	$258.8M	61.0%	271,060	9
Substandard	$165.6M	39.0%	216,863	6
Grand Total	**$424.4M**	**100.0%**	**487,923**	**15**

Overall Condition – Non-Mission Unique Facilities

Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$193.7M	24.8%	304,439	101
Substandard	$369.2M	47.2%	566.585	35
Inadequate	$218.9M	28.0%	336,946	21
Grand Total	**$781.8M**	**100.0%**	**1,207,970**	**157**

As of Sept. 30, 2019, Berkeley Lab leases or has licenses in place for ten off-site facilities totaling 316,421 gsf. In FY20, following completion of the Integrative Genomics Building (IGB) and program moves, Berkeley Lab terminated the Joint Genome Institute (JGI) leased space. Additionally, the Lab extended the Potter Street (B977) and Hollis Street/ABPDU (B978-3) leases for an additional five years in FY20. The Lab also plans to vacate the Oakland Scientific Facility (B943) in FY20. The Lab is researching potential leased warehousing space or other storage options in support of the ALS-U Project and other operational needs. As of January of 2020, Berkeley Lab also has no-fee use of 48,211 square footage of UC space at UC Berkeley.

At the close of FY19, the Lab had seven buildings and trailers in either shutdown or undergoing disposition status, totaling 17,440 gsf. Three additional assets (7C, 46D, and 79B) totaling 1,251 gsf were in standby status at that time. There is also a diesel generator and fuel tank (OSFs) in shutdown status. Four additional assets are planned to enter shutdown status in FY20, including B7, B53B, B79, and B79A; these facilities represent 26,763 gsf of space. The Lab continues to make progress in disposing non-enduring facilities, and prioritizes facilities in the Lab's major redevelopment areas.

Non-excess Building and Trailer Utilization Summary

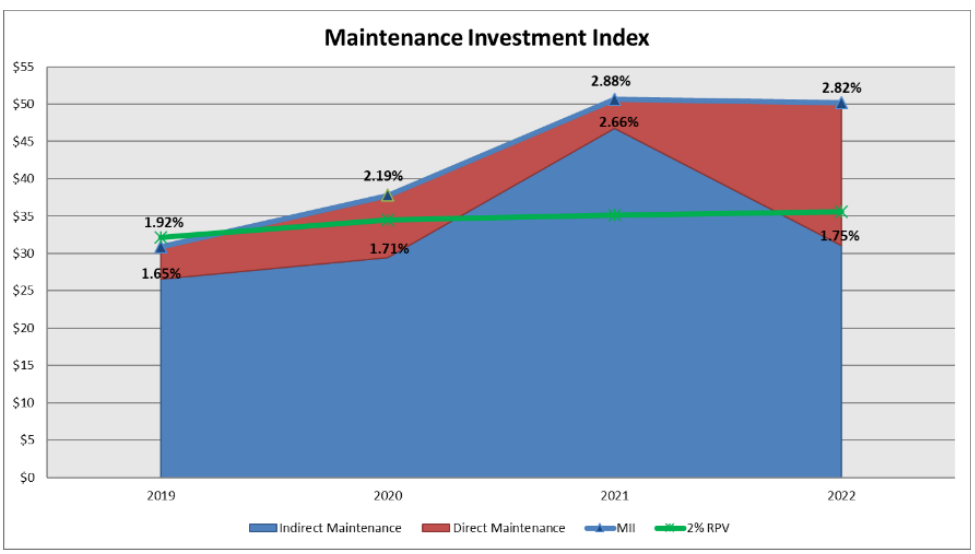
The Lab periodically surveys the use of its operational (non-excess) facilities. The non-excess building and trailer utilization summary, at the close of FY19, is summarized below. Over 93% of the Lab's facilities are either fully or over utilized, demonstrating the significant demands for adequate, mission-aligned space across the site. At the close of FY19, the 11 unutilized and underutilized spaces, representing 21,000 gsf, were all either in the process of being reassigned or being prepared for excess and disposition.

Non-excess Building/Trailer Utilization				
Category	Building	Trailer	Total	Percent
Unutilized	0	2	2	1.2%
Under utilized	3	6	9	5.2%
Fully utilized	38	7	45	26.2%
Over utilized	111	5	116	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 betterments over Berkeley Lab's long history. Figure 3 summarizes the overall asset condition of utility systems at the Lab. Of the $43.0M of inadequate Mission Critical assets, $35.4M is related to facility management control systems and $6.9M is related to natural gas piping.

Overall Condition – Utilities Condition as $ of RPV				
Condition	Mission Critical	Mission Dependent, Not Critical	Not Mission Dependent	Grand Total
Adequate	$465.8M	$22.6M	$.4M	$488.8M
Inadequate	$67.3M	$78.6M		$145.9M
Substandard	$43M			$43M
Grand Total	$576.1M	$101.3M	$.4M	$677.7M

The Lab's overall maintenance and repair (M&R) was 1.9% due to a number of non-maintenance infrastructure investment. For example, the Lab made substantial investments in moving the Joint Genome Institute from offsite leased space to the new Integrative Genomics Building, including related fit-ups of the building. The Lab invested in the conceptual development (OPC funds) of three Line Item Projects discussed in more detail below. The Lab also made investments to move personnel, equipment, and utility lines to facilitate D&D activities at Old Town and Bayview. Though these investments do not qualify as maintenance and repair investments, they are key to the long-term renewal of infrastructure across the site. Through most of the planning horizon, the Lab is projecting 2% or greater MII investment. The deferred maintenance trend is decreasing and the number of buildings rated "adequate" are increasing throughout the planning period.



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

Berkeley Lab's multiyear strategy is based on three overarching objectives that focus on optimizing mission aligned space, strengthening the continuity of critical operations, and modernizing traffic circulation, site access, and security infrastructure. These objectives, in turn, have either two or three subcomponents, as described below. Taken together, these objectives 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.

This is the fifth year of sustained mission focus around infrastructure at Berkeley Lab. As such, many of the projects planned during this period have progressed toward design and execution. A key component of the Lab's plan is maturing the interfaces between the execution of the scientific mission and infrastructure objectives. The interfaces include the tactical coordination of ongoing activities (e.g., laydown areas, outage coordination), and consider the evolving long-term mission drivers that guide strategic stewardship of infrastructure through prudent investments. To better align project delivery to strategic planning efforts, the Lab has created a new Campus Planning Department within the Facilities Division. Campus Planning provides a framework for the orderly stewardship of site, facilities, and infrastructure. Key functional responsibilities include portfolio, infrastructure, site, and environmental planning. This department's studies and analyses provide informed recommendations to senior Lab leadership and help formulate assumptions related to active project execution by better defining the long-term vision for the site. The formation of a dedicated Campus Planning Department and the project delivery improvements represent advancement of the Lab's infrastructure renewal approach.

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 Redevelopment and Charter Hill (Old Town) Redevelopment areas, with several smaller projects scattered throughout the site.

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 future building at Bayview is BioEPIC, which will bring together biological and environmental research and house exciting new research capabilities that will advance interdisciplinary priorities, such as the microbes-to-biomes initiative to examine and manipulate biological and environmental processes across scales of space and time, from molecules to ecosystems and from nanoseconds to decades. 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 Parcel 1a South Cleanup, an Environmental Management (EM) funded project, is underway and will address these site features, with completion forecast for FY21. Concurrently, the IGPP-funded Site Utilities Relocation Plan (SURP) project will reconfigure and renew pre-1970s era utilities at the Bayview cluster, ensuring reliable utility services for decades into the future. To facilitate these projects, the Lab has funded non-capital investments in FY19 and FY20 to relocate equipment and personnel from the areas that will be impacted by construction, including the demolition of an aged trailer (64B).

Redevelopment activities will continue to progress north across the Bayview cluster throughout the planning horizon. The Bayview Parcel 1b North Tunnels Cleanup, another EM-funded project, will address remaining former Bevatron facility features and contamination beyond the BioEPIC footprint. An envisioned EM-funded Bayview Cleanup Phase 2 would follow completion of the tunnel demolition and address the demolition of B56 and B64, including any local site contamination, once funding is available. This cleanup work will free up the acreage necessary to construct the third biosciences-focused facility, currently envisioned to be funded jointly between the State of California and the DOE. Additional D&D efforts farther north, to remove B55, B55A, B60, and B63 would follow, creating new acreage for the fourth and fifth biosciences-related buildings at Bayview.

Charter Hill (Old Town) Redevelopment

The Old Town Demolition Project is its final phases, including phases V, VI, and VII. These address removal of B4 and B14, removal and cleanup of B4 and B14 slabs, nearby utilities, and soil contamination, and removal of B7 and B7C, respectively. The current forecast for substantial completion is late FY21, with closeout activities occurring in FY22. Early interim uses of the newly available acreage in the Charter Hill cluster are already in place, including additional parking and laydown areas in support of projects and operations. The installation of a tensile structure in late FY20, where the former B5 once stood, will provide additional space for storing critical and temperature sensitive equipment in support of various Lab needs.

The Lab's vision includes the construction of the Advanced Materials Discovery Building (AMDB), which would house unprecedented automated accelerated materials discovery based on robotics and machine-learning algorithms coupled with theory and real-time analysis. With current capabilities spread out on different parts of the Lab and housed in substandard and inadequate infrastructure, this new facility will bring together core programs in energy storage, materials synthesis, and related research programs. The Lab's vision also includes a Charter Hill Modular Utility Plant (MUP) to serve the AMBD and other future facilities constructed in the area, as was done previously at Bayview. Following the AMDB and MUP, the Interdisciplinary Chemical Sciences Building (ICSB) would further progress towards surging the Lab's research population out of outdated and seismically poor buildings across the site, such as B46, B46A, and B70. Both of these facilities would complement the new capabilities provided by the upgraded ALS. The final phase of redevelopment could include construction at the site of the current B7, which is on grade with the ALS.

Adaptive Modernization of Existing Space

Given the high occupancy rate of existing facilities and the elevated cost of new construction across the region, the Lab is renewing efforts toward adaptive modernization of existing space infrastructure. To prioritize space improvements capable of increasing functionality or occupancy density, Berkeley Lab's Campus Planning Department will use a metrics-based approach.

The Lab has substantially completed an IGPP-funded B77A Addition Project, which creates approximately 1,900 GSF of new high bay engineering fabrication space in support of virtually every research program at LBNL and numerous projects across the DOE Complex. 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 adapting existing infrastructure, the creation of additional high bay spaces will be a high priority.

At B84, the Lab is building out existing unfinished storage space in order to create new office space to accommodate 14-16 new staff anticipated in FY21. Completion of the design and construction of this project is planned for FY20.

Several years ago, B73/B73A were vacated and placed into excess status due to their very poor seismic ratings. This year the Lab will use IGPP funding to seismically retrofit and renovate B73 (including the demolition of B73A) to create safe, modern, and occupiable laboratory and office space. This additional space will accommodate program growth in FY21 and beyond, as well as retire the institutional liabilities related to the existing deficient structures.

Two separate IGPP projects located at B77 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 is planned for substantial completion in early FY21. The second project, the B77 Engineering Facility Capabilities Modernization, will refresh and expand specialized metrology laboratory space, also allowing for additional space optimization opportunities. This project will begin design in FY20 and perform construction in FY21. The expansion and modernization of metrology lab space enables not only the measurement of individual parts, but also allows for the assembly from millimeter to meter scales with measurement accuracies down to the sub-micrometer level. In hand with the required metrology enhancements, the mechanical fabrication housed in B77 are required by science to machine to tighter tolerances. Due to tighter mechanical fabrication tolerances, the Lab is also seeking to upgrade the main machine shop with a vibration-managed shop floor, such that crosstalk between the different machine shop tools do not impact the parts fabrication. Fabrication of tight tolerance large parts and assemblies is a unique capability that is critical to DOE projects. The Lab's Engineering Division is also seeking to replace a ~40-year-old mill with a modern large scale CNC machine. Smaller maintenance projects are being executed at this complex to improve building controls, and to retire risks related to outdated electrical panel.

Electron Microscopy will enable Berkeley Lab to remain an international electron microscopy 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 broad range of programs for a diverse set of scientific challenges in areas such as materials synthesis, catalysis, earth and environmental science, soft matter characterization, and structural biology. Instruments to be developed requiring state-of-the-art facilities include ultrafast electron diffraction imaging capabilities; novel in situ, time-resolved and cryo-EM instruments; and an analytical TEM with high energy resolution.

Specialized space and infrastructure needs for information technology have been identified and early conceptual planning is in progress. Virtually all mid-tier high performance computing (HPC) is centrally provided by the Lab's IT Division in the Berkeley Research Computing (BRC) Datacenter, which houses 22 clusters, 2716 nodes, 54432 cores, and is at its maximum power availability of 885kW. End-of-life mechanical and electrical replacements at B50B-1275 are part of this overall plan, and are discussed in further detail in Objective 2. The Lab will seek to install high-efficiency 800 kW modular data center space to address the mid-tier HPC capabilities gap. In addition to the HPC demands, the Lab no longer has sufficient general-purpose data center capacity to continue to meet the diverse and growing needs of the scientific programs. General purpose data centers house non-HPC scientific servers and systems that enable scientific projects and experiments. This includes systems that provide institutional scientific services, as well as systems managed for individual projects, facilities, or experiments. The Lab has one small (walk-in closet) scale central facility for scientific colocation, and two dozen small distributed server rooms devoted to programs. These resources are effectively full. As non-HPC scientific computing needs continue to grow, the Lab requires resilient and secure general purpose datacenter space to house both dedicated and shared scientific services, such as virtual machines, storage, containers, and other servers. Additional improvements to the Lab's existing general-purpose data center space at B50B-2275 are discussed further under Objective 2.

Finally, the Lab continues to reduce inventory of trailers in poor condition. In FY19, the Lab funded the disposal of B83A and will fund the demolition of B53B in FY20. As funding allows, the Lab will continue to remove substandard and inadequate trailers on a year-to-year basis.

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, enhancing reliability, and/or increasing maintenance capabilities.

Power Shutdown Resilience

The single greatest 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, last year the Lab was forced to shut down operations for 5 business days across two separate events in October. Direct costs related to these events were approximately $1.7M per business day, or $8.5M in 2019. In addition to the productivity losses caused by the shutdowns, significant strain was placed on the Lab's aging infrastructure through repeated equipment de-energizations and re-energizations. Lab Operations and Research Area Representatives performed spectacularly and with tireless dedication in the face of very challenging circumstances. When power restoration activities commenced during the first event, 122 building-related incidents were reported, with 82% of those incidents being related to mechanical and electrical systems. The incidents highlight the importance of accelerating efforts to reduce deferred maintenance and update infrastructure to improve the Lab's ability to respond to such events in the future.

The SLI-funded Linear Assets Modernization Project (LAMP) will make major progress in improving the Lab's utility resilience. The project will seek a 50-80% reduction of the $81M of high-risk linear asset-related deferred maintenance backlog, and will create redundant system loops, where appropriate, to modernize system operations and increase utility service reliability. The planning approach is to use utility corridors where common system alignment opportunities are practical, driving installation efficiencies and increasing maintenance capabilities. Utilities include natural gas, domestic water, electrical, communication/data, storm drain, and sanitary sewer.

Several IGPP projects are in progress to improve the Lab's PSPS posture. The Sitewide Electrical Safety and Maintenance Upgrades, Phase 1 will address deficient and aged electrical equipment at two existing buildings (B50A and B70A) and switch station A3. Construction for the B70A portion of the work, as well as preparatory work at switch station A3 will begin in late FY20 or early FY21, with the B50A work planned in FY22. The B70A's dated electrical infrastructure posed special challenges for safely re-energization following the PSPS events. The Sitewide Mechanical Plant Maintenance Upgrades Phase 1 is addressing several deferred maintenance items that pose reliability risks and unnecessarily increase the cost of day-to-day maintenance activities. This project substantially completed the upgrade of boilers and controls at B62 in FY19. Engineering design for upgrading controls and cooling capabilities at B2 and upgrades to the sitewide compressed air plant at B43 will occur in FY21, with construction planned for FY21/FY22. Additional phases of the Sitewide Electrical Safety and Maintenance Upgrades and Sitewide Mechanical Plant Maintenance Upgrades are being planned for future years. Enduring buildings that are strong candidates for IGPP investments given their large deferred maintenance balances and lack of redundancy include B50A, B50B, B66, B70A, B71, B77, B88, and B90. For example, B71 mechanical, water, and HVAC system upgrades are needed to modernize the building to current standards. This includes providing redundancy for current single points of failure, replacing aging systems, and increasing capacity. The building currently does not maintain temperature well for work requiring equipment sensitive to minor temperature changes and air currents. This utility infrastructure will be more and more important as multi-program activities and user operations in the building increase, and the costs of down time or nonperformance escalates.

Another IGPP, the Grizzly Peak Transformers Installation, will provide additional capacity and redundancy to the Lab's main substation, allowing it to meet the Lab's forecasted electricity demands and improving the safety of maintenance activities. As noted previously, mechanical improvements to the existing data center at B50B are being planned to ensure cooling is maintained during PSPS events. Although the B50B data center has redundant power, it does not have redundant cooling, which required portions of the data center to be shut down during the PSPS events, impacting operational and research systems.

The Lab's resiliency planning efforts will result in additional direct funding requests over the coming months and years. For example, a feasibility study is underway to consider backup power generation options to sustain a one-week electrical utility outage, whether partially or fully (up to 70 megawatts). Some potential solutions include centralized diesel engine generation near the Lab's main substation, Grizzly Peak, onsite power production through cogeneration gas turbine engines, regional distributed diesel engine generators, and dedicated diesel engine generators at individual buildings. When appropriate, the Lab will pursue an Energy Resiliency and Independence Line Item Project to analyze alternatives, perform design, and implement the most promising solutions. The Lab will also seek GPP funding to upgrade the highest priority building controls systems across the site and replace aging emergency and standby generators. These smaller investments could provide significant benefits in a relatively short amount of time given the importance of building controls and generators to the ability of Lab Facilities personnel to rapidly and safely respond to these events, mitigating the potential for research loses. Given the significant impacts PSPS events can have, it is important to consider all potential solutions and to quickly pursue the most promising.

Improve Seismic Safety and Reduce Landslide Risks

The latest earthquake forecast, 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 30 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 LBNL site, before 2043. The Lab must prepare for this eventuality.

The Lab's 2008 Seismic Study identified 42 buildings that could be anticipated to perform poorly in a large earthquake. After more than a decade of mitigation efforts, the number of remaining buildings rated seismically poor and very poor is down to 19. Demolition of B79 will begin this year as part of a GPP funded effort to expand the Grizzly Peak Substation Yard and B73 will be seismically retrofitted and renovated in FY20/FY21 (as noted previously). The Lab has nearly completed the replacement of 11 existing balcony guardrails and 2 existing concrete rooftop pergolas located at the western edge of B50A and B50B, greatly improving the seismic safety profile of these buildings. B70 is near the top of the Lab's prioritized mitigation schedule due to its inadequate condition and poor seismic rating. Its occupants would need to be dispersed across the main campus, including the new facilities envisioned for the Old Town Site. Several other seismically poor buildings are planned to be demolished as part of the Bayview Redevelopment. Other small seismically deficient buildings and trailers are planned for demolition as indirect funding allows.

The Lab gained CD-1 approval for the Seismic and Safety Modernization (SSM) Project in late FY19 and will begin preliminary design in FY20. The project will construct a new 46,000 gsf facility to include a cafeteria, conference rooms, and space for relocating the Lab's Health Services and select Human Resource personnel. The project will seismically retrofit the second floor of B48, the sleeping quarters of the onsite Fire Department. The project will also demolish the existing cafeteria (B54), which is currently forecast for FY21. The cafeteria replacement and retrofit of B48 will improve the Lab's operational continuity in the event of an emergency, create a central hub for Operations provided services, and will improve vehicular and pedestrian circulation.

The Lab continues to seismically evaluate buildings, trailers, and non-building assets for seismic safety risks, and plans will be continually be updated to reflect the latest information. Retaining walls, hydraugers, and known slide zones are being investigated for adequacy and future projects may be initiated to address the mitigation of potential landslides. Finally, the Lab has engaged the University of

California Office of the President (UCOP) to seek funding to replace a UC owned seismically deficient overpass, called Centennial Bridge, that crosses over the Strawberry Canyon area of the Lab. Preliminary indications are that funding for design and construction will be awarded (~$15M in State funds and ~$12.5M in UC Berkeley contributed funds), with the goal of beginning construction in FY21. The project will be managed by the UC Berkeley, but will require significant Lab interfaces given the physical connectivity of the bridge and the road to the Lab site.

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

Many projects already discussed could also be applied to this subobjective, but others 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 core infrastructure elements.

The Lab is planning to substantially complete two GPP projects funded in FY18, the Supply Water (CMLC) Replacements and Storm Drain Repair/Replacements. Construction is in progress on the former, with substantial completion forecast for late FY20. The latter will begin construction in the spring, with substantial completion forecast for early FY21. The projects will retire the highest priority sections of piping that pose risks to the mission and operations.

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. Telecommunications rooms in many buildings are too small and lack sufficient power or cooling to support modern resilient network and telecommunications equipment. Investment in these spaces has been reactive to maintain existing service levels to address leaks, corrosion, rodent damage, and ground movement. A series of investments will be made over the planning horizon to address these critical technology systems.

Laser-Plasma Acceleration Infrastructure Modernization. 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. Sources of funding are being investigated.

Accelerator Science and Engineering Building. Accelerator science and engineering are closely integrated at Berkeley Lab. This close integration 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. Presently, accelerator and engineering staff are 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.

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 provide liquid in transportable dewars to other users. The DOE-OHEP has demonstrated leadership in supporting this critical need by providing funding in FY19 for the procurement of the helium liquefier; the liquefier is essential for the US MDP to deliver on its goals. To leverage the liquefier for projects and programs beyond HEP, further procurements would be required, including associated elements such as LHe storage dewars and piping for gas recovery from experimental users at the ALS and Materials Science (B6 and B2). The conceptual budget for the first phase of this work is included in the Infrastructure Investments table. Engineering would then run the cryoplant facility and support science programs within ATAP, ALS, MSD and others.

A gap table by core capability is provide in the following figure.

Core Capability Gap (Buildings and Trailers)				
Core Capability	Adequate	Inadequate	Substandard	Grand Total
SC01 Accelerator Science and Technology	0	4	5	9
SC03 Applied Materials Science and Engineering	2	0	1	3
SC05 Biological and Bioprocess Engineering	0	1	0	1
SC06 Biological Systems Science	3	1	1	5
SC09 Climate Change Sciences and Atmospheric Science	4	0	1	5
SC10 Computational Science	1	0	0	1
SC11 Condensed Matter Physics and Materials Science	0	0	2	2
SC13 Decision Science and Analysis	1	0	0	1
SC14 Earth Systems Science and Engineering	0	2	1	3
SC15 Environmental Subsurface Science	4	0	0	4
SC16 Large-Scale User Facilities/R&D Facilities/Adv. Inst.	6	3	5	14
SC18 Nuclear and Radio Chemistry	0	1	0	1
SC19 Nuclear Engineering	0	0	2	2
SC21 Particle Physics	0	0	1	1
SC23 Power Systems and Electrical Engineering	0	0	1	1
SC24 Systems Engineering and Integration	3	2	0	5
SC25 Enabling Infrastructure	86	7	21	114
Grand Total	**110**	**21**	**41**	**172**

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

This objective includes 3a) upgrading site access entry points and safety related infrastructure, and 3b) maximizing transportation and parking improvement opportunities.

Upgrades to Site Access Entry Points and Safety Related Infrastructure

The Lab is working with DOE's Safeguards and Security Program to assess the adequacy and configuration of its existing vehicular entry and egress point infrastructure elements. Though still in the earliest stages of planning, a number of events over the past decade have underscored the need to modernize these critical Lab access points. For example, both the Strawberry Gate Guard House (B33A) and the Grizzly Peak Gate Guard House (33C) were constructed in 1965 and likely do not meet today's security standards. With the planned Centennial Bridge Replacement Project likely moving forward in FY21, there may be an opportunity to improve the configurations of both these gates as part of complementary projects. Such projects would improve vehicular safety and the Lab's security posture. The Lab has also proposed, through UCOP, a Horseshoe Curve Roadway Improvement to address a steep incline and tight turn that lacks a shoulder on the uphill side and is suboptimal for receiving large trucks and Lab shuttles. This road leads to the Blackberry Gate Guard House (33B), the primary entry and egress point to the Lab.

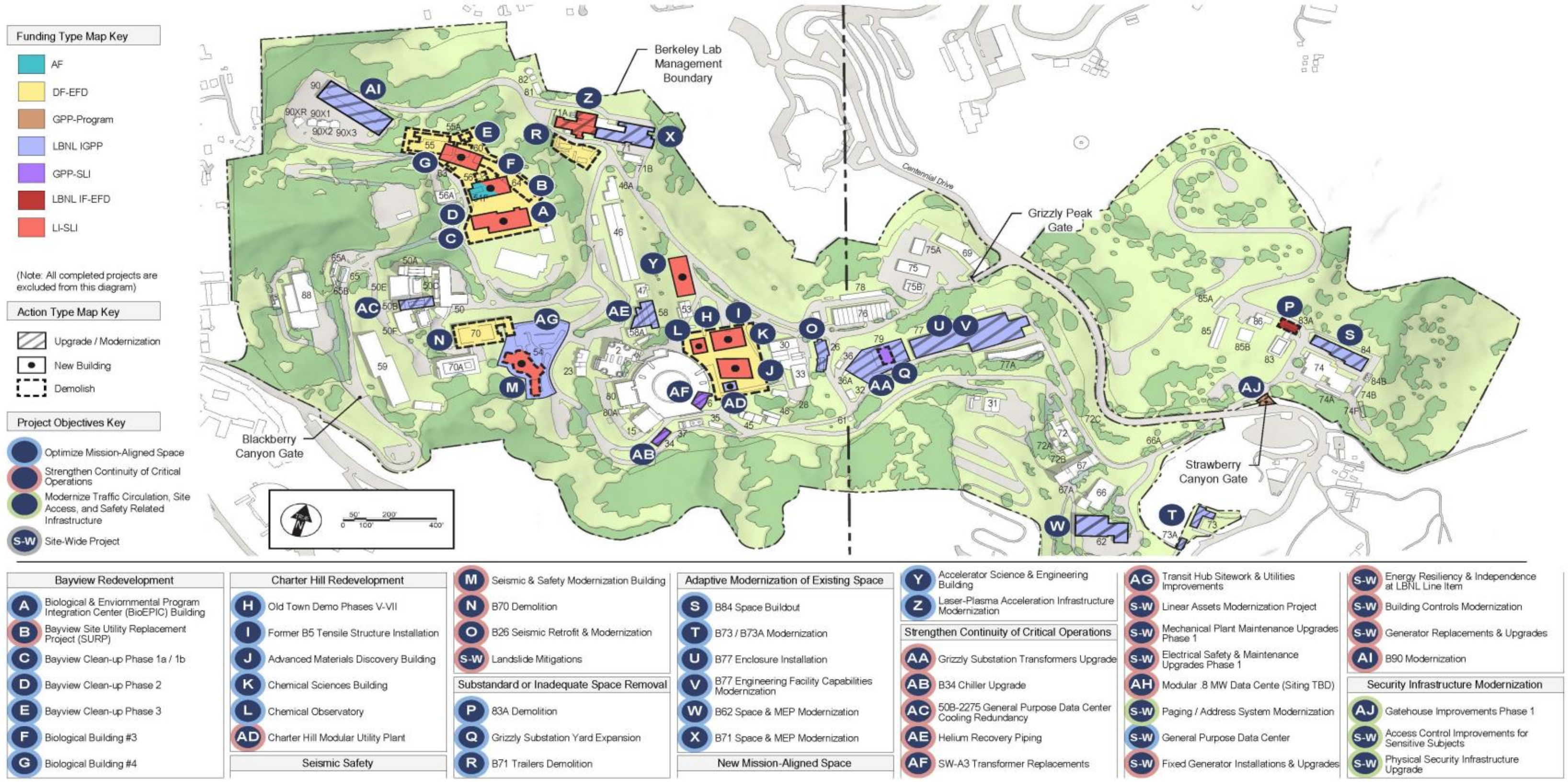
FireSAFE. The average age of fire protection systems is 26 years. Frequent equipment failures have led to costly building evacuations and operational interruptions at the Lab. The Fire and Safety Alarm Future Enhancements Project will replace and upgrade the site's existing fire and safety alarm systems nearing their end-of-life. 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.

Maximize Transportation and Parking Improvement Opportunities

The Lab's Transportation & Parking Demand program is addressing the Lab's commute challenges with a portfolio approach. By actively engaging the Lab community over the past year, challenges and opportunities have become better defined, with new ideas being actively pursued. The Lab increased shuttle services and improved routes and times to better serve community needs. The Lab also partnered with the LBNL Bike Coalition to install new bike racks in critical Lab locations and to educate shuttle riders on how to best use the shuttles' bike racks. Transportation & Parking Demand worked with Human Resources and IT to improve telecommuting options. Recently, the Lab launched a new rideshare partnership that resulted in over 400 one-way shared rides during the first four weeks of the program. The ultimate goal is to change the Lab's culture about how its population commutes to the Lab. As this will take a few years to become fully effective and sustainable, we have added parking spaces in the form of leased spaces off-site and attendant-assisted stack parking on-site. The Lab is also performing design on an IGPP funded Transit Hub Sitework and Utilities Improvements project that will relocate the main shuttle drop-off point from near B65 to the soon-to-be-constructed new Cafeteria and Welcome Center (delivered as the SSM Project). This new transportation hub will greatly improve accessibility and pedestrian safety at the site, complementing operational efforts to address the Lab's transportation and parking challenges.

Campus Overview Map

Berkeley Lab FY2020 - FY2021 | Overview and Summary-Level Needed Investments



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 FY19, the Lab has 20% of buildings by count that meet Guiding Principles, exceeding the goal of 15% by FY25. 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, which was included in the design of the recently completed Integrative Genomics Building.

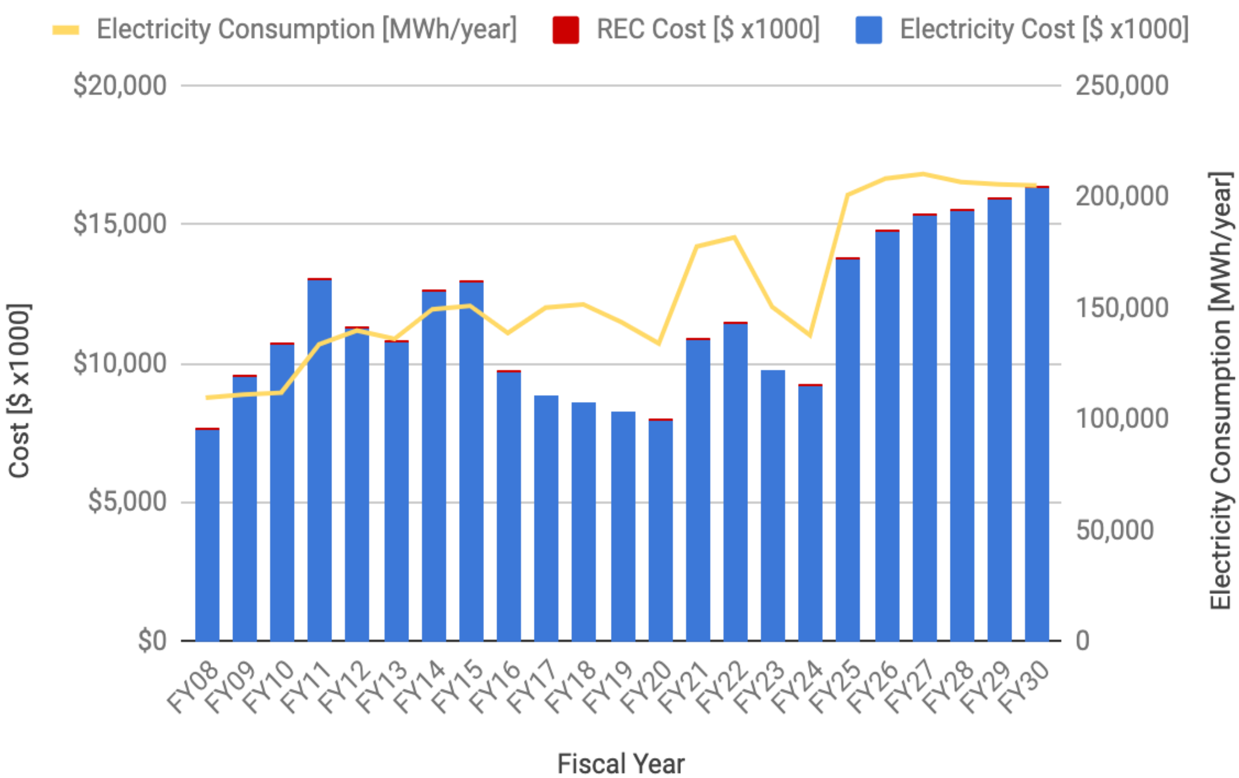
Recent highlights include:

- **Maintained Energy Savings**: As of spring 2020, Berkeley Lab is maintaining annual energy savings of 8.1 million kWh and water savings of over 19 million gallons. The savings are equivalent to the generation from a 5.2 MW photovoltaic array, which would occupy 16 football fields or 20 acres. These savings are being achieved primarily through improvements in facility operations, delivered by the Ongoing Commissioning Team and a focused team at NERSC. Energy use intensity (weather-corrected energy consumption divided by square footage) has improved 14% since FY15. Maintained efficiency savings are updated monthly at sbl.lbl.gov/data.
- **Ongoing Commissioning Team**: The Lab has formalized a dedicated cross-functional team from the Facilities Management division and Sustainable Berkeley Lab who work continuously to identify, prioritize, and resolve operational problems in buildings in order to generate energy savings and improve operations. The Ongoing Commissioning approach was recently recognized by a 2019 "Accelerating Smart Labs" Project Award given by the Department of Energy on behalf of the Better Buildings Smart Lab Accelerator. The Lab also received a 2019 Best Practice Award from the California Higher Education Sustainability Conference for advanced use of SkySpark (a building analytics platform) to support the ongoing commissioning process.
- **ISO 50001 Implementation**: The Lab has completed a two-year project to align its energy and water management activities with ISO 50001, an international energy management standard. Aligning activities with ISO 50001 is a key approach to ensure that energy and water management is strategic, effective, and persistent. The Lab completed an Energy and Water Management System Manual (working document) that describes all energy and water management practices. The Lab is currently submitting at "ISO 50001 Ready" and anticipates third-party certification in FY20.
- **Sustainability Policy**: The Lab updated its policy on Sustainability Standards for New Construction, which received a 2019 Department of Energy Sustainability Award - Outstanding Sustainability Program or Project. The Lab also issued new policy on Sustainability Standards for Operations to advance energy and water management, water conservation, as well as zero waste and waste reduction.
- **New Construction**: The Integrated Genomics Building was completed in November 2019 and is designed to meet deep energy efficiency targets (consuming only 36% of the energy used by the

previous facility it replaces), use no natural gas for space and water heating, and offset about 15% of its total energy use with rooftop photovoltaics (still to be installed). See more details about the Integrative Genomics Building (IGB) Design at sbl.lbl.gov/progress.

Historical and anticipated electricity cost and consumption data are presented below.

Figure 1. Electricity Usage & Cost Projections



Note: REC costs are difficult to see on the above chart due to their small magnitude. Values are shown in the table that follows.

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 2019 Lab Operating Costs:** $1,824.6 million
- **FY 2019 DOE/NNSA Costs:** $1,607.8 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $203.4 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 11.9%
- **FY 2019 DHS Costs:** $13.5 million

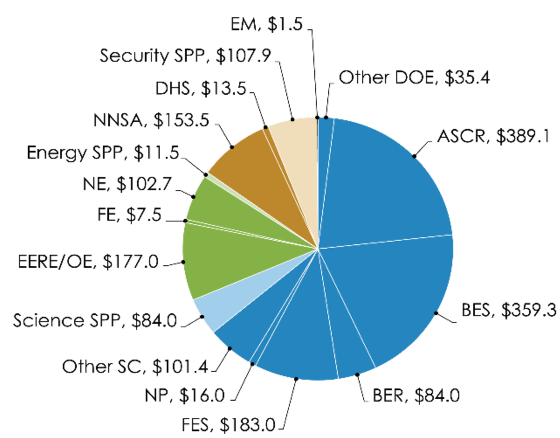
Physical Assets:

- 4,421 acres and 272 buildings
- 4.85 million GSF in buildings
- Replacement Plant Value: $67.3 B
- 1.4M GSF in 63 Excess Facilities
- 1.1M GSF in Leased Facilities

Human Capital:

- 4,856 Full Time Equivalent Employees (FTEs)
- 194 Joint Faculty
- 323 Postdoctoral Researchers
- 532 Graduate Student
- 556 Undergraduate Students
- 2,928 Facility Users
- 1,691 Visiting Scientists

FY 2019 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 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, 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 (S&T) base that catalyzes fundamental scientific advances and technology breakthroughs to support DOE's mission of addressing the nation's energy, environment, 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 production, acceleration, accumulation, and utilization of such high-intensity, high-power beams. The Spallation Neutron Source (SNS) accelerator complex, operating at 1.4 megawatts (MW) power on target, is presently 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 investigation of the dynamics of high-intensity hadron beams and the development of high-power proton targets.

Other ORNL leadership areas include expertise in negative hydrogen ion (H^-) sources and low-energy beam chopping and manipulation; superconducting radio-frequency (RF) 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 our efforts to systematically increase the power level at which SNS operates reliably.

The comprehensive 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 is now being extended into the medium-beta cavities through a recipe modification for this configuration. 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 (LACE) 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 significant reduction in the time required to complete facility turn-on after planned outages.

ORNL has constructed and commissioned a low-energy Beam Test Facility (BTF). The spare RF quadrupole (RFQ) structure has been commissioned to full power and is now installed in the main SNS linac front end; the old RFQ has been installed in the BTF and now allows the continuation of a robust program of scientific study. This program extends the FY 2019 accomplishment of the first 6D phase space measurement into a research program focused on understanding beam halo development that capitalizes on the unique high dimensionality, high dynamic range instrumentation in the BTF. The SNS accelerator complex, in combination with the Cryogenic Test Facility and the BTF, provides an essential resource to enhance accelerator science opportunities that attract, engage, and retain staff with the expertise to drive innovation in all facets 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; additional support is provided through partnerships with the University of Tennessee (UT) funded by SC's High Energy Physics program and the National Science Foundation (NSF).

Advanced Computer Science, Visualization, and Data

ORNL staff are deeply engaged in R&D to enable 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), leading several projects and participating in several co-design projects. In addition, Jeffrey Vetter, of ORNL's Future Technologies Group, leads the development tools element and is participating in the ECP Hardware and Integration focus area.

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 high-performance computing (HPC) systems. 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 OLCF, including the 200-petaflop IBM AC922 Summit, are 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. 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. 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 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 the 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 (Bredesen Center). 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 Intelligence Community (IC), 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 experimental, theoretical, and computational materials research and strongly couples a leading fundamental condensed matter and materials science program supported BES program for 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 be readily translated to high-impact applications.

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, 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. Novel processing techniques for manufacturing include advanced manufacturing of metals, alloys, and polymer composites. For example, ORNL recently demonstrated that ML algorithms can be used to optimize scan strategies, thus controlling the columnar-to-equiaxed transition during 3D printing of metals to locally control the material properties in complex geometries. In support of the Office of Nuclear Energy (NE), ORNL has initiated R&D activities for the Transformational Challenge Reactor (TCR), including exploration of materials development in conjunction with ML and advanced manufacturing tools.

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 alloys, ceramics, nanomaterials, carbon fiber and composites, nanostructured carbons, polymers, and thermoelectrics. For example, ORNL's shear thickening electrolytes have demonstrated the ability to stop a bullet[2]—work that has been granted four patents and continues with two industry-sponsored projects. Furthermore, ORNL has discovered a vapor processing route to encapsulate liquid metal in a ceramic silicon carbide shell for modular, tunable thermal energy storage for concentrating solar, nuclear, and fossil power plants.

ORNL's applied materials science and engineering program takes advantage of state-of-the-art capabilities for materials development and testing, such as SC user facilities CNMS, SNS, HFIR, and OLCF; the Carbon Fiber Technology Facility (CFTF) and the Manufacturing Demonstration Facility (MDF), both 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 demonstrated the use of ultra-high temperature ceramics as innovative plasma-facing

2 B. H. Shen et al., *ACS Appl. Mater. Interfaces* **10** (11), 9424–9434 (2018).

component materials for fusion energy systems. The system promises the use of isotope-separated transition metal diborides and transition metal carbide for enhanced lifetimes in high-radiation environments.[3]

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 to current Zircaloy-based clad materials. Overall, the core capability of applied materials science and engineering program supports the development of materials that improve efficiency, economy, and safety in energy generation, conversion, transmission, and end-use technologies. Funding comes from EERE, OE, the Office of Fossil Energy (FE), SC, 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) high-dimensional approximation and uncertainty quantification, and (4) accelerated solvers for extreme-scale architectures.

ORNL's applied mathematics capability includes extensive expertise in the development, approximation, and analysis of innovative, massively scalable, and resilient mathematical and computational approaches for scientific discovery and decision sciences. 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, physics-informed learning, and (3) demonstrated impact on applications in science and engineering. The broad scope of R&D in ORNL's applied mathematics program encapsulates both theoretical and numerical solutions of complex deterministic and stochastic systems, with immediate impact on a number of applications sponsored by SC programs. 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:

- 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. Theoretical analysis of the developed algorithms will also be conducted to demonstrate the advantages from a theoretical perspective.
- 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.
- 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.
- Strategies for model reduction, closure, surrogates, and multifidelity models.

[3] T. Koyanagi et al., *J. Am. Ceram. Soc.* **102,** 85–89 (2019).

- New optimization algorithms, including constraints reduction methods and measure-based approaches.
- 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.
- DG-IMEX framework to improve physical fidelity by including more neutrino-matter interactions, 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.

ORNL has also enabled R&D in support of SC missions by building on research for non-DOE sponsors in imaging, cybersecurity, quantum information science (QIS), nuclear engineering, materials science, neutron science, and additive manufacturing.

ORNL 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, UQ, 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.

ORNL fosters strong partnerships between mathematicians and researchers across ORNL to address the challenges faced by experimental scientists, such as deep data analytics for electron microscopy in the BES materials science program. 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 UQ; 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 biosequestration, 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 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 broad capabilities in chemical engineering, chemistry, materials science, HPC, and systems engineering to accelerate translation of research outcomes into demonstrable improvements in bioproducts and biofuels and to move bioremediation research from the laboratory to the field or pilot level. Integrated teams at ORNL bridge science to applications. ORNL uses expertise in plant sciences, microbiology, molecular biology, molecular dynamics, 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 OLCF) to address bioproduct and biofuels production.

ORNL is a recognized leader in multiple aspects 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 sequestration in soils. ORNL also leads in the use of a suite of biomass conversion processes: novel microbes and applied systems biology, computational chemistry and physics 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; and (5) development of imaging at multiple spatial and temporal scales. 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 multispectral imaging system that enables a new level of high-throughput phenotyping of plant systems. Additional bioimaging capabilities and automated sampling are future extensions of this system. CBI is leading improvements in the economics and sustainable production of biomass and its conversion to bioproducts and biomaterials. Fundamental research will rapidly advance the understanding of cell wall structure and plant feedstock systems. ORNL leads the shift in focus in bioproducts research to sustainability and a more diverse set of 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) and Biofuels, and joint projects with other national laboratories (e.g., Ecosystems and Networks Integrated with Genes and Molecular Assemblies, National Microbiome Data Collaborative, and KBase).

ORNL is expanding research on biocomplexity to facilitate understanding of the structural organization, functional dynamics, and emergent properties of complex biological systems. Capabilities in biochemical sciences, neutrons, and computing combine to 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 and modeling for interpretation of complex systems biology data. Biological systems science at ORNL also focuses on biological transformations of critical DOE-relevant pollutants and nutrients.

ORNL's neutron scattering resources can be leveraged through the Center for Structural Molecular Biology (CSMB), 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 functional architectures and local environments 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 neutron scattering, x-ray pair distribution function analysis, electrochemical measurements, and molecular dynamics simulations, to provide a fundamental understanding of the behavior of room- temperature ionic liquids inside carbon electrodes with complex pore architectures and surface chemistries.[4]

Designing new materials for efficient chemical separations is a strength of the ORNL Chemical and Molecular Science program. ORNL has recently developed a cost-effective and efficient cycle for direct air capture of CO_2 by focusing on amino acid–based sorbents that promote CO_2-crystal formation,[5] and previous work on direct air capture crystallization methods is being adapted for efficient capture of CO_2 in flue gas.[6] Utilizing ML and AI to understand and predict fundamental chemistry in carbon capture, separation, and catalysis is a growing emphasis for ORNL.

The neutron scattering expertise in ORNL's Chemical and Molecular Science program is also enhancing our fundamental understanding of legacy waste at the Hanford site and the catalytic reaction mechanism in hydrogen production. As part of the Interfacial Dynamics in Radioactive Environments and Materials EFRC led by Pacific Northwest National Laboratory, a series of quasi-elastic neutron scattering measurements were conducted on highly concentrated, high-alkaline aluminum-bearing solutions, in which researchers showed that the identity of the electrolyte can have dramatic effects on the

[4] H. Chen et al., *Adv. Funct. Mater.* **29,** 1906284 (2019).

[5] N. J. Williams et al., *Chem.* **5**, 719 (2019).

[6] K. A. Garrabrant et al., *Ind. Eng. Chem. Res.* **58**, 10510 (2019).

nucleation behavior of solid phases.[7] By coupling inelastic neutron spectroscopy with infrared and x-ray photoelectron spectroscopies and computational approaches, the long-debated reaction mechanism of the water gas shift reaction was resolved, providing new insights into optimization of industrial hydrogen processes.[8]

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. 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 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 and applications to BER and NP programs are closely coupled to the chemical and molecular science core capability.

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) 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. Recent results include new molten salt–based processes that dramatically lower the required temperature and, therefore, the cost for synthesizing graphite from amorphous carbonaceous materials. Stable isotope research and production depend on utilization of specialized or potentially novel feedstock chemicals not available commercially, including 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 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 (CMI). Separations methods have been developed for intra-lanthanide separations protocols using preorganized phenanthroline-base ligands.[9] In addition, EERE-funded research on carbon fibers has focused on ways to use lignin, a renewable industrial by-product, to improve thermoplastics. For example, ORNL has developed a way to

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[7] T. R. Graham et al., *J. Phys. Chem. B.* **122**, 12097 (2018).

[8] F. Polo-Garzon et al., *J. Am. Chem. Soc.* **141**, 7990 (2019).

[9] M. A. Healy et al., *Chem. Eur. J.* **25,** 6326–6331 (2019).

efficiently disperse lignins within a thermoplastic matrix using zinc chloride salt[10] which results in a 100% increase in tensile strength and an order of magnitude rise in Young's modulus (stiffness).

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 recovery and recycle 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.

With 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.

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.

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) 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 development of better strategies for model evaluation and connection 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,

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[10] S. Barnes et al., Macromol. *Rapid Commun.* **40,** 1900059 (2019).

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 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 ARM program. With over 1.8 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. The team recently deployed a ship-based data system for the ongoing Multidisciplinary Drifting Observatory for the Study of Arctic Climate (MOSAiC) campaign conducted from an icebreaker near the North Pole and successfully processed data from the Cold-Air Outbreaks in the Marine Boundary Layer Experiment (COMBLE).

ORNL infrastructure supporting climate change science and atmospheric science includes leadership-class computing through 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), US Air Force (USAF), and the USDA's Forest Service (USDA-FS) 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. 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, that 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 of new nanomaterials; closing the carbon cycle, predictive understanding of microbial, molecular, cellular, and whole-organism systems; simulation of nuclear fission and fusion systems; 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 that addresses problems which are only tractable using HPC for companies of all sizes, including SmartTruck Systems, GE, Rolls-Royce, Ford, Arconic, and Boeing.

Example applications under active development for current and future leadership computing platforms include DCA++ for simulation of superconducting materials; QMCPACK for simulation of electron structure of atoms, molecules, and solids; AMPERES for multiphysics simulation of electrochemical and renewable energy storage; Kokkos development for performance portable use of diverse HPC, and DataTransferKit, a parallel solution transfer service code for multiscale, multiphysics simulations. ORNL support for the ECP Applications Development (AD) focus area includes leadership of 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 contributions to another 10 of 24 ECP AD projects, including E3SM development and wind power (ExaWind).

These capabilities are applied to deliver integrated, scalable solutions to complex problems of interest to DOE and other sponsors, including materials design, advanced manufacturing, electrical energy storage (batteries and supercapacitors), 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, and EERE. Other offices and agencies, including OE, DoD, IC, HHS, and NSF, also sponsor or collaborate on activities that leverage DOE investments in computational science.

Condensed Matter Physics and Materials Science

ORNL has world-leading capabilities for predicting, synthesizing, characterizing, and ultimately controlling materials systems over broad temporal and spatial scales. This makes 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. The scientific themes of this 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. ORNL has specialized expertise in synthesis of single crystals, thin films, artificial heterostructures, alloys, nanophase materials, polymers, and polymer composites. For example, precision synthesis of quantum heterostructures enabled the discovery of a large orbital polarization in correlated $LaNiO_3/SrCuO_2$ heterostructures by deliberately modifying the interface.[11] Synthesis of a $CsYbSe_2$ crystal and its study by neutron scattering found a magnetic signature that indicates its candidacy for a quantum spin liquid ground state.[12] The quantum materials synthesis effort will be focused on the discovery of novel topological and correlated quantum materials using the new spin- and angle-resolved photoemission spectroscopy for understanding their electronic structures. A study of the interfacial layer structure in polymer nanocomposites demonstrated that preadsorbing polymer chains to nanoparticles significantly improves their dispersion in polymer nanocomposites.[13]

[11] Z. Liao et al., *Nature Commun.* **10,** 589 (2019).

[12] J. Xing et al., *Phys. Rev. B* **100,** 220407(R) (2019).

[13] A. C. Genix et al., *ACS Appl. Mater. Interfaces* **11,** 17863 (2019).

Neutron scattering is employed to gain an understanding of quantum matter, dynamics of light elements, energy storage materials, and polymers. A recent study observed a novel nonlinear mechanism for stopping heat-carrying phonons in a perfect crystal of thermoelectric PbSe.[14] In addition, neutron scattering was used to reveal the diffusion behavior of H^+ and Li^+ ions individually in cubic $Li_{6.25}Al_{0.25}La_3Zr_2O_{12}$,[15] providing insights into the properties of solid electrolytes used in aqueous lithium batteries.

Enabled by electron beam atom-by-atom manipulation, two QIS projects were recently initiated to create, enhance, and stabilize entangled and correlated quantum states through direct control over dopants, defects, and material geometry.[16] Electron microscopy is being used to modify and characterize materials at the atomic scale in order to "quantum functionalize" them. Understanding fundamental nanoscale processes that drive qubits and quantum sensors with topological and superconducting materials is also an ongoing research area.

Leadership capabilities in materials imaging, including in situ electron microscopy and spectroscopy, scanning probe microscopy modalities, atom probe tomography, and chemical imaging, are made available through the CNMS user program. A scanning probe microscopy study discovered quadruple-well ferroelectricity in layered $CuInP_2S_6$ crystals based on a structural phase that doubles electrostatic polarization owing to the van der Waals gap.[17] Developing deep learning networks from scanning transmission electron microscopy (STEM) is also an active research subject to advance automated image analysis and recognition of the defects in solids.[18]

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 [(QMC] and Locally Self-Consistent Multiple Scattering [LSMS]) that take advantage of OLCF. Powerful algorithms are used to calculate the ground state properties of low-dimensional models inspired by iron-based superconductors and characterized by having several active orbital degrees of freedom in addition to magnetic spins.[19] ORNL is developing approaches to apply these codes to next-generation exascale computation as part of a BES Computational Materials Science project and an ECP project focusing on QMC. A joint ASCR-BES project supported through SciDAC is also being conducted to develop a computational framework for controlled and unbiased studies of strongly interacting electron systems in quantum materials.[20,21]

The Energy Deposition Defect Evolution EFRC led by ORNL focuses on elucidating the origin of radiation damage using a set of high-entropy alloys combined with atomic-level characterization and computational approaches. This project has provided invaluable information for designing the next generation of radiation-resistant alloys for nuclear and other applications and will be ending in FY 20.

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[14] M. E. Manley et al., *Nature Commun.* **10,** 1928 (2019).

[15] X. Liu et al., *Energy Environ. Sci.* **12,** 945 (2019).

[16] O. Dyck et al., *MRS Bull.* **44,** 669 (2019).

[17] J. A. Brehm et al., *Nat. Mater.* **19,** 43 (2020).

[18] M. Ziatdinov et al., *Sci. Adv.* **5,** 9 (2019).

[19] J. Herbrych et al., *Phys. Rev. Lett.* **123,** 027203 (2019).

[20] S. Li et al., *Phys. Rev. B* **100,** 020302(R) (2019).

[21] P. Laurell and S. Okamoto, *npj Quantum Mater.* **5,** 2 (2020).

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 visual analytics, data analytics, ML and deep learning, database architectures, secure communications, signals analysis, and information security to (1) collect, share, intelligently store/retrieve, analyze, and classify enormous and heterogeneous collections of data; (2) create knowledge from disparate and heterogeneous data sources; and (3) understand, defend against, and defeat known or unknown adversaries to protect the nation's energy, economic, and security infrastructures.

Cybersecurity is a domain where human-centric operations drive the efficacy of network security architectures. ORNL has substantial capability in developing technologies that optimize and enhance the defensive value of cybersecurity operations. Outcomes from this core capability are translated from R&D to deployment through partnership with operational cyber infrastructure and co-located expertise. ORNL is successfully transferring technologies based on rigorous mathematical results to address cyber and information security challenges. Tools such as Situ (cyber situational awareness), Oak Ridge Cyber Analytics (ML-based network security for DoD), Akatosh (forensics), Beholder (cyber-physical protection), and others have been licensed to multiple parties or operationally fielded within the US government. In addition, ORNL is developing a new capability 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 software vulnerability discovery.

Information science and data play a crucial role in both scientific discovery and mission-oriented decision making. The grand challenge is how to collect, organize, and structure the complex and voluminous data so it is useful and informative for end-use scenarios. Solutions to this problem 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, data curation, smart storage/retrieval, and feature engineering that leverage resources such as OLCF, the 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 allow for deep learning on HPC systems, providing unparalleled insights into the behavior of malicious and nefarious cyberspace actors.

QIS R&D is providing game-changing capabilities for secure communications and control systems, especially in protection of the electric grid, where new programs have been awarded by the Cybersecurity for Energy Delivery Systems R&D program of DOE's Office of Cybersecurity, Energy Security, and Emergency Response (CESER). The combination of these cybersecurity and quantum communication capabilities spans areas such as cyberphysical systems protection, trusted and secure communication architectures, and persistent threat detection and mitigation in networks. Further, ORNL develops mathematical methods for identifying the impacts of complex attacks on cyber infrastructures, including software-defined networks, and game-theoretic strategies for ensuring infrastructure resilience in the presence of intentional and incidental disruptions. This capability extends to supercomputing, where assurances in computational 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), classified HPC systems, the Center for Trustworthy Embedded Systems, the Vehicle Security Laboratory, the Resilient Cyber Physical Systems Laboratory, 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 cyberphysical 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, IC, the US Department of Transportation, DHS, the US Department of Veterans Affairs, 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 system–based decision science, including geospatial decision support tools that aid national security sponsors in making decision 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 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 ORNL's expertise in geospatial Bayesian decision support systems, particularly in the area of building intelligence, ORNL is hiring Chris Krapu (from Duke University).

ORNL uses geographic information science for decision and risk analyses of critical infrastructure expansion and population mapping. 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, IC, 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 supports 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 consequence assessment, 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, military, and IC missions.

To support ORNL's multimodal data decision science and analysis core capability with their ML and data analytics expertise, ORNL has hired Nisha Srinivasan, Robert Zhang, Colin Smith, and David Cornett.

The 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 utilized 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, IC, the Federal Emergency Management Agency, NRC, 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) applying highly sensitive tracers in CO_2 capture and storage to validate the integrity of CO_2 geosequestration; (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 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 of 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 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 use.

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 OLCF, state-of-the-art greenhouses, field and laboratory facilities (including the Environmental Science Laboratory, Aquatic Ecology Laboratory, Mercury SFA Field Site, and the Y-12 Integrated Field Research Challenge site), JIBS, 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 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) delivery of a predictive understanding of complex, heterogeneous, multiscale environmental systems to describe uranium fate and transport in subsurface systems (e.g., through the ENIGMA consortium's demonstration of the role of groundwater hydrogeochemistry on the day-to-day population shifts in local subsurface microbial communities); (2) field- to molecular-scale geochemistry and microbiology to elucidate the coupled physical and biogeochemical processes that govern mercury transformations in headwater streams and their surrounding watersheds; (3) state-of-the-art subsurface hydrology and reactive transport model development; 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 state, flux, 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.

Elizabeth Herndon, previously at Kent State University, has joined ORNL as an environmental geochemist whose research incorporates methods such as field sampling, mesoscale laboratory experiments, and analytical techniques.

This core capability comprises a wide range of state-of-the-art facilities, including the Critical Interfaces SFA Field Site, the Y-12 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 utilized. 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 that 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.

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 (FnPB) is available at SNS. Significant investments in instrument improvements, sample environment, and data analysis capabilities make ORNL's neutron scattering instruments world leading. Construction of the Versatile Neutron Imaging Instrument (VENUS) at SNS, now 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 STS at SNS is planned. The Proton Power Upgrade (PPU) and STS projects leverage DOE's investment in neutron sciences. The PPU will increase the neutron peak brightness and flux at the SNS First Target Station, thereby increasing scientific capacity and capability on currently oversubscribed instruments. The PPU project also provides the platform for the STS. PPU construction has begun. ORNL is pursuing CD-2 and CD-3b approval for remaining PPU construction activities and CD-1 approval for STS in FY 2020.

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 will be well positioned for the next 20 years following the planned installation of a new beryllium reflector with a design that supports improved neutron production while maintaining performance for neutron scattering. ORNL is evaluating upgrade paths for HFIR to sustain its world-leading capabilities. Options under consideration include pressure vessel replacement and alternative moderators and fuels.

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 operations. 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. ORNL's other strategic HPC resources include the Cray XC40 Gaea system, operated for NOAA to facilitate multiagency cooperation and R&D partnerships across the climate research community. Through a strategic partnership with USAF, ORNL provides mission-critical regional and global weather products that maximize America's war fighting power through the exploitation of timely, accurate, and relevant weather information. The research portion of this partnership has developed sophisticated weather models for advanced architectures through acceleration of Air Force models using techniques that can be leveraged within DOE. The partnership relies on ORNL's National Center for Computational Sciences to provide high-availability, production-hardened HPC systems and services.

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 (1) rapid synthesis and characterization via a pulsed laser 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 (CL) microscope that offers angle, polarization, temperature, wavelength, spatial, and time-resolved CL microscopy. CNMS has acquired a Raith VELION nanofabrication system, a combined focused ion beam (FIB)/scanning electron microscope 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 and 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 hiring a dedicated CNMS staff chemist to develop and improve deuteration methods for small molecules that are critical for neutron experiments of biomaterials and polymers.

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 project at SNS, the MAJORANA Demonstrator project, the Material Plasma Exposure Experiment (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, expertise in mass spectrometry has contributed to the development of large-scale stable isotope enrichment systems. Expertise in the analysis of stress, strain, and thermal effects in composite materials, fluid dynamics, and dynamic analysis of rapidly rotating devices has 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 after-treatment development).

Mechanical engineering capabilities at ORNL have been used to developed remote systems for SNS, INMC, and, most recently, the Facility for Rare Isotope Beams (FRIB) at Michigan State University. 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. 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 focuses for ORNL's nuclear and radiochemistry research are the nuclear engineering design of advanced targets for efficient production of isotopes and 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. For example, development of methods for the separation of berkelium-249 from californium-252 enabled the discovery of four superheavy elements, including tennessine. Other actinide separations techniques, such as those for the separation of decay-enriched californium-251 and curium-248 from californium-252 sources, are supporting the search for new superheavy elements in the approach to the island of stability. These capabilities have also enabled the development of specialized sources (including radioisotope power sources and sources used in the generation of specific nuclear signatures) and have inspired new ultra-trace characterization methods (such as isotope dilution mass spectrometry). ORNL's nuclear chemistry and enrichment expertise is also involved in maintaining and improving our nation's 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 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 is also examining long-term needs for radiochemistry facilities to support increasing demand for radioisotopes for use in medical, industrial, and research applications. ORNL is the nation's sole producer of californium-252 and high-specific-activity nickel-63, both of which are important in security and industry. Capabilities also exist for recovery of actinium-225, an increasingly important medical isotope, from thorium-229. ORNL radiochemists use hot cells and radiological facilities to process and characterize other important radioisotopes, such as selenium-75 used in radiography, nickel-63 used in explosives detection, barium-133 used as a calibration source, and medical isotopes actinium-227, tungsten-188, strontium-89, and lead-212. ORNL has established production capability for delivery of actinium-227 for medical applications and has launched an effort to identify the resources needed to meet the increasing demand for this radioisotope. Funding provided by NASA supports production of plutonium-238 for use in radioisotope power supplies and heat sources for planetary science missions. An automated target-processing system for the Pu-238 Supply Program is enabling plutonium oxide production from about 50 to 400 g/year.[22]

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

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[22]R. M. Wham et al., "Automation of Neptunium Oxide-Aluminum Target Fabrication," presented at NETS 2019—Nuclear and Emerging Technologies for Space, Richland, WA, February 25–28, 2019. Available at http://anstd.ans.org/NETS-2019-Papers/Track-5--Radioisotope-Power-Systems/abstract-118-0.pdf (accessed April 2, 2020).

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 development of new materials and systems for fission and fusion, taking advantage of specialized facilities and core capabilities in materials science, chemistry, chemical engineering, computing, 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 project (referenced in Section A.13), which will enable a full demonstration of the potential for combining advanced manufacturing, data science, and materials science to accelerate development of advanced nuclear energy systems. Cutting-edge data science and computation may allow autonomous sensor and control systems, as well as utilize ML for component, system, and material design and optimization. ML has been heavily utilized at ORNL to improve reactor performance, enabling new operational regimes and improved safety and economics.

ORNL’s nuclear engineering expertise is critical to the continued viability of the nuclear power industry, including improved operations and life extension of the existing fleet.[23,24] ORNL’s expertise in the design and post-irradiation examination of HFIR irradiation capsules is used to study reactor materials and accident-tolerant fuels.[25] 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,[26] materials, and salts; improved instrumentation and controls; regulatory research; thermal-hydraulic experiments; and innovative system concepts. ORNL is the world leader in MSR 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

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[23] A. Abd-Elssamd et al., *ACI Mater. J.* **117** (1), 265 =–277 (2020).
[24]R. Montgomery et al., *Nucl. Sci. Eng.* **193,** 884–902 (2019).
[25] N. M. George et al., *Ann. Nucl. Energy* **132,** 486–503 (2019).

[26] C. M. Petrie et al., *J. Nucl. Mater.* **526,** 151783 (2019).

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.

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 enabled reliable, high-fidelity solutions for large-scale, complex problems. The ORNL-led Consortium for Advanced Simulation of Light Water Reactors (CASL) has 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 under CASL, is being leveraged to provide scientific understanding and solution of 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 has hired Vittorio Badalassi, a world-leading expert in computational thermodynamics, who is establishing a coordinated strategy for development of computational fluid dynamics codes, with the expectation that he will contribute to the development of engineering simulation capabilities and support design and safety analyses for advanced nuclear reactor concepts.

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 several sources, including NE, SC, NNSA, DHS, the Defense Threat Reduction Agency, NASA, NRC, and other government agencies.

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.

Nuclear Physics

ORNL's core capability in nuclear physics makes crucial contributions to DOE's NP portfolio, in both discovery science and applied programs. It spans theoretical and experimental research that is relevant to DOE's mission of developing an understanding of nuclear matter and fundamental symmetries 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 is making crucial contributions to the detector operation and data analysis. ORNL 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 using a germanium detector invented at ORNL and developed with NP support. At the FnPB beamline at the SNS, the ORNL-led search for nEDM provides a complementary probe of the matter-antimatter asymmetry. Data analysis for the n-^{3}He experiment has been completed with publication pending. Combined with the NPDGamma results, it provides the most precise measurement of parity violation in hadronic weak interactions. Nab, the next experiment at the beamline, will make the most precise measurement of the electron-neutrino correlation parameter during a neutron decay. The experiment is on track to start commissioning and begin data acquisition in the fall of 2020.

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. A search for the superheavy element 119 is under way at RIKEN using curium-248 targets and digital electronics supplied by ORNL.

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 soon 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 has unique expertise in the design and development of specialized electronics and detectors relevant to research at the Large Hadron Collider (LHC) at CERN 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. This expertise will be applied to the development of detectors for the future Electron Ion Collider.

ORNL has initiated a program to resolve the computing problem for the detailed simulation of detector response for collider experiments in particle and nuclear physics. This program intends to use the HPC systems at ORNL to achieve an order of magnitude speedup of the simulation process.

ORNL's nuclear data program includes cross-section measurements, 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 technologies for isotope enrichment are being developed using electromagnetic isotope separation and gas centrifuge isotope separation. Major advancements have been achieved in both technologies underpinning the SIPF and SIPRC projects. These technologies will be matured, with a specific aim at lighter gases for the centrifuge technology. Efficient production pathways through advanced separation chemistry are being developed for radioactive isotopes.

Funding in this area originates from SC and defense programs (NNSA and SPP sponsors).

Plasma and Fusion Energy Sciences

ORNL is DOE's lead laboratory for fusion nuclear science and fusion materials, which are required to fully enable fusion energy. ORNL scientists are experts in pellet fueling systems and are responsible for addressing challenges associated with closing the fusion fuel cycle, a requirement for a fusion pilot plant. Materials scientists at ORNL conduct experiments to support development of alloys and silicon carbide composites, which 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. These radiation-tolerant materials will be required to make a fusion pilot plant reliable and economical. ORNL's core capability in plasma and fusion energy sciences, 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 well positioned to support the recommendations of the National Academies' Committee on a Strategic Plan for US Burning Plasma Research.[27] ORNL addresses the Committee's first recommendation, "the United States should remain an ITER partner as the most cost-effective way to gain experience with a burning plasma at the scale of a power plant," through its leadership of the US ITER Project, its R&D and fabrication of US contributions to ITER, and its active participation in research related to burning plasmas and ITER technology. ORNL addresses the Committee's second recommendation, "the United States should start a national program of accompanying research and technology leading to… a compact pilot plant that produces electricity from fusion at the lowest possible capital cost," by leadership and collaborations developing the fusion technologies needed for a compact pilot plant.

The recommendations made by the APS Division of Plasma Physics Community Planning Process indicate that ORNL's position in fusion nuclear science and materials is also key to the priorities likely to emerge from the 2020 FES Advisory Committee Long-Range Strategic Plan.

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 as noted in the 2018 National Academies report. US hardware contributions include the world's highest-stored-energy pulsed superconducting magnet; superconductor for ITER toroidal field coils; a 1 gigawatt cooling water system; high-power, long-pulse plasma heating systems; electrical power system components; 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.

ORNL has made progress toward the demonstration of the science and engineering to sustain a magnetically confined plasma with the properties needed for a compact fusion pilot plant. In parallel with US ITER efforts, ORNL applies its broad experimental and theoretical expertise in plasma science, strong synergies with materials in extreme environments, and computational science programs to develop materials, components, and power exhaust and particle control solutions that can meet the demands of a burning plasma environment and enable fusion energy. ORNL scientists and engineers are building MPEX to address the challenges associated with exposing materials to high-energy, high-density

[27] National Academies of Sciences, Engineering, and Medicine, *Final Report of the Committee on a Strategic Plan for U.S. Burning Plasma Research,* National Academies Press, Washington, DC, 2019.

plasmas. 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.

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 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 testing the source concept for MPEX.

ORNL continues to hire leading experts in nuclear fusion and fusion engineering, including Kathy McCarthy, Director of the US ITER Project, and Mickey Wade, Director of the Fusion Energy Division.

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 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 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 (EPB) reinforces this core capability by providing real-world understanding and commercial-scale implementation of emerging technologies. ORNL's Grid Research, Integration, and Deployment Center (GRID-C) 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, removing "range anxiety" and long charging times because the 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 (IoT) including connected sensor and internet framework, 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 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 of combustion processes, understanding materials properties for advanced manufacturing, 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, Proto-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 CMI), 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, 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 the world's premier research institution, ORNL will attract and retain a diverse staff with the highest potential, training and equipping them for realizing professional growth and delivering impactful scientific breakthroughs. We will also invest in infrastructure and resources, including state-of-the-art equipment, needed to drive a premier research institution.

ORNL will steward and advance capabilities at a set of DOE user facilities in nanoscience, neutron scattering, high-performance computing (HPC), advanced manufacturing, building technologies, electrical grid, and transportation to provide world-leading research capabilities for researchers in academia, government, and industry. To drive the scientific underpinnings of new technologies, new tools are needed to bridge length and time scales to understand how atomic-scale structure and dynamics impact mesoscale properties. These efforts will take full advantage of the current Proton Power Upgrade (PPU) project at the Spallation Neutron Source (SNS), which will provide exceptional capabilities for studying the structure of materials at highest resolution while requiring far less sample. The increased power of the PPU, coupled with the Second Target Station (STS), will provide the world's highest peak brightness cold neutrons and will yield unprecedented capabilities for studying material dynamics and hierarchical structures. These advances at the SNS connect strongly with expanded synthesis and characterization capabilities at the Center for Nanophase Materials Sciences (CNMS) in both polymers and quantum materials, as well as with the core DOE programs at ORNL. Potential upgrades are being assessed 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. ORNL is preparing to lead the exascale computing revolution by delivering the Frontier system at the Oak Ridge Leadership Computing Facility (OLCF) and examining approaches to realize next-generation, extreme-scale heterogeneous computing.

ORNL will invest in new capabilities to sustain leadership in eight science and technology (S&T) initiatives (listed in Table 4.1 and described in the subsections below) to drive S&T preeminence in these areas. In addition to these areas, we will utilize Laboratory Directed Research and Development (LDRD) resources to advance multidisciplinary discovery and innovation to integrate these S&T initiatives and address the global challenge of closing the carbon cycle. ORNL will produce scientific discoveries and technical breakthroughs that support this goal through the co-design of materials and processes, and in doing so, contribute to the development of sustainable carbon-based economies. We will focus on two primary thrusts: (1) combined carbon capture–separation–conversion to high-value products and (2) chemistries that use captured CO_2 for processing higher level polymers. (See also Appendix C.)
To meet this challenge, we envision a new data-driven approach for discovery that moves beyond Edisonian processes to accelerate the pace of scientific discovery. This approach will integrate HPC, computational simulation, analysis, data science, and experiments to provide unprecedented opportunities for science. This will allow scientists to continually learn and update their predictions based on data from an array of interoperating and interdependent instruments and experiments facilitated by data and computing at the edge. The outcomes of this initiative are anticipated to have broad impact, including (1) accelerated and improved imaging and scattering capabilities; (2) smart, "self-driving" experiments and synthesis processes; (3) real-time model-experiment loops; (4) inverse approaches to materials design; and (5) control of metastable and non-equilibrium states to realize new materials and processes.

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 5,000 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 194 operational buildings (4.4M gross sq. ft. [GSF]) owned by the DOE Office of Science (SC), 1 operational building (0.02M GSF) owned by the DOE Office of Nuclear Energy (NE), and 77 operational buildings (0.38M GSF) owned by DOE's Office of Environmental Management (EM), reflecting the multiprogramatic support of ORNL's infrastructure. Fifty-one buildings in shutdown status, owned by SC, EM, and NE, represent 0.30M GSF of ORNL's building inventory. A total of 16 SC-owned buildings (0.13M GSF) are awaiting disposition, having been excessed to DOE, and seven SC-owned buildings (0.05M GSF) are in a standby status awaiting repurpose or reuse. UT-Battelle has extensive experience interfacing with EM contractors (e.g., with UCOR, the EM cleanup contractor), as they have executed numerous EM projects in the middle of the ORNL central campus. Active coordination with EM contractors will continue and grow as decontamination and decommissioning (D&D) activities accelerate across the ORNL site. UCOR will establish a larger presence onsite in FY 2020 as characterization and mitigation begins in the central campus area for an increase in scope of D&D activities.

All SC mission-unique facilities (1.2M GSF) have an adequate condition rating. Of SC's non-mission-unique facilities, 91% are rated adequate, with the balance rated substandard. Substandard buildings, typically more than 50 years old, will be modernized. For SC's operating Other Structures and Facilities (OSFs), 88% are rated adequate with the remaining 12% rated substandard. Building 4500N (363,980 sq. ft.) is the largest substandard building on campus, with $4.7 million in operating costs and repair needs of $28 million. This facility and aging plantwide utility systems (i.e., substandard OSFs) are important focus areas for modernization.

Research that requires ready access for industrial partners is conducted in off-site leased facilities (10 facilities totaling 0.32M GSF). ORNL's Hardin Valley Campus, about 7 miles from the main campus, hosts the Manufacturing Demonstration Facility (MDF); GRID-C, including the Battery Manufacturing Facility; and the National Transportation Research Center. The Carbon Fiber Technology Facility is located at a separate site in Oak Ridge, 5 miles from the main campus. ORNL's leased space portfolio is evaluated frequently to ensure best support of mission needs and to identify consolidation or reduction opportunities. There was no change to the leased space portfolio in 2019; however, ORNL has renewed the lease for Union Valley in 2020. 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, Oak Ridge National Laboratory, Oak Ridge, Tennessee), and ORNL's *Site Wide Master Plan* can be found at https://services.ornl.gov/ronweb/Media/ORNLswmp.pdf.

Campus Strategy

ORNL's campus strategy is focused on advancing distinctive scientific missions. The execution of this strategy relies on achieving four primary objectives:

1. Advance science and energy leadership.
2. Establish a modern, adaptable infrastructure to support research.
3. Return the ORNL Central Campus to productive science missions.

4. Reduce excess facility liabilities.

These four objectives will be accomplished, in part, by successfully addressing critical infrastructure needs identified through ORNL's Mission Readiness process and will culminate in the planned facilities and infrastructure investments shown in Fig. 6.1. ORNL will continue to evaluate changes to campus strategy in regard to new office and parking construction as the "new normal" evolves. Construction of new office space and parking have been pending final evaluation.

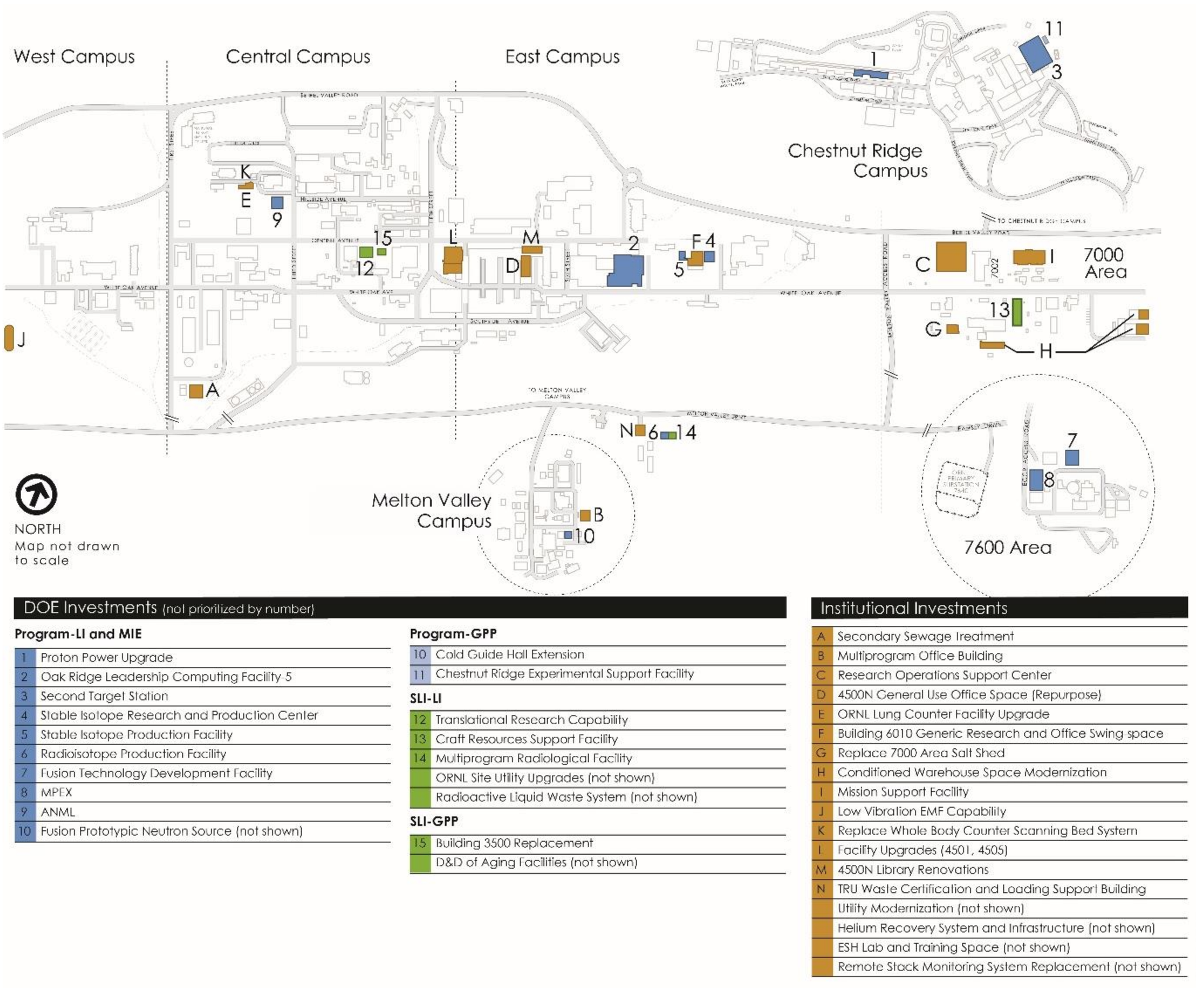


Figure: Proposed facility and infrastructure investments

The figure above indicates how DOE and institutional investments to advance ORNL's scientific and technical capabilities could transform the nerve center of the ORNL campus into modern research space. The following investments are shown.

Six programmatic line item construction projects:

- Spallation Neutron Source (SNS) Proton Power Upgrade (PPU) project, supported by DOE SC Basic Energy Sciences (BES) (CD-1 and CD-3a and CD-3b approved)
- SNS Second Target Station (STS), supported by BES (CD-1 in process)
- Stable Isotope Production and Research Center (SIPRC), supported by DOE SC Nuclear Physics (NP) (CD-0 approved)
- Radioisotope Production Facility, supported by the Office of Isotope R&D and Production (IRDP) (CD-0 in process)

- Advanced Nuclear Materials Laboratory (ANML), supported by NE
- 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-3a approved, CD-2/3b approved)

Three Major Item of Equipment (MIE) projects:

- Stable Isotope Production Facility (SIPF), supported by IRDP (progressing toward CD-2/3 equivalent)
- Material Plasma Exposure Experiment (MPEX), supported by FES (CD-1 approved)
- Fusion prototypic neutron source (FPNS), supported by FES (proposed for FY 2023)

Five Science Laboratories Infrastructure (SLI) line item (LI) construction projects:

- Translational Research Capability (TRC) (CD-3a approved, CD-2/3b in process)
- Craft Resources Support Facility (CRSF), (CD-1 approved, status delegated)
- Radioactive Liquid Waste System (CD-0 approved)
- Site Utility Upgrades (proposed for FY 2022–FY 2029)
- Multiprogram Hot Cell Facility (proposed for FY 2023–FY 2025)

Two programmatic General Plant Projects (GPPs):

- Chestnut Ridge Experiment Support Facility, supported by BES (proposed for FY 2021–FY 2023)
- High Flux Isotope Reactor (HFIR) Cold Guide Hall, supported by BES (proposed for FY 2021)

Two SLI GPPs:

- Building 3500 Replacement (proposed for FY 2022–FY 2023)
- D&D of Aging Facilities (proposed for FY 2022-FY 2023)

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.

Advancing the impact and application of neutron science

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 54 years and is a key scientific asset with capabilities unlikely to be eclipsed by new reactor designs. Upgrading HFIR with a new pressure vessel and making strategic facility improvements would improve and extend the reactor's capabilities for at least another half-century at a fraction of the cost of new construction. Longer-term sustainment of HFIR capabilities includes replacement and refurbishment of critical components.

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, a sample environment, and equipment.

Scaling computing and data analytics to exascale and beyond for science and energy

Leadership-class computing underpins nearly all scientific disciplines. Thus, continued development of ORNL's high-performance computing (HPC) infrastructure as part of 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 2020 and acquisition, installation, and operation of an initial exascale system, Frontier (OLCF-5), in 2021–2022. To leverage significant prior investments (about $100 million) in power and cooling water systems, Frontier will be housed in Building 5600, and Building 5800 will be reconfigured to increase power and cooling capabilities 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 to the edge, ORNL has created the Scalable Distributed Data Infrastructure initiative with a mission to capture, store, and curate data and metadata from various sources in scalable fashion, requiring significant enhancements to the optical fiber network and transmission capabilities to instruments at distributed locations across the laboratory. To mitigate this infrastructure capability gap, institutional investments are planned for high-bandwidth network capability.

Discovering and designing 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 our quantum materials and quantum information science (QIS) initiative (see Section 4.3). To support increasingly sensitive imaging equipment, institutional funds have been allocated to provide a low-vibration, low-electromagnetic field capability. In preparation for the TRC facility, a $93 million investment, ORNL has successfully completed CD-3a with CD-2/3b in process.

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.

Achieving breakthroughs in nuclear science, technologies, and systems

ORNL's nuclear capabilities support a broad range of efforts: several SC programs (NP, FES, and BES), other DOE programs (NE and the National Nuclear Security Administration), 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 at BWXT. In addition, a new permanent beryllium reflector and four new beam tubes are being fabricated in preparation for the beryllium reflector replacement outage scheduled to begin in FY 2024.

- *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 consistently funding INMC operation would ensure long-term sustainability and compliance with DOE's nuclear safety standards. The demand for new approaches to realizing next-generation nuclear energy systems has driven an effort to pursue mission need approval (CD-0) by NE for the ANML, a radiological facility, to expand ORNL's capabilities for world-class nuclear-related materials research, development, analysis, testing, and qualification. Also, ORNL is initiating plans to construct a Multiprogram Hot Cell Facility proposed for FY 2023–FY 2025, which will position ORNL to continue and expand its nuclear R&D work in the next decade. These new capabilities will enable D&D of some nuclear facilities currently operating in the Central Campus as scheduled by EM.
- *Fusion Prototypic Neutron Source.* A fusion prototypic neutron source has been identified by the recent American Physical Society Division of Plasma Physics Community Planning Process as a high-priority facility for fusion energy, and FES has indicated that development of a mission need statement may occur in late FY 2020. Options to repurpose existing ORNL facilities are currently being evaluated and would require additional resources (e.g., power, water cooling). ORNL will continue to support FES in this effort.
- *Fusion Technology Development Facility.* ORNL is developing plans for the Fusion Technology Development Facility (proposed for 2025), which will enable advancement in several key fusion technology areas, including power exhaust and particle control, fusion blanket and fuel cycle, and heating and current drive research. This facility will require investment in new infrastructure, including a new building, multiple flexible laboratories, high bay space, and sufficient utilities to support a diverse R&D program.

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 a number of 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 a number of 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 Production Facility (CD-0 in process) 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

Revitalizing ORNL's 7000 area as a 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 and houses 600 craft personnel. Modernization of this area began in 2013–2014 with construction of an IGPP-funded shipping and receiving facility. The Research Operations Support Center (ROSC), which will centralize and co-locate security and fire response personnel, is under construction using IGPP funds with an estimated completion date of December 2020. ROSC will allow the lab to exit and D&D two Central Campus facilities. SLI-GPP investments to address longstanding environmental challenges to our fabrication and machining operations have been completed. This renovated space houses state-of-the-art fabrication equipment, increasing capabilities for larger parts and assemblies procured through institutional investments. Institutional investments are also planned to construct a new Mission Support Facility. The Craft Resources Support Facility, which received CD-1 approval in April 2020, will provide modern facilities in the form of a vehicle garage and shops for sheet metal workers, carpenters, mechanics, and electricians, thereby enabling the D&D of 10 or more 1950s vintage facilities.

Modernizing ORNL's utility systems

Reliable, efficient, and maintainable utility infrastructure provides the foundation for successful scientific achievement. High-performance, reliable electrical, fiber, potable water, and other utilities are critical to the numerous DOE missions conducted at the laboratory. Continuous, uninterrupted operation of ORNL facilities provides researchers with cutting-edge scientific tools that support in-depth research and drive 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 installed as part of the Manhattan Project are becoming increasingly inefficient and difficult to maintain, resulting in more frequent need for emergency repairs complicated by obsolescent parts, which is an increasingly difficult challenge. These factors combine to increase costs while decreasing reliability and efficiency. Further, the aging systems were not designed to support modern research. Although preventive maintenance and institutional investments have maintained a high level of service, they cannot address large-scale modernization. To correct deficiencies in utility systems (electrical, fiber, potable water), an SLI LI is proposed for FY 2023 (CD-0 in process). This investment will modernize the highest-risk deficiencies identified by utility system stewards through condition assessments and inspection.

Managing radioactive waste

In the past, ORNL has relied on EM infrastructure for management of gaseous, liquid, and transuranic debris waste from nuclear and radiological facilities. This 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 the existing infrastructure once legacy waste missions are completed. With this deadline as motivation, ORNL has been developing independent capabilities to achieve waste management self-sufficiency. IGPP investments have created a remote-handled waste loading station at REDC, and investments have been made to construct a local high-efficiency particulate air filtration system and exhaust ventilation stack at Building 3525 to enable its removal from the EM-operated central stack. The Building 3525 ventilation system is planned to be operational in early FY 2021. In the near term (2022–2023), ORNL needs to obtain storage facilities from EM and adapt them for packaging transuranic waste as EM completes its transuranic mission in Oak Ridge. 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 established. Effort over the past few years has been devoted to waste minimization to reduce the capital investment required to provide this important capability.

Enabling biological and environmental research

Construction of a greenhouse/headhouse (approximately $6.1 million) will be completed in 2020, providing modern-day, automated phenotyping equipment to support the Center for Bioenergy Innovation, Next-Generation Ecosystem Experiments–Arctic, Spruce and Peatland Responses Under Changing Environments, and other environmental systems studies for rapid, data-rich collection and assimilation.

Objective 3: Return the ORNL Central Campus to Productive Science Missions

ORNL's strategy to revitalize the Central Campus includes five primary components: (1) construct the TRC, (2) construct or renovate an existing facility for ANML, (3) renovate or replace Building 3500 to provide modern office space near several important scientific facilities, (4) vacate 1940s-vintage mission support facilities, and (5) advocate for accelerating EM cleanup work.

Modernization of the ORNL Central Campus, which contains some of the laboratory's oldest facilities, is crucial to the execution of rapidly growing research programs. The planned removal of several aging facilities by EM is a key step in returning the Central Campus to productive science missions. ORNL is actively coordinating with EM D&D contractors to prevent barriers on the site in support of this objective.

ORNL's plan for this campus is to support EM in timely demolition and removal of decrepit facilities and associated contaminated soils, revitalize existing utility infrastructure, and construct a series of modern facilities to link the previously updated ORNL East and West campuses. Actions needed to realize Central Campus revitalization include (1) construct the TRC, (2) construct the ANML, (3) replace aging facilities, (4) vacate and demolish 1940s-era mission support facilities, and (5) advocate for a strong EM funding profile necessary to achieve cleanup efforts.

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 for HPC infrastructure in Building 5800. ORNL has received CD-3a approval with CD-2/3b in process.

Construct ANML

ANML is being proposed to support development of materials designed to withstand extreme environments (e.g., temperature, pressure, chemical, radiation, plasma) and to develop approaches leading to "born qualified" materials for these environments. ANML is envisioned as a radiological facility providing world-class capabilities for R&D, analysis, testing, and qualification of materials to surpass current performance limits and to extend service life in extreme environments. ORNL is working with NE to establish a Mission Need Justification.

Replace aging facilities

A proposed FY 2022 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 deferred maintenance.

Vacate and demolish aging mission support facilities

Upon completion of the ROSC in the 7000 area, ORNL will vacate the fire station (Building 2500, built in 1943) and the protective force station (Building 3037, built in 1951). Three other Central Campus buildings (Buildings 2518, 2523, and 2621) are all more than 55 years old. Collectively, these facilities represent 45,000 sq. ft of excess space that can be vacated and demolished.

Advocate for a strong EM funding profile

ORNL's Central Campus, a prime location for future development, houses a number of excess facilities that are awaiting final demolition. The presence of these aging facilities hinders modernization and mission delivery and increases liabilities and risks. Modernization of the Central Campus will be most quickly realized if facility demolition is accompanied by associated contaminated soil removal, thereby allowing immediate redevelopment. 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. Continuation of a strong EM funding profile is key to ensuring ORNL's ability to deliver on its mission.

Objective 4: Reduce Excess Facility Liabilities

ORNL currently expends approximately $2.5 million annually to address environmental and safety risks associated with SC excess facilities. Demolition of these facilities would free up these funds and reduce future expenditures needed to prevent further degradation. Further, several of these facilities are barriers to modernization.

Working with DOE's Excess Contaminated Facilities Working Group, ORNL has prioritized excess facilities into four groups:

- ORNL-managed SC and NE facilities at the Y-12 National Security Complex (Y-12),
- SC facilities in ORNL's Central Campus,
- 7000 area facilities (see Objective 2 above), and
- Balance of buildings for demolition.

SC and NE facilities at the Y-12

Due to deteriorated condition and size, ORNL facilities at Y-12 represent the highest ORNL cost risk. EM is preparing three Biology Complex facilities (Buildings 9207, 9210, and 9401-1) for demolition, which is scheduled to begin in FY 2020. Preparation of Buildings 9201-2 and 9204-1 for demolition will follow.

Former SC facilities in ORNL's Central Campus

SC has transitioned several Central Campus buildings to EM (Buildings 3003, 3010A, and 3080 in 2019; Buildings 3034 and 3036 in 2020). The presence of hazardous materials in these structures presents a risk to staff, mission, growth, and laboratory modernization and blocks prime real estate from redevelopment. To address these concerns, EM is planning a campaign in the Central Campus for the removal of the 3026 C&D Hot Cells, Isotope Row, and the research reactors (Buildings 3005, 3010, and 3042).

7000 area facilities

Demolition preparation work (e.g., characterization, abatement, personnel moves, and material cleanout) is taking place in FY 2020 to make way for construction of the Craft Resources Support Facility

(CRSF). Facilities slated for demolition in FY 2021 to clear space for construction of the CRSF include Buildings 7035A, B, C, E, and F; 7105; 7770; and 7033.

Balance of buildings for demolition

SC has recently transitioned Buildings 7600, 7609, 7610, and 7014 to EM to prepare for demolition. ORNL continues to clean up and dispose of abandoned facilities and experiments throughout its campus. For example, Building 3606 was recently demolished to prepare a site for construction of the TRC.

Future Infrastructure Gaps within a 10-Year Window

New greenhouse space is needed to support secure biosystems design, bio-design goals, and robotics systems for automated sampling, in addition to mass spectrometry and advanced, high-throughput imaging equipment.

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 17 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, 99 projects have been completed at a total cost of $224 million. Over the next decade, we expect to continue investing $25 million–$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. Thirty-three percent of ORNL's operational non-mission-unique facilities, representing approximately 34% of the total GSF, are more than 50 years old and carry nearly 48% of deferred maintenance.

Site Sustainability Plan Summary

The ORNL Site Sustainability Plan (SSP), submitted in December 2019, 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 8% from the FY 2008 baseline. ORNL will be challenged to meet any future GHG reduction goals because of mission-driven growth in energy demand.
- Energy use intensity (EUI) has decreased by 33.9% since FY 2003 and by 3.4% since FY 2018, exceeding the 1.0% year-over-year reduction target.
- Water use intensity (WUI) has decreased by 30.1% from FY 2007 and by 9.4% from FY 2018, exceeding the 0.5% year-over-year target. ORNL will continue to aggressively identify and repair leaks and seek creative solutions to reduce consumption.

High Performance Sustainable Buildings (HPSBs)

ORNL maintains a portfolio of 15% of applicable buildings that meet all HPSB Guiding Principles (GPs). ORNL has documented GP compliance for 20 applicable buildings and expects to meet or exceed the FY 2025 DOE goal of 17% HPSB inventory.

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. Projected annual savings include 12,358 million watt-hours of electricity; 17 million watts of electrical demand; 707,019 million Btu of natural gas; 18,864 million Btu of fuel oil; and 170 million gallons of water, all of which contribute to lower EUI and WUI.

Electricity Use, Historical Cost, and Cost/Use Projections

Figure 6.2 shows electricity use and cost for ORNL, including SNS and leased facilities. Estimated costs include escalation in Tennessee Valley Authority and municipality rates through FY 2031.

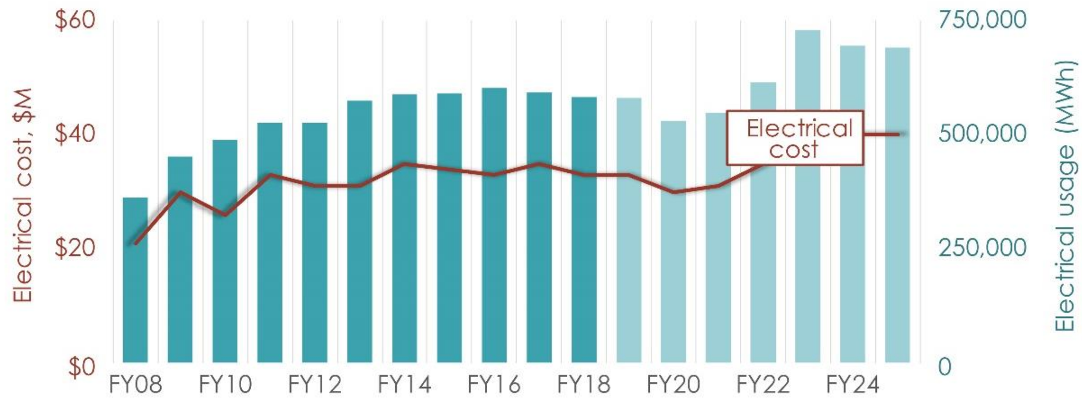


Figure: Electricity cost and use history and projections

Renewable Energy Credit (REC) cost projections

In FY 2019, ORNL purchased RECs to supplement on-site renewable energy generation from its five solar arrays and to achieve 9% renewable energy, thereby exceeding the statutory target of 7.5% of electrical energy consumption from renewable energy. Growth in electrical consumption is driven by HPC and other programs, and a significantly larger REC purchase will be required to achieve the target. ORNL will continue to investigate the economic feasibility of on-site renewable energy projects.

PACIFIC NORTHWEST NATIONAL LABORATORY

Lab-at-a-Glance

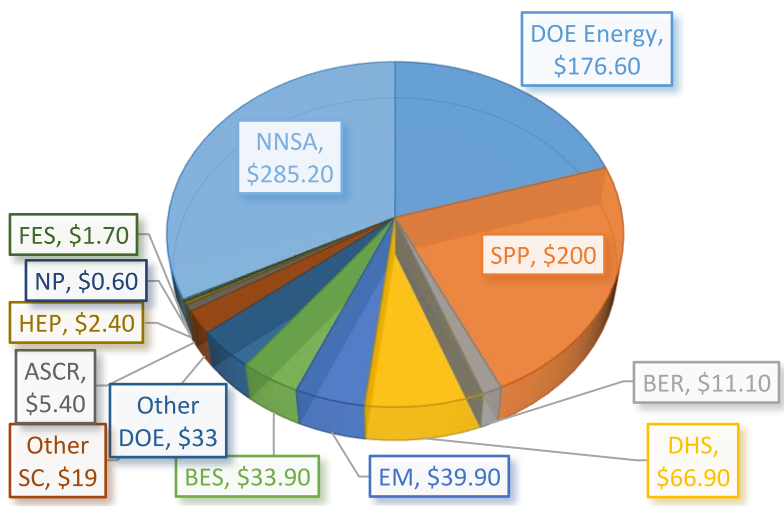
Location: Richland, Washington
Type: Multi-program Laboratory
Contractor: Battelle Memorial Institute
Site Office: Pacific Northwest Site Office
Website: www.pnnl.gov

- **FY 2019 Lab Operating Costs:** $938.3 million
- **FY 2019 DOE/NNSA Costs:** $708.7 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $200 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 21.3%
- **FY 2019 DHS Costs:** $66.9 million

Physical Assets:
- 549 acres and 76 buildings (DOE & Battelle Facilities)
- 1,180,712 GSF in buildings
- Replacement Plant Value: $934M
- 968,580 GSF in 30 Leased Facilities
- 166,477 GSF in 11 Battelle Buildings

Human Capital:
- 4,301 Full Time Equivalent Employees (FTEs)
- 150 Joint Appointments
- 287 Postdoctoral Researchers
- 414 Graduate Student
- 398 Undergraduate Students
- 1,557 Facility Users
- 71 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



Mission and Overview

Pacific Northwest National Laboratory (PNNL) draws on signature capabilities in chemistry, Earth systems, and data analytics 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 are inspired by biology to design catalysts and chemical pathways for new fuels, feedstocks, and energy storage materials. In Earth systems, we work to improve the predictive power of DOE's Earth system models, emphasizing Earth systems in transition. In data science, we combine machine learning (ML), data visualization, and modeling to create new knowledge from "Big Data." PNNL operates two DOE user facilities—the Environmental Molecular Sciences Laboratory (EMSL) and the Atmospheric Radiation Measurement (ARM) user facility, to advance knowledge of Earth system processes.

PNNL research enhances energy resiliency. We apply expertise in system situational awareness and high-performance contingency analysis to North American electric grid functions to design, test, and evaluate technologies for grid security, resiliency, and optimization. We apply chemistry and materials science capabilities to develop advanced energy storage solutions for grid resiliency

PNNL's national security capabilities are rooted in our Hanford heritage. We integrate expertise in data analytics, applied mathematics, and computational science to protect U.S. critical energy and defense infrastructures from emerging cyber threats. Our nuclear science capabilities advance nonproliferation, nuclear and radiological security, cleanup of radiological and hazardous wastes, fuel processing and disposal, nuclear forensics, and production and delivery of medical isotopes.

In 2015, PNNL began a 10-year, internally funded, $250M facilities transformation plan. To date, PNNL has invested approximately $148M in this recapitalization and is on track for a total investment exceeding its goal.

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.

Stewardship of core capabilities is an essential responsibility. To understand and manage this, PNNL has begun assessment of the health of its core capabilities using multiple indicators in an Integrated Capability Management framework that addresses health/quality of our 1) staff, 2) facilities and infrastructure, 3) equipment and assets, and 4) research portfolio. Each of these four critical components is assessed against six questions:

1. Sufficiency: Do we have enough?
2. Quality: Do we have the best?
3. Risks: Is the team/portfolio/collection of assets and infrastructure resilient?
4. Weaknesses: Do we have gaps/weaknesses?
5. Mitigating Factors: Are we pursuing mitigation strategies to address our risks and weaknesses?
6. Prognosis: Is the near-term expectation for the health of this capability improving, staying steady, or declining? What is the demand forecast?

PNNL's *Integrated Capability Management (ICM) Program Description Document – April 2019* 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.

Chemical and Materials Sciences

Chemical and Materials Sciences includes core capabilities in 1) chemical and molecular science, 2) condensed matter physics and materials science, 3) applied materials science and engineering, and 4) nuclear and radiochemistry.

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, multi-component systems.

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. 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, enabling 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), EM (environmental remediation), NNSA (nonproliferation), 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 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 quantum effects and mitigating materials degradation due to environmental factors. The Laboratory has domain expertise in the synthesis of nanostructures, biomolecular materials 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 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 materials, both inorganic and organic; the most advanced imaging 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, which was renewed at the end of FY 2018, and in the Center for the Science of Synthesis (CSSAS), an EFRC led by UW, which was newly 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.

This capability forms the basis for PNNL's sponsor-funded, fundamental science programs in synthesis and processing, biomolecular materials, 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, 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 optimum and leadership effort is attending to this. Some existing space shortfalls will be addressed with 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 device 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, biofuels, redox flow batteries, and many other clean energy technologies. PNNL holds domain expertise in materials characterization; materials theory, simulation, design, nucleation, and synthesis; solid phase processing methods for the fabrication of alloys and semi-finished products; the role of defects in controlling material properties; and materials performance in hostile environments, including the effects of radiation and corrosion. This capability includes the ability to engineer enabling nanostructured and self-assembled materials, as well as tailored thin films, ceramics, glasses, metal alloys, composites, and biomolecular materials. PNNL is also leveraging this capability to develop advanced waste forms (e.g., glass, ceramic, metallic, cementitious), key process control models, and tactical processing strategies to assure safe and successful operations for the immobilization and processing of nuclear wastes around the DOE complex.

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, solid oxide fuel cells, solid-state lighting, absorption cooling, lighter-weight vehicles, next-generation reactors, magnetics, separations, and nuclear waste management. 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 Facility, the Advanced Battery Facility, and the Solid-State Lighting Test and Analysis Facility. PNNL is currently in the planning stage for a new OE-funded battery materials development facility to consolidate and augment existing PNNL capabilities. 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 and the Vehicle Technologies Office's Battery500 and LightMat consortia.

Health: Scholarly output continues to be strong with multiple publications in high impact journals (i.e., *Science* and *Nature*). This core capability benefits from strong partnerships (joint appointments plus two joint institutes). Increased demand in this core capability has created a staffing gap that is being addressed through intensive recruiting. Available office and laboratory space is not keeping pace with the growth of research portfolio and staff, but will eventually be addressed by the ESC and GSL. There remains a need for additional high bay space.

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. This year, a system called Xenon International won awards for its engineering accomplishments and international impact. In 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 wasteforms, 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-Defense Nuclear Nonproliferation R&D office relies heavily on these capabilities for next-generation nuclear detection systems, along with the Defense Threat Reduction Agency (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.

Computational and Mathematical Sciences

Advanced Computer Science, Visualization, and Data

PNNL has depth and breadth of expertise in advanced data analytics; energy-efficient computing; performance, power, and reliability modeling; exploration and design of novel computing architectures; and runtime and system software. Specific domain areas include predictive modeling and simulation of complex architectures, programming models, resiliency, AI/ML, 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 and materials science.

PNNL has advanced the state-of-the-art in the application of deep learning 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. 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 AI to DOE mission priorities, such as cybersecurity and electric grid resilience. PNNL is making new investments in AI, including exploring the mathematical foundations of AI to support 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 for visual analysis of high-volume streaming data and visual interfaces for interactively building machine learning classifiers and evaluating AI performance. PNNL is also making significant advances in graph analytics, including hybrid architectures for exploiting large graph datasets and algorithms for scalable graph query on multi-threaded systems.

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 supercomputer, the Constance institutional computing cluster, the Marianas cluster (including Tonga, a state-of-the-art NVIDIA DGX-2 system) optimized for machine learning workloads, and Newell, an experimental IBM Power9 testbed for on-ramping codes to Oak Ridge National Laboratory's Summit; private research cloud and public cloud access through Amazon's Amazon Web ServicesBIL, Microsoft's Azure and Google's Cloud Platform; testbeds for IoT and industrial internet-of-things (IIoT) devices and new FPGA and advanced reduced instruction set computer 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 the 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 has improved with good gender diversity; however, compensation competitiveness 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, recent investment in machine learning hardware have provided up-to-date capabilities, and replacement of the HPC system is in progress.

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. More recently, through investments from BES and internal LDRD, PNNL has been exploring the application of quantum computing platforms to applications in computational chemistry and materials science. PNNL maintains strong capabilities in 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.

Multidisciplinary teams of domain and computer scientists and applied mathematicians have long been an elemental part of the research process at the Lab. For example, as part of developing NWChem, PNNL pioneered engaging teams of computational scientists to create a 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. This same integrative, co-design-based approach now is being employed to develop advanced computational models at multiple length and time scales for the power grid, high energy physics, materials science, and climate, to name only a few. Moreover, PNNL has been a significant contributor to various DOE Scientific Discovery through Advanced Computing (SciDAC) projects. These teams continue to adapt to the changing computing landscape through efforts such as the Exascale Computing Project, which includes developing NWChemEx as well as exascale applications in other domains, such as machine learning and power grid applications.

Internal LDRD investments have focused on bringing together interdisciplinary teams of data scientists, computer scientists, data 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 domain-aware machine learning methods that can be applied to a wide range of DOE problems. PNNL-developed codes, such as NWChem, are also heavily used on DOE's Leadership Computing Facility systems and at the National Energy Research Scientific Computing Center.

Staff members are housed primarily in CSF, Information Sciences Building (ISB)1, ISB2, ETB, EMSL, and MATH buildings. This capability leverages support from PNNL's applied mathematics and advanced computer science, visualization, and data core capabilities, and receives support from programs in ASCR, BES, BER, EM, and EERE.

Health: Solid project portfolios for all DOE-SC sponsors. Adequate staff numbers; infrastructure, and equipment are good.

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, AI/ML, complex information modeling, data analytics, decision and control 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, PNNL is developing capabilities in domain-aware machine learning, as well as physics-informed methods for parameter estimation and uncertainty quantification as a part of several projects funded by ASCR, BER, and FE. These techniques focus on solutions for nonlinear and high-dimensional systems, and include surrogate and multi-fidelity modeling for both forward prediction and inverse models. PNNL is developing 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 is pursuing innovative research in the analysis and integration of complex, high-dimensional data. PNNL mathematicians are advancing 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 is also designing extreme-scale machine learning and data mining algorithms, including supervised learning algorithms (e.g., deep learning, support vector machines), unsupervised learning algorithms (e.g., auto-encoders, spectral clustering), reinforcement learning, and PhILMs (methods where physics laws are used in addition to data to train deep learning algorithms). In addition, PNNL is developing 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 machine learning, signature discovery, causal reasoning, and game theory— enables domain scientists to generate novel hypotheses in both static and streaming applications. Most of the research in data sciences and machine learning is currently funded by internal investment as well as from external sponsors such as DOE-ASCR, DoD, and NNSA.

PNNL also has an emerging capability in the applications of discrete mathematical techniques to a range of problems in the DOE mission space. PNNL uses these capabilities to solve crosscutting problems of national interest. PNNL is heavily invested in solving issues related to large-scale graph analysis (e.g., data fusion), time evolution of discrete structures, and the development of network invariants and their applications. PNNL researchers leverage emerging capabilities in QIS to develop quantum algorithms for combinatorial optimization. PNNL applied mathematics researchers are located in ISB1, ISB2, Biological Sciences Facility (BSF), CSF, ETB, 3860, and our Seattle offices.

Health: Staffing, portfolio, infrastructure, and equipment are all good.

Cyber and Information Sciences

The Laboratory conducts research and develops technology that bring scientific approaches to cyber operations and defense, to give 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 analytic techniques to extract value from data. Research, engineering, and analysis staff are nationally and internationally recognized in cybersecurity, resiliency, the development of secure design principles for control systems for and validation of industrial 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 (ICS), OT, and 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 for DOE complex cyber defense and the 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, 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, 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 has also developed a world-class deep learning capability that applies emerging machine learning techniques 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, and DHS.

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 private sector recruitment of relevant hot skills and the associated high compensation levels, makes this core capability one of three being addressed through intensive recruiting and cross-training. Currently, there is insufficient federally owned office and laboratory space for research in data exploitation workflow and provenance in the extreme-scale science, energy, and security domains; however, PNNL plans to renovate unutilized 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 in 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 decision support under resource constraints. 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 field testing, evaluation, and performance assessment; programmatic risk assessment; geo-spatial decision analytics and visualization; 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, Bonneville Power Administration (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, so recruitment and retention remain a matter to watch.

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 system science 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, MSL, 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, and integrated human-Earth system models, including the Global Change Assessment Model, the Weather Research and Forecasting model, and the Energy Exascale Earth System Model, as well as in integrating modeling and observational systems that span multiple disciplines 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, FE, National Aeronautics and Space Administration (NASA), EPA, National Oceanic and Atmospheric Administration (NOAA), and other sponsors.

Health: Key leadership gaps and staffing needs (e.g., JGCRI Director, Senior Coastal Modeler, 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.

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 from surface waters. 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 from seawater, 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. Nearly one-fourth of the staff are postdocs/graduates, and 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 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 MSL, 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 (EGS), technology development for nuclear waste repositories, and remediation of contaminant plumes.

For EM, PNNL applies an integrated experimental and modeling approach to resolve technical issues necessary to inform decisions for environmental remediation, waste management, and closure. PNNL has teamed with other laboratories to develop the Advanced Simulation Capability, a state-of-the-art scientific approach that uses integrated toolsets for understanding and predicting contaminant fate and transport in natural and engineered systems. PNNL leads the Deep Vadose Zone-Applied Field Research initiative, providing the technical basis to quantify, mitigate, and monitor natural and post-remediation contaminant discharge from the vadose zone to groundwater. Outcomes include advanced prediction, characterization, remediation, and monitoring approaches for addressing residual soil and groundwater contamination at DOE facilities, as well as the protection of regional water resources and aquatic ecosystems.

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 now exploring potential carbon storage in the sub-seafloor Cascadia basin basalt offshore of Washington State. PNNL has key roles in FE's National Risk Assessment Partnership and in the new EGS Collab 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, ETB, and MSL.

Health: Scholarly output trend is improving. Over one-half of the staff have 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 and infrastructure are good, but an equipment refresh is needed.

Biological Systems Science

Through PNNL's biological systems science core capability, the Laboratory is developing a mechanistic 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 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 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. Investments from the Microbiomes in Transition (MinT) LDRD investment have developed into programmatically supported core capability to understand the metabolic activities of complex microbial communities and how metagenomes translate to the function of a microbial community, as well as to illuminate the microbiome's role in plant, animal, human health, and biogeochemical cycling. Investments in synthetic biology have expanded PNNL expertise in applying fundamental systems biology knowledge into new strategies for biodesign of new functions to advance BER 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.

In combination with other core capabilities, including chemical and molecular sciences; environmental subsurface science; advanced computer science, visualization, and data; applied mathematics; and large-scale user facilities/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 structure and activity 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; CSF; the Bioproducts, Sciences, and Engineering Laboratory (WSUBSEL); MSL; the Aquatic Research Laboratory; Life Sciences Laboratory 1 (Gnotobiotic Animal Facility); the Microbial Cell Dynamics Laboratory; and EMSL. 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. Three senior positions were recently filled. There is sufficient lab and office space. Portfolio is growing through increased programmatic support by both BER, NIH, and new funding from DARPA and DTRA. Infrastructure and equipment are good; capital equipment through internal and programmatic investments (X-ray Nanotomography, Cryo-EM) is expanding the bioimaging capability. Workhorse equipment that support multiple sponsors (mass spectrometers and NMRs) is aging, and the path for replacement is unclear.

Engineering

Biological and Bioprocess Engineering

Leveraging capability in biological and bioprocess engineering, PNNL is developing technologies and processes to convert biomass and waste materials into fuels and chemicals that will reduce our nation's dependence on petroleum. Biomass sources include lignocellulosic materials (e.g., corn stover and wood wastes) and other waste materials (e.g., water treatment plant wastes and other industrial 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. Research spans from a 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.

PNNL's biologists, chemists, and chemical engineers specialize in fungal processing, catalysis and reaction engineering, algae growth and processing, separations, process engineering, techno-economic and life cycle analyses, and resource assessments. PNNL's technical areas of expertise include fast pyrolysis for converting biomass to bio-oil, hydrothermal liquefaction for conversion of wet materials 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 houses unique indoor, climate-controlled raceway ponds 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 maintains a significant IP portfolio, providing a pathway for technology commercialization. The PNNL team has seven distinguished inventors, each with 14 or more awarded U.S. patents, for a total of 82 bio-based U.S. patents since the year 2000. 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. Thanks to 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. PNNL provides leadership in biological and bioprocess engineering to the EERE Bioenergy Technologies Office, EM, academia, and industry. Industrial partners include companies such as Archer Daniels Midland, Genifuel, and LanzaTech.

Health: All areas are strong, with a stable publication record. Portfolio currently is strongly dependent on EERE-BTO; however, collaboration with industry is expanding, and a collaboration with DOE-IN and WSU increases the ability to leverage this capability to address the needs of a broader sponsor base.

Power Systems and Electrical Engineering

PNNL has internationally recognized capabilities spanning the entire electric power grid. Staff at PNNL have deep expertise in conventional and variable generation of electricity, 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, by better planning, operating, and controlling of modern power grids for enhanced resilience and reliability. Primary supporting disciplines include power system, electrical, and control engineering; computational science; cybersecurity; data analysis; and mechanical engineering. With a focus on system-level issues, PNNL is the national leader in defining the inherently 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 integration, energy storage, distribution system modeling, and grid cybersecurity. PNNL's expertise in grid simulation and analytics enables high-performance grid monitoring and control at 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 resources. PNNL's expertise in advanced control theory, application, and testbeds supports advances 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 smart appliances, 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), CESER, ARPA-E, DHS, ASCR, DoD, the U.S. Department of State, and private industry.

Health: Better-than-expected success in hiring over the past 12 months (~60 new hires) and reduced attrition has addressed previous year's immediate skills gaps, but also has created immediate need for additional office space in Richland, Seattle, Portland, and Arlington. Both near-term and longer-term plans are being operationalized to address this. Transactive campus infrastructure and addition of thermal storage and new batter installations are contributing significantly to the health of this capability.

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 energy and nuclear and radiological security. 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 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, 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 technology, and conducting large-scale technology demonstrations. 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), Office of Fossil Energy (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 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, and chemists specializing in disciplines including 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. Other distinctive areas of expertise include radioactive and non-radioactive nuclear waste treatment (from milligram to ton-scales), encompassing slurry transport and mixing, glass melting, advanced rheology, and fluid dynamics for complex multiphase systems.

PNNL successfully applies its chemical engineering capabilities to a broad array of challenges, including the development and commercialization of NOx reduction units for automobile emissions control; the development and application of software to predict the thermal and structural performance of spent nuclear fuel storage and transportation systems; the development of novel heat pumps and building systems to increase energy efficiency; and the invention and development of micro-technology-based reactors and separations systems for applications such as fuel cells and solar natural gas reforming. Current research focus areas include biomass and fossil fuel conversion to fuels and chemicals, as well as subsequent fuel upgrading; nuclear waste processing and immobilization research; and cost-effective start-up and operation of the Hanford Waste Treatment Plant.

This core capability supports sponsor-funded research by the DOE-SC (BES), as well as DOE's Applied Energy Offices, including EM, EERE (VTO, BETO, GTO, SETO, and FCTO), FE, NE, NNSA, and ARPA-E. PNNL's chemical engineering capability is also leveraged in support of research funded by DHS and DoD.

Health: Publication record is strong, including several in *Science* and an R&D 100 Award. High hazard biofuels research currently conducted in high bay space on south campus (PDL-W) requires relocation to north campus, which may be delayed by funding limitations. Ultimately, PNNL is planning a new federally owned facility located in a higher hazard zone to support these experimental test stands. Lack of available office space is a significant issue in PSL and LSL2, and an emerging concern at BESL.

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 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 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 of 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 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 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 lead the scientific community toward a predictive understanding of molecular processes controlling the flux of materials that underpin biological and ecosystem functions. Research in EMSL focuses around two science areas—biological sciences and environmental sciences. 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 strives for a predictive and ultimately controlled understanding of biology. The science focuses on biological "machines" and processes in and among microbes (archaea, bacteria, and algae), fungi, and plants. EMSL research focuses on improving the mechanistic understanding of how genetic information is translated into processes across temporal, spatial, and organizational scales—molecules, organisms, consortia, multispecies communities, and ecosystems. This helps advance the accurate metabolic reconstructions and predictive models needed to understand nutrient flux in the environment and improve strategies for designing plants, fungi, and microbes for biofuels and bio-based products.

The Environmental Transformation and Interactions Area focuses on mechanistic and predictive understanding of fundamental physiochemical, ecological, hydrological, biogeochemical, plant, and microbial processes in terrestrial and subsurface ecosystems, the atmosphere, and their interactions from molecular- to ecosystem-scale. EMSL provides the experimental, computational, and simulation expertise to investigate the cycling, transformation, and transport of critical biogeochemical elements (e.g., C, N, S, P, Mn, Fe, and Ca), contaminants, and atmospheric aerosols. Coupled experimental and modeling approaches will accelerate mechanistic understanding of soil-microbe-plant-atmosphere processes and their interdependencies across molecular, field, atmospheric, and ecosystem scales to ultimately inform models of land-atmosphere interactions at larger scales. Through the integration of field, laboratory, and computational approaches, EMSL users gain new knowledge of molecular-scale phenomena that can be parameterized, scaled, and integrated into models designed to understand complex biological and environmental systems across many spatial and temporal scales.

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 and JGI sponsor joint user calls 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. 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 ARM (described below) and BES-funded light sources. EMSL also collaborates with other user facilities through the new Society for Science at User Research Facilities. This capability is funded by BER.

Health: Quality of staff and research portfolio are both strong. Research equipment health remains strong. A strategic equipment reinvestment plan is in process, which will guide future equipment acquisition. EMSL roof is nearing the end of its useful life and plans for replacement are in process. EMSL is in the process of planning for the use of space that will be available when Physical and Computational Science's Directorate (PCSD) staff move to the ESC.

ARM Research Facility

The world's premier ground-based observatory for atmospheric science research, the ARM Research Facility, is a DOE user facility that provides a global network of instrumented fixed, 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 sites are located in the United States 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 National Center for Atmospheric Research Community Earth System Model and 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 U.S. Southern Great Plains site, 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 recent Cloud, Aerosol, and Complex Terrain Interactions (CACTI) 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. FY 2020 represents a strong focus on the Arctic, as both mobile facilities are deployed for Arctic experiments, while ARM continues to operate two sites on the North Slope of Alaska. The first mobile facility is deployed to coastal Norway for a study of the cloud systems formed over the north Atlantic during cold-air outbreaks. The second mobile facility is deployed on the German icebreaker, Polarstern, for a major international campaign in which observations will be taken for a year as the icebreaker drifts with the ice around the Arctic Ocean.

Following these polar deployments, the first ARM mobile facility will be deployed to Houston, Texas for another study centered on deep convection. That campaign will begin in April of 2021 and will feature the second deployment of the scanning C-band precipitation radar.

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 under way. To replace the G-1, PNNL has followed the CD process (DOE O 413); and following CD-2/3 approval, purchased a Challenger 850 regional jet in May 2019. The Air ARM Project Team is now proceeding with plans for the aircraft modification for research. 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.

PNNL leads the development of UAS capabilities within ARM. PNNL has procured a very capable mid-size UAS that can carry payloads of up to 100 pounds as high as 18,000 feet for periods of up to eight hours. This mid-size UAS is currently undergoing instrument integration and testing with plans to use the platform to study aerosols at the ARM Southern Great Plains site.

PNNL is responsible for the overall technical direction of the ARM Facility'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 G-1 Replacement aircraft has CD-2/3 approval and has received full capital funding. The aircraft Request for Proposal pre-purchase inspection contract/aircraft modifications statement of work is in progress. A new ARM hanger to be constructed in late 2019 will consolidate space and will improve storage conditions. Shortages in high bay space and field test sites will be needed to execute our programs; these are being addressed. Staff and portfolio are good.

Science and Technology Strategy for the Future/Major Initiatives

Scientific Vision

PNNL draws on signature capabilities in chemistry, Earth systems sciences, and data analytics to advance scientific discovery and create solutions for the nation's toughest challenges in energy resiliency and national security.

As with all national laboratories, PNNL has broad scientific depth. We are, however, particularly recognized for our expertise in catalysis and chemical conversions, climate and subsurface science, and machine learning and data analytics. These enable PNNL to tackle complex problems that span fundamental research questions to challenges in operational application.

In chemistry, we are pursuing bio-inspired design and synthesis rules to develop new catalysts and explore chemical pathways that enable the sustainable manipulation and transformation of carbon and other elements, reinventing the key chemical transformations of molecules found abundantly in waste streams to convert them into principal feedstocks for fuels, materials production, and energy storage.

PNNL's long history in Earth sciences—atmospheric processes, microbiology, and environmental systems science—has positioned us well to build the science basis for an integrated whole-Earth system model spanning molecular to global scales, from the subsurface to stratosphere and the coast to desert. Our work in Earth sciences draws heavily on our traditional strengths in chemistry, biology, atmospheric sciences, and environmental subsurface sciences, as well as on integrating theory and experimentation with field validation, and with computer modeling and simulation across scales.

Originating from a national-security-driven need to illuminate and understand relationships in large volumes of text, PNNL has developed strong capabilities in the mathematics, statistics, data analytics, ML, artificial intelligence (AI), and computer science disciplines that underpin both compute- and data-intensive technologies. We bring this expertise to bear on all our research challenges, accelerating discovery in these and paying particular attention to problems—such as materials discovery or grid optimization—that are best solved by integrating AI and ML into HPC scientific simulations, augmented by graph analytics and fueled by big data sets.

PNNL also is leveraging our traditional strengths in computational chemistry, application data analytics, and HPC, as well as our expertise in atomically precise and ultrapure materials, to shape our contribution to the emerging field of quantum information science. Specifically, we are advancing quantum computing algorithms and programming models that run on new quantum computing platforms and demonstrate the power of quantum computing with quantum-accelerated applications in advanced materials and catalysts, our traditional areas of strength in energy sciences.

PNNL's signature strength in the resiliency of the North American electric grid draws naturally from our strengths in chemistry/catalysis and data analytics, as well as capabilities that include our Electricity Infrastructure Operations Center (EIOC), which accesses and analyzes streaming situational data concerning the physical state of the U.S. grid using actual grid data provided by utility partners. Here, our goals are two-fold. The first is the modernization of the electric grid through the development of highly complex models and tools that are appropriate to an interconnect-scale and -speed system, and which are sufficient to access grid operational conditions and predict threats to its reliability, resiliency, and security. Our second goal, soon to be greatly enhanced by the construction of GSL on the PNNL campus, is the development of low-cost ($120/kWh) grid battery energy storage.

Our understanding of the workings of a key critical infrastructure—the U.S. electric grid—coupled with our strengths in data analytics and our extensive work in threats to our national security, has led to an obvious focus on the cybersecurity of critical infrastructures. PNNL operates the Cybersecurity Risk Information Sharing Program (CRISP), the only extant example of a critical infrastructure situational awareness system operating at scale, and the Cyber Intelligence Center (sponsored by the Department of Homeland Security [DHS]), which has long been central to the U.S. government's efforts to generate, steward, and use information about adversary tactics and techniques. Our research focuses on the development of mechanisms that will drive autonomous decision-making into the critical infrastructures themselves—in our view, the only way that we will ultimately be able to match the speed and flexibility of emerging cyberattacks.

Finally, PNNL's history with nuclear materials production on the Hanford Site, as well as our focus on radiation detection spread over many decades, and investments in unique facilities that enable us to work with radioactivity at the benchtop scale and pilot scale have led us to the goal of mastering all aspects of radiation dynamics and nuclear materials production—a goal that allows us to contribute significantly to national needs in nuclear energy, nuclear waste disposition, the science underlying the nuclear stockpile, and our ability to detect and counter adversarial nuclear proliferation efforts.

In addition to the major initiatives summarized in the following pages of this plan, PNNL is exploring the addition of a bioscience major initiative for incorporation in its FY 2022 plan. Such an initiative would integrate and interpret molecular and cellular-scale data from multi-omics experiments, imaging, and chemical biology using data analytics, machine learning, and modeling to develop functional maps of biological communities. We would apply this approach to explore biosystem resiliency to environmental perturbations, the mechanisms by which the persistence of traits is maintained or inhibited in organisms and systems, discover molecular signatures predictive of pathogenicity and disease outcomes, and engineer biological systems to produce valuable materials and chemicals.

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 on the Hanford Site. PNNL also conducts operations at the soon-to-be DOE-owned PNNL campus in Sequim, Washington. Additionally, PNNL has a presence in multiple offsite locations, including 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.

Real Property Assets. As of September 30, 2019, PNNL consists of

- 35 DOE-owned (10 by EM and 25 by SC) buildings (1,180,712 gsf) and 23 OSFs on 580 acres (549 acres PNNL and 31 acres EM)
- 11 BMI-owned buildings (166,477 gsf) and 21 OSFs on 232 acres, including 117 acres in Sequim (65 acres of land and 52 acres of tidelands)
- 30 buildings from third-party leases and agreements (968,580 gsf)

As part of the PNNL contract, Battelle provides DOE with exclusive use of the Battelle-owned buildings for PNNL purposes. Battelle buildings comprise 10 percent of PNNL's laboratory space (square feet) and are provided to the government at cost. DOE and Battelle have reached a contractual agreement to transfer the Battelle-owned buildings and land in Richland and Sequim, WA to DOE on or before the end of FY 2022.

Utilities. The utility and distribution systems that serve PNNL's Richland campus, the PNNL Sequim Campus, and PNNL-operated buildings in the Hanford 300 Area are provided by various suppliers and currently have an overall asset condition of *adequate*. All utilities consumed by PNNL in both Richland and Sequim have the necessary capacity to meet the current DOE mission. The water and sewer infrastructure in the Hanford 300 Area is owned by DOE and managed by PNNL; the City of Richland is the provider of the water, sewer, and electric service on the PNNL Richland Campus and of the electrical service in the Hanford 300 Area. Natural gas for both the Hanford 300 Area and the PNNL Richland Campus is provided by Cascade Natural Gas. For the PNNL Sequim Campus, the septic system and water distribution system are owned by BMI and currently have an overall asset condition of *adequate*. There is no centralized gas utility system at the PNNL Sequim Campus. The water and sewer systems at the Sequim Campus are currently adequate, but are operating at capacity.

Condition/Utilization. The FY 2019 condition and utilization assessment designated all 35 (1,180,712 gsf) federally owned, active, operating buildings as *adequate* relative to mission. A total of 34 of 35 buildings were designated as *utilized,* none were designated *underutilized,* and one (Battelle Inhalation Laboratory [BIL]; 17,621 gsf) was designated as *unutilized* and *standby*. The assessment also designated 39 of the 41 (1,021,900 gsf) non-federal, active, operating buildings as *adequate* relative to mission; two (113,227 gsf) were designated as *substandard*; and none were designated as *inadequate*. All of the 41 non-federal buildings were designated as *utilized*; none were designated as *underutilized* or *unutilized.* Actions to resolve the unutilized and/or substandard buildings are described in the Campus Strategy section.

The program for addressing underrated electrical equipment was expanded to include performing an Extent of Condition evaluation across the PNNL Richland and Sequim Campuses. This evaluation has been completed. In addition to the original BMI facilities, a total of 10 buildings were determined to have underrated electrical equipment. Of these, we have completed mitigation actions on four, and the remaining facilities are scheduled for completion in FY 2020.

Deferred Maintenance. PNNL's current deferred maintenance for all federal assets (DOE-SC and EM) stands at $10.3M, and the overall condition index is 95. DOE began the process of acquiring all current BMI facilities during FY 2019, which will increase PNNL's overall deferred maintenance and replacement plant value. This transition is planned to be completed by the end of FY 2022. These buildings have a low deferred maintenance balance relative to their replacement value. Because of this, PNNL is expecting little change to the campus' overall condition index.

Campus Strategy

PNNL's campus strategy is driven by a need to enable PNNL's major initiatives, sustain the health of our core capabilities, and support key programs and sponsors. Campus planning consists of understanding the mission need, assessing the state of readiness, determining the facilities and infrastructure gap consistent with the Integrated Capability Management review, assessing alternatives, and developing and implementing the strategy. The facility and infrastructure investments discussed in the balance of this section of our Lab Plan are presented as they support two objectives:

- Objective 1 − Mission Alignment: Support mission alignment by providing the physical environment that meets current and emerging program research needs required to deliver vital mission impacts.
- Objective 2 − Optimize Functionality, Reliability, Utilization, and Operating Costs: Support optimization of facility and infrastructure capabilities to enable research operations.

Across these overarching objectives, however, our strategy is guided by the following near-term goals.

Consolidate the PNNL Footprint on Federal Land and in Federal Buildings

PNNL currently is engaged in a multi-year effort to facilitate DOE's acquisition of Battelle-owned buildings and land that currently comprise approximately 10 percent of the Laboratory's footprint. The figure below illustrates our vision for the PNNL campus at the end of FY 2031, showing increased federal ownership (DOE-SC) of buildings and land. In support of this transition, PNNL will continue to invest significant internal funds to renovate, repurpose, and optimize utilization of existing underutilized facilities on the PNNL campus. Consistent with this goal, PNNL is also taking advantage of opportunities provided by reuse of EM-owned Hanford 300 Area buildings to support the PNNL mission.

Use of Leased Facilities

In FY 2019, PNNL's enhanced emphasis on hiring and retention bore fruit—the Laboratory increased head count by approximately 7 percent net new staff and is planning for a 4.5 percent increase in FY 2020, as well as a 4 percent increase in each of the following four years. This pace of growth will place significant strain on office space at the Laboratory, which is currently operating at or near capacity. To address both immediate and longer-term needs, as well as increase available workstations, PNNL is pursuing short-term leases while continuing a strategy for constructing federally owned facilities. The mid- to long-term strategy of reducing reliance on third-party leases includes line item and direct-funded opportunities, in addition to piloting novel space-usage models attractive to the next generation of researchers. The use of short-term leases will enable PNNL to right size the amount and type of available workstations as staffing levels fluctuate over time.

Appropriately Locate Hazardous Work

As part of the overall consolidation and revitalization of the PNNL Richland Campus, PNNL is working to site ongoing and planned hazardous research to the appropriate hazard zone (low, moderate, high), away from public encroachment. This will improve PNNL's ability to mitigate hazards and constraints on the south end of the PNNL Richland campus, while enabling the ability to perform concurrent low-hazard operations. In the mid- to longer-term, PNNL is exploring, via its Integrated Capability Management effort, opportunities to co-locate other categories of work, such as those that involve sensitive or emerging technology or computing, to build layers of security and collaboration into our physical campus.

Modernize the PNNL Sequim Campus

As stated earlier, DOE and Battelle have reached a contractual agreement to transfer the Battelle-owned buildings in Richland and Sequim, WA to DOE on or before the end of FY 2022. In support of this decision, PNNL is taking necessary actions to modernize the facilities and infrastructure of the site, as well as making investments that will prepare and support its future uses.

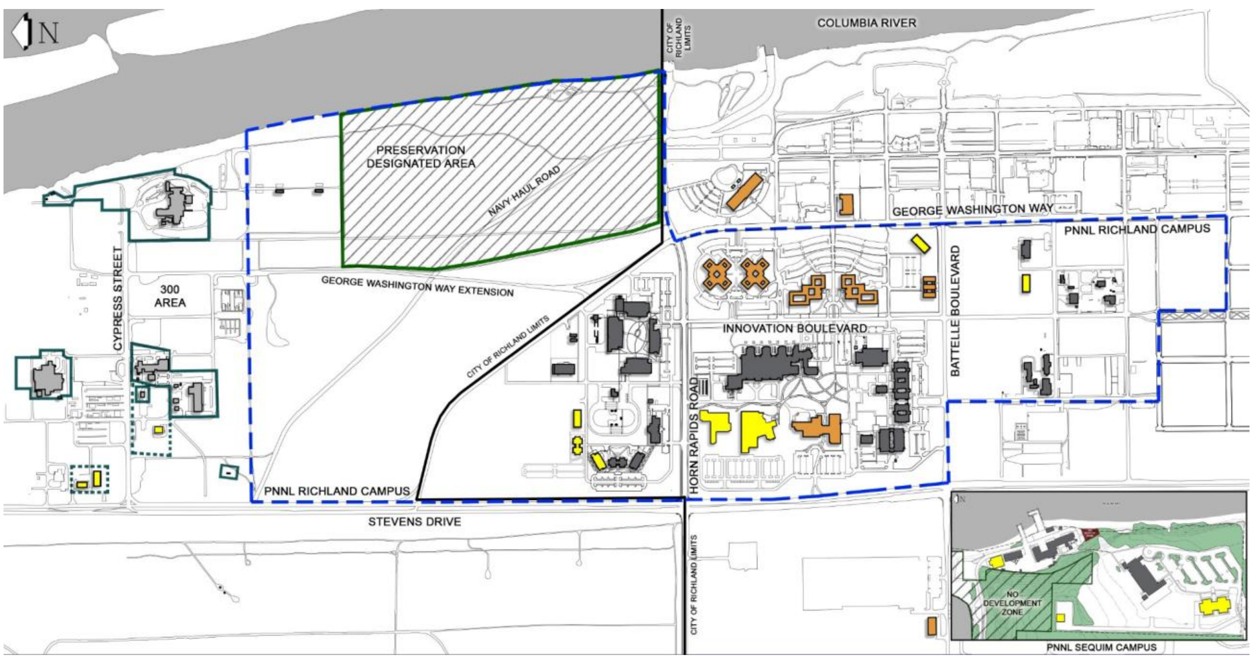


Figure: PNNL 10-year campus strategy site map for FY 2031, showing land ownership, the PNNL Richland Campus area, and proposed and notional new construction; the inset shows the PNNL Sequim Campus

Ongoing and Proposed Investments

Ongoing and proposed projects and investments in support of our two facility and infrastructure objectives are summarized in the following pages of this plan. Investments cross-walked by core capability are shown in Table 4. The type, timing, and alignment of capital investments are summarized in Table 5. Table 6 provides the Integrated Facilities and Infrastructure crosscut data per the Integrated Facilities and Infrastructure Guidance definitions.

Objective 1 – Mission Alignment

The following projects support critical programs/initiatives, strengthen the Laboratory's core capabilities, and assure a mission-ready environment.

New Construction and Modernization of Existing Facilities

The **Energy Science Capability (ESC)**, a DOE-SC SLI funded $93M line item, will enhance basic and applied research programs that are pursuing novel catalyst design and molecular-level control of chemical transformations. The ESC will deliver an ~139K gsf facility consisting of 52 laboratory modules, 200 workstations, and collaboration space. This project has received a CD-2/3 authorization. Design is being finalized, and construction will be initiated in the spring of FY 2020. Construction is scheduled to be completed in late FY 2021. Following completion, PNNL will invest $4–5M over two to three years to consolidate laboratory space onto the campus by vacating third-party leased facilities.

The **Grid Storage Launchpad (GSL),** a DOE-OE funded facility, has received CD-1 approval at $75M total project cost; it will enable validation, acceleration, and collaboration of next-generation grid-scale energy storage materials and technologies under realistic grid operating conditions. The GSL's key performance parameters have not yet been finalized, and performance specifications are being developed to support the current intention for ~85K gsf of laboratory, workstation, and collaboration space.

EMSL investments will be completed in anticipation of the ESC project completion; the EMSL Operations Team is working collaboratively with the ESC Project Team to plan for the future integration of each buildings' missions. Through these planning efforts the EMSL Operations Team is proposing two GPP projects to be direct funded by their BER sponsor. Both of these projects will allow EMSL to maintain operational efficiencies and mission alignment within the EMSL user facility.

- *Additional Water Cooling for EMSL Computing:* Planned to initiate in FY 2021, this project will integrate EMSL's HPC cooling system with the proposed Heat Transfer Building 1 (HTB1) that is planned to be constructed as part of the ESC project. This system will provide waste heat to be used to temper single pass air needed at ESC and GSL.
- *EMSL Facility Backfill and Expansion:* Planned to initiate in FY 2022, this project plans to backfill space vacated in EMSL once the capability relocations into the ESC project have been completed. This plan includes the repurposing of approximately 13,000 SF to accomplish four key objectives: 1) grow science areas of strategic importance to EMSL, 2) incorporate new capabilities that benefit EMSL, 3) unpack/relocate current laboratories to promote safe and efficient research, and 4) create core lab spaces to consolidate equipment and capabilities that cross-cut EMSL's Integrated Research Platforms.

The **Outdoor Collaboration Area in the center of campus** is a proposed project on the PNNL Richland Campus that will create an area in the central campus to support outdoor events, improve pedestrian access, and provide informal gathering/collaboration spaces.

A **suite of projects in support of our Nuclear Science and Engineering** core capability is under way or envisioned to expand and modernize the nuclear chemistry and detection R&D in 325RPL and the 3420 Radiation Detection Laboratory.

- *Replace 325RPL Hoods and Ductwork (420/525) with Acid Resistive Equipment:* Soon to be under way in 325RPL, this project will replace deteriorated fume hoods and ductwork with modern equipment, thus allowing the continued use of existing research labs. This $2M to $3M project is anticipated to be initiated in FY 2020.
- *Reconfigure 3220 to Support Office Space:* Currently, 325RPL is operating at capacity, with insufficient room for office growth. The pending transfer of 3220 from EM-Hanford

management to PNNL will allow PNNL to reconfigure this space to support the 325RPL facility. PNNL is proposing a $500K to $1M project to reconfigure 3220. This project is anticipated to initiate in FY 2021.

- *325RPL Lab 52 Renovation:* PNNL will be investing direct sponsor funding to renovate Lab 52 to accommodate a sponsor funded instrument used to support Defense programs.
- *325RPL A-Cell Window Refurbishment:* Under consideration for 325RPL, this project would clean out and refurbish the 325RPL A-Cell to repair three shielded viewing windows with failing gaskets that result in oil leakage from the assembly. This would be a $3M to $4M project, and it is envisioned to occur within the next three to five years.
- *Quiet-Type Research Space with Adjacent Rad-Chemistry Space:* PNNL is exploring opportunities to grow and expand existing capabilities in production verification and materials characterization within 325RPL. If realized, this will require construction of quiet-type research space and adjacent rad-chemistry space.

The office space inventory. PNNL is proposing future campus development projects to reconfigure existing space and create new workstations to support the increasing demand, including the following:

- *Maximize utilization by repurposing existing space* to address immediate, urgent office space demand. Spaces identified within the Laboratory include locations in the Mathematics Building (MATH), LSB, Computational Sciences Facility (CSF), and Environmental Technology Building (ETB). In addition, PNNL will pursue opportunities to pilot novel configurations that are attractive to the newest generation of scientists, while enhancing collaboration.
- *Construct Richland North Office Building:* PNNL is proposing to construct an approximately 26K gsf office facility to support current and future mission needs on the northern end of the PNNL Richland Campus. This $12M to $13M Minor Construction (MC)-funded project is anticipated to initiate in FY 2022.
- *Construct South Campus Office Building:* PNNL is exploring the possibility to construct an approximately 18K gsf office facility on the perimeter of the south end of the PNNL Richland Campus to support relocating support staff out of concentrated research focused areas of campus. This realignment effort would provide additional research space near high-density laboratory areas of campus.

PNNL's Sequim Campus. PNNL is planning future investments at the Sequim Campus to prepare and optimize the site for current and future R&D activities in support of DOE missions. These investments include the following:

- *PNNL Sequim Campus Water/Sewer Conversion:* The current PNNL Sequim Campus water/sewer infrastructure (artesian well and septic tank) limits potential development at the site. Converting the PNNL Sequim Campus from the legacy well and septic tank configuration to the City of Sequim utilities is, thus, a critical first step in enabling any future development at the PNNL Sequim Campus. This $2M to $4M MC-funded project is expected to be initiated in FY 2021.
- *PNNL Sequim Campus Storage:* The existing PNNL Sequim Campus includes no available space for research and building operations to store and manage critical spare parts and equipment needed to maintain continuity of operations. PNNL proposes to build a general campus storage facility and associated outdoor laydown space that would accommodate proper storage and maintenance of large equipment when not in use. This $2M to $3M MC-funded project is expected to be initiated in FY 2023 or sooner.
- *PNNL Sequim Campus Revitalization:* PNNL is planning to revitalize the facilities at the PNNL Sequim Campus, including a remodel of existing space and the acquisition of new space. This would include a new office/collaboration building, marine laboratory space, and large

equipment/high ceiling space to support research activities. PNNL will pursue all funding sources, including direct sponsor investments.

- *PNNL Sequim Campus Access Improvements:* PNNL is proposing an infrastructure development project to improve the overall accessibility of the PNNL Sequim Campus. This proposed project scope would address aquatic access to the Sequim Bay, pedestrian travel between shorelines and uplands, parking and sidewalk improvements, and vehicle access to the proposed uplands storage and laydown space. PNNL will pursue all funding sources, including direct sponsor investments.

Foster the health of PNNL core capabilities. PNNL's Integrated Capability Management process regularly identifies facility and infrastructure needs/gaps that are or have the potential to weaken any of PNNL's 19 core capabilities. In addition to the items identified in Table 4, the following projects are being proposed for future development opportunities:

- *Nuclear Chemistry:* PNNL has identified a future need for additional nuclear chemistry space and is considering the construction of a new nuclear chemistry building to support forecasted growth in PNNL's Nuclear Engineering and Nuclear Radiochemistry core capabilities. In the interim, this demand would be partially met via repurposing existing space, such as the 331 Building.
- *Quiet and Clean Chemistry:* The Lab continues to evaluate the amount and type of specialized chemistry space and our need for growth. One area of projected shortfall is in the specialized chemistry lab space needed to make the exquisitely precise chemical measurements that are a hallmark of PNNL's science. This could be accommodated through repurposing of existing lab space, additions to existing facilities, or a new chemistry lab.
- *Research Testbed:* PNNL is considering the construction of a large outdoor space on the PNNL Richland Campus, with required utilities to support large-scale research projects that are not conducive to being conducted inside a facility. This space is proposed to be several acres in size and will be supplied with enough power and access control to allow flexibility to serve as a general-purpose research space.

Leasing Facilities and Office Space

PNNL's lease portfolio consists of approximately 970K gsf supporting both institutional and programmatic needs. Programmatic leases are tied to individual sponsor needs or projects and are terminated when the need has ended. Institutional leases, by contrast, support a broader range of sponsors and needs; thus, they should be considered from a longer-term cost-benefit perspective and to support mid-range flexibility driven by varying staffing levels. Institutional leases should have a determined path to ownership, support a strategic relationship, and support short-term growth needs or those that are identified as a benefit to DOE through a cost/benefit analysis. PNNL's long-term goal is to limit over dependence on third-party leased facilities. An unintended consequence of past attempts to drive vacancy rates to a minimum across the Laboratory and of using very conservative growth estimates is that we delayed the initiation of leases that might have helped mitigate our current, acute demands. Thus, in the projects highlighted below, we reflect a strategy by which we enter into leases as necessary to minimize the chance of overbuilding and by incorporating the remodeling and/or construction of facilities to address mid- to longer-term needs.

PNNL is working on or has proposed the following projects:

- *Near-Term Solution:* PNNL is pursuing a two-pronged approach to meet current office space demand at the PNNL Richland Campus. This approach includes both temporary modular office rentals and multi-year office leases.

- Office Lease Space: PNNL will acquire new office space through the execution of a new third-party lease in proximity to the PNNL Richland Campus. PNNL is proposing to construct a new federally owned office facility. The continued need for this office lease will be re-evaluated at the end of the construction of proposed federal office space (see below), estimated for completion in FY 2024.
- Construction of Federal Office Space: PNNL is investigating the possibility of constructing new federally owned office space on the Richland campus to obviate the recurring need to lease facilities and to avoid their costs.

- *ARM Aerial Facility (AAF):* The existing programmatically leased hangar (at the Port of Pasco) is being replaced with a new programmatically leased hangar for the AAF. The new hangar will house the G-1's replacement (Bombardier Challenger 850), mission support equipment, staff, instrumentation, and UASs. The new hangar will be fully capable of supporting the new aerial platform and will accommodate the equipment and activities previously provided by two existing substandard hangars. It also will better support the mission of the Bombardier Challenger 850 by enabling instrumentation to be easily configured at the hanger.
- *Applied Process Engineering Laboratory (APEL):* APEL is a laboratory/office building located off the PNNL Richland Campus. The long-term goal is to vacate the APEL leased facility within the next five years by backfilling existing space on campus. Vacating APEL also supports PNNL's leasing strategy to minimize the overall footprint of third-party leases (54,000 gsf), generating savings of $1.2M to $1.5M annually. Initially, PNNL is proposing a project to remodel Life Sciences Laboratory 2 (LSL2) labs 404–424, which will soon be federally owned, by converting unusable LSL2 lab vivarium space into ventilation-intensive, general-purpose wet laboratory spaces. This $4M to $5.5M MC-funded project is expected to be initiated in FY 2021. Additional investment projects are being planned in support of exiting APEL on this timeline.
- *PNNL Seattle Office*: The PNNL Seattle office is located in the heart of Seattle's South Lake Union district. Its location alongside leading tech companies, research institutions, and universities is often cited by staff as a major attraction of PNNL and is an ongoing source of intellectual engagement with neighboring institutions. PNNL's leased space in this office currently is over-subscribed; thus, we will explore opportunities to take advantage of additional contiguous space as it becomes available.
- *Enhanced Security Facility (ESF)*: PNNL currently leases a third-party facility providing space in which to conduct work requiring enhanced security. Although this facility is not envisioned as part of the long-term solution for our enhanced security needs, PNNL plans to invest overhead funds to support short-term needs at this location. In the mid-term, we are evaluating options for expanding the enhanced security facilities required by our multiple sponsors, with the eventual objective of exiting this lease. Long-term, PNNL is exploring opportunities for a separate, direct-funded facility that would include laboratory space and support sensitive and secure research with related support staff and equipment.
- *PNNL Seattle ESF Modifications*: PNNL is proposing expanding secure space at the PNNL Seattle facility. These modifications will support meeting the mission needs of the PNNL Seattle campus.
- *The SALK Facility*: The SALK facility currently is home to the Tritium Target Program (TTP). SALK is an office building with open areas; the open areas were converted to support electronics lab work. Our near-term strategy involves relocating the TTP to a DOE-owned facility, ultimately vacating this lease.

Objective 2 – Optimize Functionality, Reliability, Utilization, and Operating Costs

PNNL continues to invest in the necessary maintenance, repair, and renewal to sustain our building and infrastructure assets in a mission-ready condition; provide the physical environment that meets current and emerging research needs; optimize campus functionality, reliability, and utilization; and improve research operations while maintaining or reducing operating costs.

The following general-purpose building or parcel-specific projects support this objective:

- *Federalization of the PNNL Campus*: PNNL is focused on executing the DOE and Battelle contractual agreement to transfer the Battelle-owned Richland and Sequim, WA facilities to DOE-SC by the end of FY 2022. DOE and Battelle have also agreed that DOE has the right to acquire or lease Battelle-owned land in Richland and Sequim, WA, and DOE has agreed to fully exercise this right on or before the end of FY 2035, subject to the availability of funds. This agreement results in DOE acquiring 21 Battelle-owned buildings and approximately 347 acres in Richland and Sequim, WA. To date, the Pacific Northwest Site Office (PNSO) and Battelle successfully transferred 10 buildings and 115.6 acres. The remaining parcels will be transferred to DOE-SC ownership, based on funding availability.
- *Take Advantage of Opportunities Provided by EM-Owned 300 Area Buildings*. PNNL is partnering with DOE's Richland Operations Office (DOE-RL) and the EM-managed Hanford Site to gain operational control of an expanded footprint within the existing Hanford 300 Area to support the PNNL mission. In FY 2020, PNNL has reached an agreement with DOE-RL to take over management control of 339A, converting this building to valuable lab space and taking on management and operations (M&O) responsibilities. In the near-term, PNNL has requested agreement from DOE-RL to take over management control of 3220, supporting office space growth needs and high ceiling space shortages in the 300 Area. Over the long-term, PNNL will be negotiating agreements to manage and occupy the existing 3212 facility, which would add valuable large instrument space. In addition to facility acquisitions, PNNL is reviewing opportunities to manage and operate additional land areas in support of the PNNL mission.
- *Discovery Hall Horizon Room Acoustics*: PNNL is proposing to increase the overall acoustical performance in multiple locations on the PNNL Richland Campus. The first of those projects will improve the acoustics in the Horizon Room in Discovery Hall by limiting the sound transmitting between the various conference rooms. This approximately $500K to $750K MC-funded project is planned to initiate in FY 2020.
- *Repurpose Guest House*: The PNNL Guest House is currently configured as dormitory/hotel space to accommodate visitors to the Laboratory. This building was initially constructed in 2001 to support the EMSL user facility, as well as PNNL students and interns. Operating the Guest House as a hotel has become more difficult. In alignment with PNNL's strategic vision, dormitory wings of the facility will be converted to office space, creating roughly 50–60 new workstations, leaving the center of the facility as existing hotel space. This $2M MC-funded project is anticipated to initiate in FY 2020.
- Reconfigure 339A to Support Research: PNNL has gained operational control of the existing DOE-EM 339A facility in the Hanford 300 Area. We will be initiating a $500K to $1M MC project in FY 2020 to remodel this facility to house research currently residing in the third-party facilities. Like all PNNL occupied 300 Area facilities, once this facility is no longer useful to this mission, it will be turned back to DOE-EM for disposal and remediation.
- *Repurpose Storage in the Laboratory Support Warehouse (LSW) to High Bay*: PNNL's Integrated Capability Management process has identified a need for high ceiling and high bay space to support research under way in and near the Physical Science Facility complex. To address this need, PNNL is proposing an MC project to repurpose the existing LSW storage warehouse to high ceiling research space. This facility is ideally located and possesses the basic infrastructure to support high ceiling research needs. This project will require adding additional power and potential ventilation to the existing facility. This $1M to $2M MC-funded project is anticipated to initiate in FY 2023.
- *Build a Richland Storage Warehouse*: PNNL is proposing to construct a new general-purpose storage warehouse on the south end of the PNNL Richland Campus (consistent with our strategy of migrating low-hazard activities to the south end of the campus) to replace the space lost to

the creation of the high ceiling facility. This $3M to $4M MC-funded project is anticipated to initiate in FY 2021.

- *Repurpose Battelle Inhalation Laboratory (BIL)*: PNNL will conduct an analysis to evaluate the existing conditions of the BIL facility in contrast to current Lab operating needs to determine the most cost-effective reuse option for PNNL's only unutilized facility. Once the analysis is complete, PNNL will propose an MC project to invest in repurposing the unutilized BIL facility to best align with the institutional needs of the overall campus strategy.

The following general-purpose infrastructure projects support this objective:

300 Area Infrastructure Investments: PNNL operates multiple facilities that are strategically placed in the Hanford 300 Area. Much of the infrastructure supporting these facilities is beyond its useful life (65 years old) and requires investment to support PNNL use to FY 2046 and beyond.

- *300 Area Waterline Replacement*: Originally designed to support the entire operating Hanford 300 Area, the existing potable water supply line that supports the remaining PNNL facilities is significantly oversized, which creates operational challenges. This $2M to $3M MC-funded project is proposed to be initiated within the 10-year planning horizon.
- *Steam-to-Hydronics Conversion*: PNNL is planning a steam-to-hydronics conversion project to replace failing heating infrastructure for three key Hanford 300 Area facilities. In addition to updating aging infrastructure, this project will attain institutional energy savings and, where feasible, increase the use of renewable energy sources. This $5M to $7M effort will be executed building by building over the 10-year planning horizon, reducing PNNL's deferred maintenance by $2.29M.

PNNL Richland Campus Infrastructure Investments:

- Condenser Water System Replacement: PNNL cooling ponds are critical to providing the chilled water necessary to meet the cooling requirements for comfort, facility equipment, and research equipment in LSL2, LSL2A, Battelle Auditorium (AUD), Research Operations Building (ROB), MATH, Physical Science Laboratory (PSL), and Engineering Development Laboratory facilities. The pond spray heads and pumps are at the end-of-life and need to be replaced to support the current mission. This $1M to $1.2M MC-funded project is proposed to be initiated in FY 2020 and will reduce PNNL's overall deferred maintenance by $540K and an additional $440K of repair needs.
- Steam-to-Hydronics Conversion: PNNL is planning a steam-to-hydronics conversion project to replace failing heating infrastructure for three additional key Richland Campus facilities. In addition to updating aging infrastructure, this project will attain institutional energy savings and, where feasible, increase the use of renewable energy sources. This $5M to $7M project will be executed building by building over the 10-year planning horizon and will reduce PNNL's overall deferred maintenance by $2.27M. PNNL will pursue SLI-general plant project (GPP) funding for this project. If SLI-GPP is unsuccessful, other funding sources will be pursued.
- Richland North Infrastructure: PNNL is proposing an MC-funded infrastructure development project north of Horn Rapids Road. This project will allow PNNL to be prepared for future development on the PNNL Richland Campus. This $2M to $3M MC-funded project is proposed to be initiated in FY 2022.
- Roof Replacements: Leveraging PNNL Plant Engineering's Condition Assessment Surveys of all facilities, PNNL has established a systematic approach to prioritize, fund, and execute roof replacement projects for those that have reached the end of their design life. PNNL leverages the mission need, deferred maintenance, and cost to repair and/or replace each roof in determining the prioritization. This approach is designed to reduce PNNL's overall deferred maintenance backlog while maintaining a mission-ready campus. In FY 2020, PNNL proposed the

replacement of the 318 roof, which will result in an overall deferred maintenance of $2M. The EMSL roof will be replaced during the current planning horizon.
- Campus Sidewalks and Parking Addition: To assure a mission-ready campus, PNNL is planning to make continual investments in the PNNL Richland Campus sidewalks and parking areas. This investment will refresh campus infrastructure to support pedestrian transportation across the PNNL Richland Campus.

Site Sustainability Plan Summary

Fundamental to the S&T outcomes that we deliver every day is our commitment to sustainability—a responsibility that we take seriously. 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 nation.

From innovative best practices in sustainable operations to environmentally focused scientific breakthroughs, PNNL is committed to making our world a better place to live for many generations to come. In FY 2019, we achieved several sustainability milestones, which are highlighted below.

Innovative Approach to Sustainability

PNNL was recognized for the 2019 DOE Sustainability Award for the Innovative Approach to Sustainability for our Voting-based Control for Occupancy Comfort and Energy Savings project.

This innovative project represents a joint effort between our researchers and sustainability engineers using occupant feedback to make real-time thermal comfort adjustments and to modify building operation set points for continuous work environment improvements. This approach is easy to sustain and is reproducible for other labs. The three-month pilot turned into a 12-month pilot with additional QuickStarter funding. After 12 months, PNNL saved more than 8,000 kWh (~5 percent) of electricity, more than 400 MMBtu (~34 percent) of natural gas, and approximately 70 tons in chilled water compared to the prior year, all while increasing occupants' comfort and optimizing building operations by enabling real-time feedback through interactive operations.

Better Building Smart Labs Accelerator Partner/Sustainable Buildings

PNNL is part of 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 of buildings and laboratory spaces as "Smart Labs." To date, PNNL has qualified one building and 20 laboratory spaces using the Smart Labs evaluation tool. PNNL plans to repeat this process for new facilities and existing buildings, where appropriate. For example, PNNL is in the process of preparing another new facility for the start of construction in early spring of 2020—the ESC building. This facility will be the next sustainable laboratory building compliant with the 2016 Guiding Principles and equipped with controls and sensors enabling Smart Labs operation.

Currently, PNNL has 10 (or 493,367 gsf) of 21 (or 1,149,481 gsf) applicable buildings compliant with the Guiding Principles. This is approximately 48 percent by building count, or 43 percent by total square footage.

Water Management

PNNL has reduced its water intensity by 67.4 percent compared to the FY 2007 baseline, which is a 2.9 percent year-over-year decrease. This accomplishment was achieved primarily due to water conservation and efficiency efforts. PNNL's newest building, Discovery Hall, was designed to meet the Federal Guiding Principles and was expected to exceed a 20 percent reduction from the allowed baseline water usage. The actual reduction from this building was 43 percent, which was more than double the expected reduction. PNNL has also added new, energy-efficient chillers in EMSL, a high energy, mission-specific facility, to further reduce its overall potable water consumption. PNNL's potable water use intensity since 2007 is provided in the figure below.

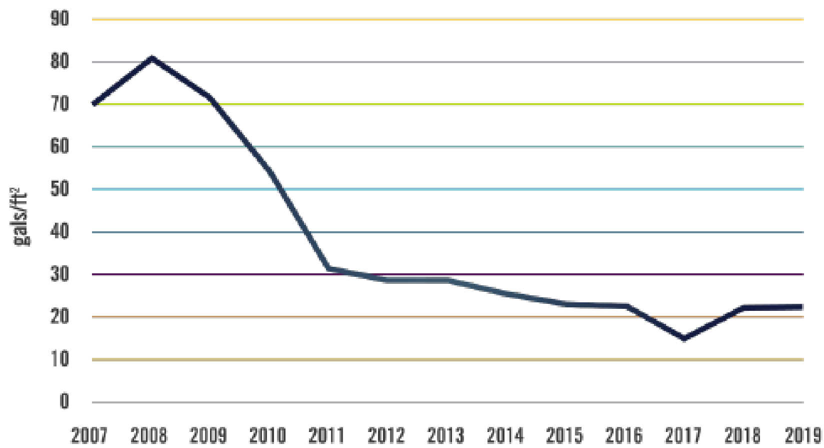
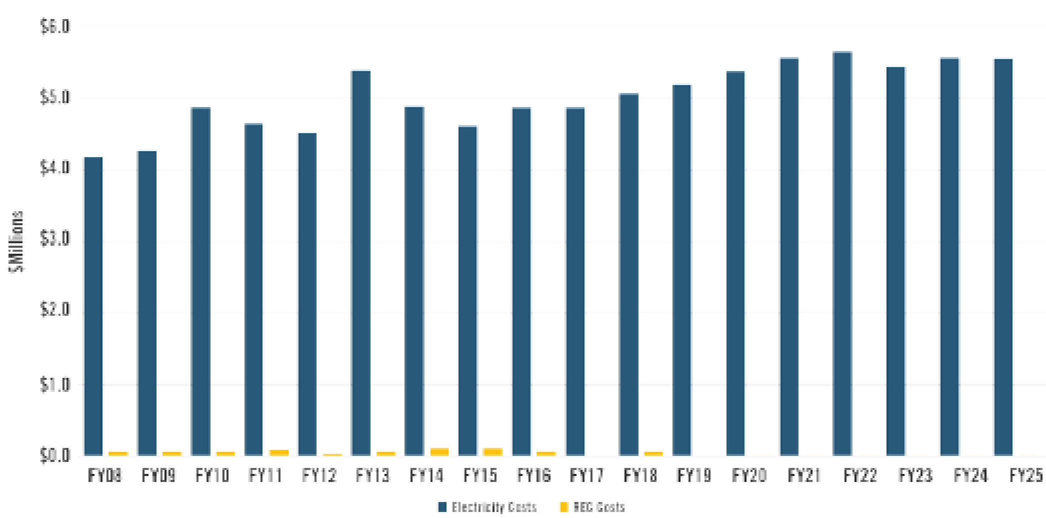


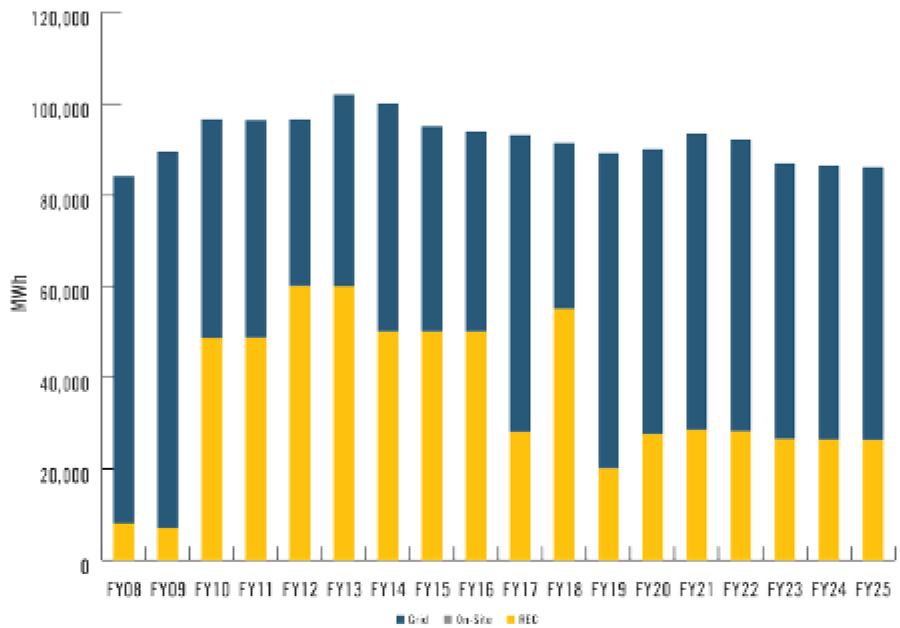
Figure: Potable water use intensity in gals/ft^2

Renewable Energy

In FY 2019, PNNL procured enough renewable energy certificates (RECs), combined with the onsite renewables, to offset 23 percent of its electrical use and 17 percent of its total electric and thermal energy.

Aside from RECs, PNNL has several onsite solar arrays. The solar hot water heater installed at EMSL produces approximately 160,000 Btu/hr (peak output) and is dedicated to the lunchroom and associated restrooms, fulfilling the majority of that area's hot water needs. Several small solar photovoltaic (PV) arrays power various air and water monitoring stations throughout the campus; these have not been counted toward the goal. In addition, PNNL operates a 125 kW PV array at the EMSL building, which includes charging stations for electric fleet vehicles and is used for several R&D projects. The figures below illustrate PNNL electricity and REC costs, as well as electricity usage and cost projections.




120,000
100,000
80,000
60,000
40,000
20,000
0
MWh
FY08 FY09 FY10 FY11 FY12 FY13 FY14 FY15 FY16 FY17 FY18 FY19 FY20 FY21 FY22 FY23 FY24 FY25
Grid
On-Site
REC

PRINCETON PLASMA PHYSICS LABORATORY

Lab-at-a-Glance

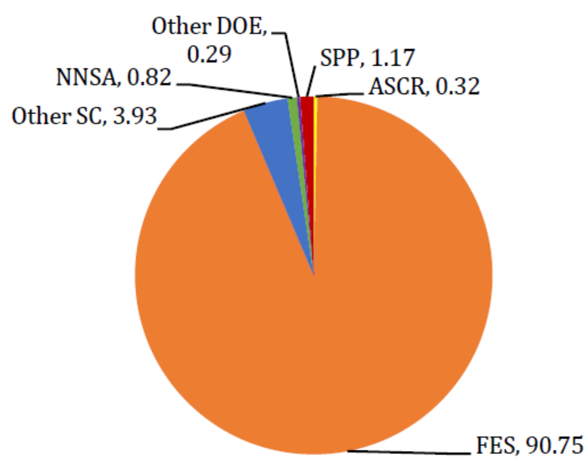
Location: Princeton, NJ
Type: Single-program Laboratory
Contractor: Princeton University
Site Office: Princeton Site Office
Website: www.pppl.gov

- **FY 2019 Lab Operating Costs:** $97.28 million
- **FY 2019 DOE/NNSA Costs:** $96.11 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $1.17 million
- **FY 2019 SPP as % of Total Lab Operating Costs:** 1.2%

Physical Assets:
- 90.7 acres and 30 buildings
- 758,000 GSF in buildings
- Replacement Plant Value: $744.1 M

Human Capital:
- 531 Full Time Equivalent Employees
- 7 Joint Faculty
- 36 Postdoctoral Researchers
- 45 Graduate Students
- 24 Undergraduate Students
- 318 Facility Users
- 28 Visiting Scientists

FY 2019 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 managed by Princeton University since 1951. 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 industries of the future; and (3) to further the scientific understanding of plasmas from nano- to astrophysical- scales.

PPPL's five core capabilities reflect its expertise and the role it plays in the DOE missions:

- Plasma and Fusion Energy Sciences
- Systems Engineering and Integration
- Large Scale User Facilities/Advanced Instrumentation
- Mechanical Design and Engineering
- Power Systems and Electrical Engineering

For nearly seven decades, PPPL has been a world leader in magnetic confinement experiments, plasma science, fusion science, and engineering. PPPL is 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. The Laboratory is evolving however, 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 of the future. Princeton University and PPPL develop the workforce of the future by educating and inspiring world-class scientists and engineers to serve the laboratory and national interest. PPPL also develops its operations staff (64% of total) to deliver its mission efficiently and rigorously.

Core Capabilities

The Princeton Plasma Physics Laboratory (PPPL) has five DOE-designated core capabilities and two proposed new capabilities 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* (proposed new)
7. Condensed Matter Physics and Materials Science* (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 *industries of the future*. 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 two new core capabilities:

- Computational Science
- Condensed Matter Physics and Materials Science

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 2019, 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 have collectively authored or co-authored dozens of white papers and initiative proposals for the CPP across all areas of the field, and 28 of whom were in attendance for the CPP-Houston meeting. PPPL was host to a town hall for the CPP in 2019. Successfully designing, constructing, and operating a world-leading "next-generation facility"—a charge defined as an outcome of the recent Houston meeting—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.

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. These contributions and more are described more fully in the Science and Technology Strategy for the Future section.

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

Following successes with the NSTX-U Recovery Project, PPPL is well positioned to lead the systems engineering of new fusion facilities to incorporate innovative designs for reduction of capital costs. Systems Engineering and Integration principles are ingrained in PPPL's daily work processes for design to field integration, with consideration for technical risk and failure modes throughout the engineering lifecycle.

Systems engineering is application-agnostic, as it can be applied to different types of systems from power plants to computer chips. Therefore, PPPL's engineering expertise is quite valuable for future research and development activities, independent of direction. Systems engineering is fundamental in the design of a next generation nuclear fusion plant, which may be maintained and managed, real-time, in a distributed environment via a virtual representation or "simulation" of the machine. PPPL has plans to materially contribute to ITER diagnostic design and fabrication and to commercial industry needs and standards using integrated simulations and virtual prototyping for experimentation and testing, once platforms and tools are implemented at PPPL. Integrated simulation environments allow for: enhanced communication between scientists and engineers, thus reducing technical risk; remote maintenance, to avoid exposure to hazardous environments; and the importing of data from instrumentation associated with test stands, prototype efforts, and experiments.

PPPL developments of note in FY 2019 include:

- NSTX-U has further extended the applications of systems engineering to help define and track granular requirements through design, develop interface control documents to ensure subsystems interact correctly, and is on the verge of developing test plans to confirm the system has been recovered correctly. Additionally, a small-scale, integrated solution using a commercial Multiphysics tool COMSOL is being piloted on NSTX-U. The initial focus is on system-element boundaries from inception, rather than at completion, to reduce errors.
- PPPL is leveraging existing operational and experimental computation experience to develop Distributed Instruments, potentially enabling 5th Generation (5G) wireless technology for computing to the edge in many diagnostic and control applications. Additional work is being done to develop a small, inexpensive 5G enabled sensor meshes for mass deployment, to further acquire large data sets to be analyzed by machine learning techniques. PPPL's capacity to innovate and execute novel, tightly coupled, electronics and software solutions for scientific applications is a core competency. With additional experience in delivering experimental data to fast or near real-time computational resources to obtain meaningful, scaled, results that benefit real-time control, PPPL will serve as a valuable partner to industries exploring new applications.
- PPPL has developed automated mechanisms to transfer and analyze large data sets in post pulse scenarios to quickly inform operators and research personnel of the effects oftheir experiments. This capability may be used to mirror NSTX-U experimental data in ITER's Interface Data Structure (IDS), enabling the development and porting of PPPL's analysis code and use of ITER's native format through the creation of a local ITER Data System in a proof of concept.
- PPPL is currently studying the effects of neutron radiation on electronics and the materials used in their construction to optimize type and placement of equipment in areas of high flux.

Systems engineering also formed the support frame for the conceptual design and cost and schedule of the proposed permanent magnet stellarator.

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 and Lithium Granule Injector 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.
- 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.

Mechanical Design and Engineering

PPPL has developed a modern, rigorous design-by-analysis approach that is integrated into its engineering planning, quality assurance, and project management principles, preparing for new opportunities to analyze, design, test, validate, and enable operation of advanced engineered systems and devices. This approach is achieved by defining a design path, aligning the depth of the analysis with the level of maturity and risk in the design.

Through the extensive and thorough design reviews and quality control for NSTX-U Recovery, PPPL has benchmarked its engineering design practices with experts from U.S. national laboratories for better alignment to industry standards and project management best practices. The PPPL Engineering organization, as a whole, has been well-reviewed by senior staff from other U.S. national laboratories and partners from international fusion research centers, and has made important organizational and functional changes based on their insight and recommendations.

During the manufacturing phase of NSTX-U Recovery, PPPL will further modernize and integrate advanced fabrication tools with Computer-Aided Design and Manufacturing (CAD and CAM). This will improve machining capabilities and reduce risk in the project delivery by providing prompt and flexible response to unpredictable and urgent requests.

Anticipated, future developments include:

- case studies and market studies to identify requirements for a Virtual Engineering platform to serve PPPL's functional needs and develop designs that can be more efficiently manufactured;
- using cloud computing to tap into diverse analytical tools, as suitable;
- hiring and training additional manufacturing engineers with CAD/CAM capability to perform simulations and parametric design and modeling, and to debug design and machining issues;

- allocating space during conceptual design of PPPL machines to investigate various manufacturing options that are drastically different;
- developing PPPL's expertise in study and application of semiconductors and nanofabrication;
- partnering with Alkali Consulting and Tokamak Energy (TE) to procure and assemble components of test designs and designs; and
- collaborating with TE to develop installation constraints, engineering support, and deploy designs in ST40.

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) transformer. This transformer has been selected in conjunction with the Laboratory, to support the future experimental pulsed loading requirements. The capacity of the main switchyard transformers is sufficient to support the NSTX-U power pulse loading 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 virtual 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.

Proposed New Core Capabilities

PPPL is increasing efforts to strengthen and/or diversify into research areas embodied in two new core capabilities:

- Computational Science
- Condensed Matter Physics and Materials Science

The Laboratory's and Princeton University's expertise in nanofabrication science is considerable (especially in low temperature plasmas). Leadership in this science and technology area will require a multidisciplinary set of capabilities that PPPL is committed to strengthening and growing. Thus, PPPL seeks to formally establish a new core capability in **Condensed Matter Physics and Materials Science** through strategic hires. Similarly, PPPL has been at the forefront of developing numerical capabilities for fusion prediction, analysis, and design, and for plasma simulation, in general. However, PPPL wishes to be further recognized as a leader and therefore seeks to formally establish a new core capability in **Computational Science** with help from Princeton University and through hiring of data scientists, applied mathematicians, and other computational numerical specialists. The laboratory expects to establish these two 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 radical advanced fusion concepts and technologies through computer simulation and targeted experiments. The Laboratory is collaborating with private fusion companies and foundations to move its fusion science and technology toward market viability.
2. The second mission is to advance the science of nanoscale fabrication for industries of the future. 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 plasmas from nano- 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 some of the most important problems in Astrophysics and Space physics. For example, the collaborative experiment, FLARE, is being constructed to unravel the mysteries of magnetic reconnection that powers many natural explosive events.

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 enduring 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 of 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 758k gross square feet (GSF) of the Princeton University Forrestal Campus, 30 government-owned buildings, two temporary office trailers, and one off-site pump house. 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 2019 and there are no current plans for transactions in FY 2020.

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, and
- Telecommunications.

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.

Infrastructure Data Summary

Total Building Assets	**30**
Total Other Structured Facilities (OSF)	27
Total Deferred Maintenance 2019 ($)	**$71.4M**

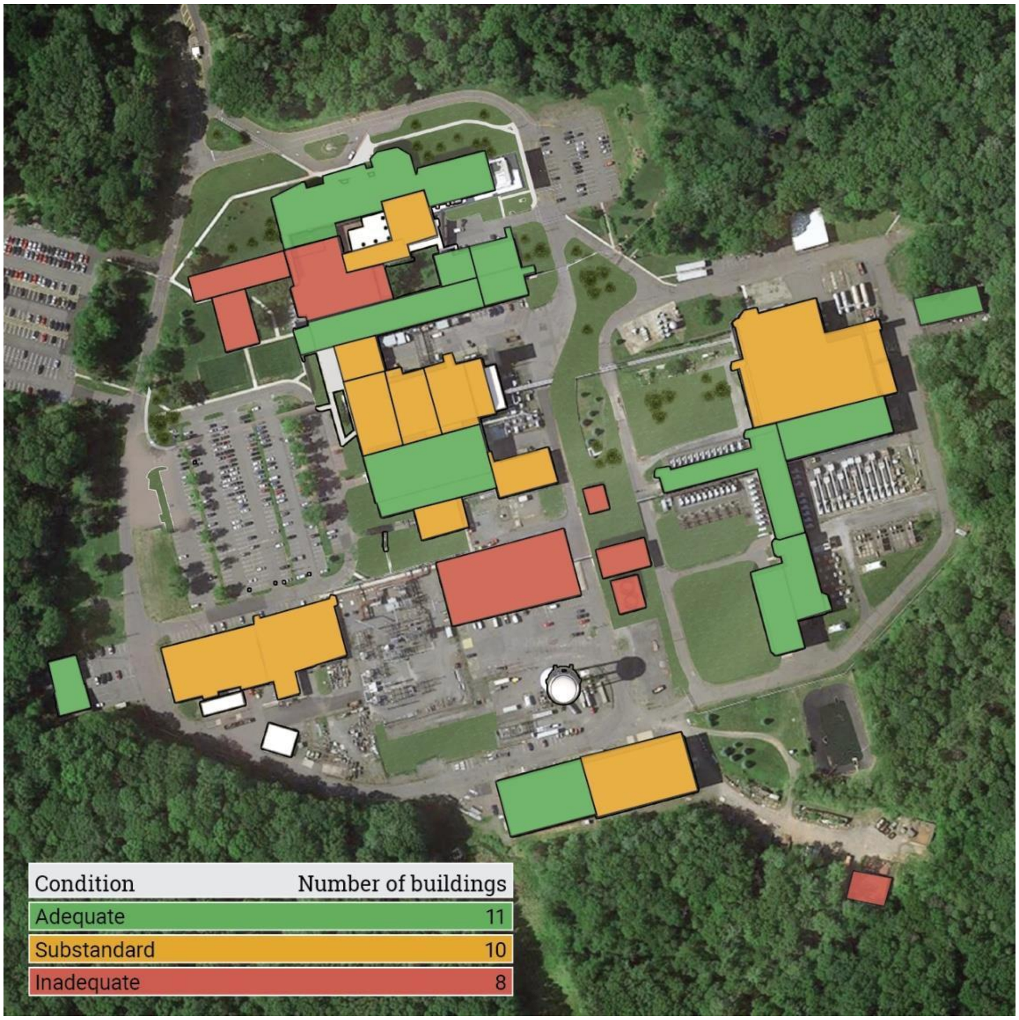


Figure: Building Condition

As identified above, 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 $10 million of the current General Plant Projects (GPP) portfolio is in construction, with another $10-12 million in design. The Laboratory is preparing for CD-1 approval of more than $200 million in SLI Projects. These projects will enhance PPPL's resiliency and improve efficiency by leveraging artificial intelligence for operations.

The only gross square foot reductions under consideration at this time are associated with the SLI construction of the Princeton Plasma Innovation Center (PPIC). PPIC will update two existing, "inadequate" buildings (Theory Building and the Administration Building), and the Critical Infrastructure Recovery & Renewal (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 unutilized 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 further 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 must continue to renovate existing facilities and provide reliable, efficient systems in new and planned facilities. 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, the physical, "usable" footprint of the Laboratory will need to grow, too.

The FY 2020 Maintenance and Repair (M&R) budget projections are expected to be below those of FY 2019. CD-0 approvals for the planning of two SLI Projects were initiated in FY 2019. When completed, these projects will replace old, inefficient buildings (one 40+ years old and one 62+ years old); provide a new modern research building with nominal maintenance needs and high operating efficiencies; and replace/modernize ~$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.

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. Additionally, the GPP pipeline of projects has grown. The campus strategy is currently at a pivotal point in which new science diversification plans are being defined. The final plan for campus strategy is subsequently being developed to address this new vision in a comprehensive plan that will also address DM.

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 Princeton Plasma Innovation Center (PPIC), Critical Infrastructure Recovery & Renewal (CIRR), and Tritium System Demolition and Disposal (TSDD) – to co-locate these staff populations and resolve functionality issues; however, additional renovations and infrastructure assessments are needed to support future research. 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 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.

PPPL's five existing Core Capabilities, as well as two newly proposed capabilities are:

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*

**Proposed New*

These seven total capabilities, as well as the five science 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 science initiatives and will support continued growth in both established and proposed new core capabilities.

Gap Analysis

Planning Objectives	Gaps/Risks	Impacted Science Initiative	Impacted Core Capability
Increase Reliability/ Capability of User Facility	NSTX-U lacks adequate infrastructure to support user facility needs. • Pursue projects to update systems (HVAC, controls, roofs). 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 construction of Liquid Metal Development Lab.	**1, 4**	**1, 3, 5**
Advance Industries of the Future	PPPL lacks modern lab space and clean rooms to continue nanofabrication research and to pursue new Quantum Information Science (QIS) R&D. • Design PPIC to provide space for diagnostics and actuators for FLARE, a PM Stellarator, superconducting magnet research, and fabrication and testing space. • Construct PPIC to offer modern lab spaces, collaboration spaces, and office spaces. • Complete TSDD project and re-envision TFTR Test Cell as well as surrounding area as new Fusion Research Technology Hub (FuRTH) in support of partnerships with private industry.	**2, 4, 5**	**1–4,** 6,* 7*
Enhance Laboratory Operational Reliability/Safety	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 PPIC's Collaboration and Visualization Hub (CVHub). PPPL does not offer enough space to accommodate both large collaborations and provide a safe, social distance. • Remodel existing space for immediate and safe use for all groups. • Implement the CIRR Project to improve utility and IT infrastructure.	**3, 4, 5**	**1, 2, 3,** 6*
Enhance Laboratory Operational Efficiency	Existing, usable building spaces and offices are oversubscribed and cannot accommodate the staff growth necessary for mission execution. • Open PPIC to provide 233 new seats for staff and flexible, mobile infrastructure to accommodate changing needs. • Existing spaces are not able to co-locate or "cluster" collaborators and mission-focused research teams. • Construct new building within the FuRTH to accommodate internal and external user growth and provide proximity to experiments.	**2, 4, 5**	**1, 3, 5,** 6*
Diversify PPPL's Research Portfolio	PPPL lacks space for new staff, external partners, and users of different science disciplines. • Construct PPIC to offer modern lab spaces, collaboration spaces, and office spaces. • Construct new building within the FuRTH to accommodate general growth of staff and users. • Transform underutilized, existing spaces into new Science and Technology Interaction Center (STIX) to foster collaborations.	**2, 4, 5**	**1–5,** 6,* 7*

Based on this gap analysis, the Laboratory has identified the infrastructure priorities necessary to close these gaps and support Mission Readiness.

To *Increase Reliability* of PPPL's *User Facility*, NSTX-U, PPPL will focus on the replacement of NSTX-U's HVAC systems and roofs. As further described in the FY 2020 Campus Plan, the CIRR project will update the transformers to support power loads when NSTX-U becomes operational. Success of NSTX-U relies on the timely execution of these CIRR project plans.

PPPL's New Liquid Metals Development Building

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 five pounds is urgently needed. 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, as an important concept paper is being reviewed by ARPA-E for potential science funding support. The proposed new, or remodeled structure will be encased in steel and designed to the National Fire Prevention Association (NFPA) 484 standard to ensure operational safety.

The Princeton Plasma Innovation Center (PPIC)

NSTX-U's immediate program needs also include additional office spaces to accommodate growth in scientific and engineering staff, as well as visiting scientists. PPIC will not offer new spaces in time for initial start-up, 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 industries of the future* 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 abovementioned 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.

Two existing experimental spaces are slated for upgrades in FY 2020 to accommodate active research for SPP and CRADA partners while the Lab awaits the opening of PPIC and the delivery of the necessary small- and medium-bay labs for expanded research in this area. Scientific staff also depend heavily on the availability of Princeton University laboratories and partners to support research that cannot currently be conducted on site.

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 2025, the completion of the RCC and CVHub (2026) 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:

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)

Even with the large number of highly anticipated improvements, many deficiencies still remain that impact research operations. 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.

A proposal to retrofit the former TFTR Test Cell is forthcoming. The Fusion Research and Technology Hub (FuRTH) will include the newly available test cell space, created through completion of the Tritium System Demolition and Disposal (TSDD) Project, and an adjacent building to support its scientists and engineers. The TSDD Project will 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 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.

Figure: FuRTH Test Cell

A small, new office building will 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), to accommodate on-site private industry research partners. This new building will provide two levels of working spaces to accommodate:

- researchers and technicians employed by these collaborating companies;
- PPPL researchers and operations staff supporting this research; and
- additional PPPL staff necessary for supporting growth of research programs.

Science and Technology Interaction Center (STIX)

PPPL also looks forward to the successful completion of the full scope of CIRR projects in order to support external academic partners on current research projects as growth in experimental research populations, long-term national and international collaborators, and shorter-term facility users and visitors is anticipated. Existing spaces often prevent teams and departments from being co-located, creating inefficiencies and collaboration hurdles. Transforming the former Harold P. Furth Library, the aged fitness center, and a large portion of the PPPL computer center (PPPLCC) into a new academic collaboration center, the Science and Technology Interaction Center (STIX), will allow for increased interaction among researchers in a centralized location. This remodeled space will provide the needed workspaces for Princeton University users, official visitors and assignees, and graduate student populations.

These infrastructure proposals are further detailed in PPPL's FY 2020 Campus Plan.

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 our EMS objectives and targets.

PPPL's FY 2019 Scope 1 and 2 Greenhouse Gas (GHG) emissions were 86.5% below the FY 2008 baseline, far below the annual goal of 31%, primarily due to a lack of fugitive sulfur hexafluoride (SF6) emissions from experimental power systems. Scope 3 GHG emissions were 9.2% below the FY 2008 baseline primarily due to lower site electricity usage and associated transmission and distribution (T&D) losses. Emissions from employee commuting and business travel are both higher than baseline.

PPPL continues to exceed federal recycling goals for both municipal solid waste (MSW) and construction and demolition (C&D) waste by achieving recycling rates of 76.5% and 70.5%, respectively. 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.

PPPL has one existing Leadership in Energy and Environmental Design (LEED)-certified building. This is equivalent to approximately 16% of PPPL's total GSF, meeting the site's target of at least 15% of square footage meeting the Guiding Principles. PPPL is planning for the new Princeton Plasma Innovation Center (PPIC) to meet the Federal High Performance and Sustainable Building (HPSB) Guiding Principles and meet the LEED-Gold criteria, subject to available funding.

Figure: Artist’s rendering of the new entry to PPPL with the Princeton Plasma Innovation Center (PPIC)

Between FY 2003 and FY 2019, PPPL’s energy intensity decreased from a baseline of 176 thousand British Thermal Units per gross square foot (kBtu/GSF) to 151 kBtu/GSF – a reduction of 14%. Recent energy use intensity (EUI) data show an uptick in consumption (1.5% from FY 2018 to FY 2019) which is attributed to on-site construction activity, inefficient buildings and equipment that are well past their life expectancy (increasing deferred maintenance), and lack of prior year energy-reducing project investment. PPPL has reduced per-capita potable water consumption by almost 40% between FY 2007 and FY 2019. 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. 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.

SLAC NATIONAL ACCELERATOR LABORATORY

Lab-at-a-Glance

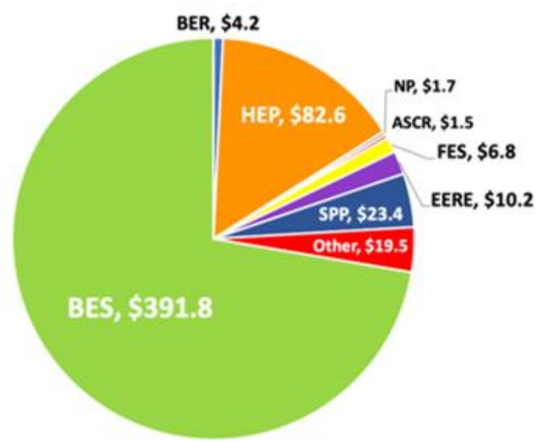
Location: Menlo Park, CA
Type: Multi-program Laboratory
Contractor: Stanford University
Site Office: SLAC Site Office
Website: www.slac.stanford.edu

- **FY 2019 Lab Operating Costs:** $541.5million
- **FY 2019 DOE/NNSA Costs:** $518.1 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $23 million
- **FY 2019 SPP as % Total Lab Operating Costs:** 4%
- **FY 2019 DHS Costs:** $0.4 million

Physical Assets:
- 426.3 acres and 150 buildings
- 1.8M GSF in buildings
- Replacement Plant Value: $3.1 B
- 1,170 GSF in 1 Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:
- 1,620 Full Time Equivalent Employees (FTEs)
- 22 Joint Faculty
- 227 Postdoctoral Researchers
- 241 Graduate Student
- 121 Undergraduate Students
- 2,608 Facility Users
- 22 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



Mission and Overview

SLAC National Accelerator Laboratory is a vibrant multi-program laboratory whose mission is to explore how the universe works at the biggest, smallest, and fastest scales and invent powerful tools used by scientists around the globe. As a U.S. Department of Energy (DOE) national laboratory, 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 is the world-leading laboratory in X-ray and ultrafast science due in large part to our X-ray user facilities: 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.

Since our founding in 1962, SLAC has made breakthrough discoveries that have established our leadership in high energy physics. SLAC continues to lead major scientific advances toward understanding the physics of the universe, with international leadership in all five science drivers of the Particle Physics Project Prioritization Panel (P5), including probing the nature of dark energy with the Vera C. Rubin Observatory, previously known as the Large Synoptic Survey Telescope (LSST).

With five decades of excellence in accelerator physics, SLAC is the leader in advanced accelerator concepts and drives the development of critical accelerator technologies with a broad range of applications.

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), the Stanford-SLAC cryogenic electron microscopy (cryo-EM) facility, and the National Institutes of Health (NIH)-funded cryo-EM facility located in the Arrillaga Science Center (ASC).

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. To do this, SLAC leverages our location in Silicon Valley and our strong relationship with Stanford University (Stanford).

Stanford manages the Laboratory for DOE's Office of Science (DOE-SC) and bolsters our research, education, and operations. SLAC jointly operates three institutes and two research centers with Stanford. Together with Stanford, SLAC educates and develops the U.S. scientific workforce in key technological areas.

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 user facility. 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 will the addition of the undulator Beam Line 12-1. This new beamline, which targets micro-beam macromolecular crystallography, will form a structural biology gateway between SSRL and LCLS and allow us to integrate multimodal imaging with the cryo-electron microscopy (cryo-EM) facility at SLACe.

Cryo-EM. SLAC operates one of the world's leading centers for cryo-EM research and technology development; the six 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 serves the international science community and Stanford, operates four of the instruments. Two others are made available to the scientific community at the National Institutes of Health (NIH)-funded Stanford-SLAC Cryo-EM Center (S^2C^2). We are adding new capabilities that, 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, section A 1.2 below.

Particle Physics facilities and instruments. See "Particle Physics" core capability, section A 1.5 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.

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, coherent X-ray light sources – both free-electron lasers (FELs) and storage ring light sources – and instruments for UED and ultrafast electron microscopy (UED/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 upgrade (LCLS-II) and LCLS-II high energy upgrade (LCLS-II-HE) are implementing high-repetition-rate superconducting accelerator technology to increase the repetition rate of the FEL from 120 Hz to 1 megahertz (MHz). In contrast to the pulsed superconducting European X-ray Free Electron Laser (European XFEL), the LCLS-II superconducting radio-frequency (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 research and development (R&D) program aims to achieve complete control of the beam's spectral and temporal X-ray 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 X-ray seeding to narrow the spectrum of wavelengths within a single pulse; generation of higher-power FEL beams and much shorter pulses; generation of multiple colors and pulses of X-rays at the same time; and advancements in techniques, diagnostics, and optics for ultrafast science. 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. Our collaboration with Argonne National Laboratory (ANL) on cavity-based X-ray free electron laser (CBXFEL) R&D is developing technologies that have the potential to increase the brightness of X-rays from LCLS-II and LCLS-II-HE by one-to-two orders of magnitude.

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 hard X-rays from LCLS-II-HE; improving the brightness by a factor of four would nearly double the spectrum of wavelengths it could generate. 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 CW SRF electron sources and plasma-based sources and is collaborating with Lawrence Berkeley National Laboratory (LBNL) on an upgrade of the LCLS-II RF gun. This work is critical for the success of future X-ray experiments, UED/UEM, and even future particle colliders.

Advanced acceleration and RF acceleration R&D. SLAC plays an internationally unique role in the development of beam-driven PWFA. To maintain our leadership in this increasingly competitive field, we are developing FACET-II, the follow-on facility to FACET. 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.

SLAC's capability and innovation in RF accelerator technology are tapped by federal agencies, industry, and laboratories around the world. SLAC is the only laboratory in the DOE system with the integrated capability to conceive, design, prototype, and test the full technological chain of RF accelerators, from RF sources to structures. Through system-level optimization (*e.g.* cryogenic copper RF structures and heavy beam loading), and basic R&D efforts (*e.g*. in materials and topologies), our program focus is improving the cost-capability curve of RF accelerators. SLAC had the lead laboratory organizing role for the 2019 DOE Basic Research Needs Workshop on Compact Accelerators for Security and Medicine sponsored by DOE-SC and DOE-NNSA, NIH, the U.S. Department of Defense (DOD), the Defense Advanced Research Projects Agency (DARPA), and the U.S. Department of Homeland Security (DHS). SLAC also co-edited the workshop report published in January 2020.

SLAC's leading expertise in THz science and technology has extended the reach of our RF accelerator program and delivered unique capabilities in diagnostics, beam manipulation and gradient, and for example, in generating compressed electron bunches. New directions include the development of novel THz power sources and their integration with accelerators, as well as THz-based high-brightness electron sources.

Accelerator test facilities. SLAC's test facilities also include the following.

The low-energy Accelerator Structure Test Area (ASTA) facility. ASTA is a small bunker and test stands equipped with multiple high-power RF sources, flexible laser systems, and excellent temperature stabilization. This facility allowed efficient development of our UED capability.

The medium-energy Next Linear Collider Test Accelerator (NLCTA). The NLCTA provides critical support for vital R&D programs, including SRF gun studies for LCLS and LCLS-II, DOE-HEP-sponsored high-gradient structure testing, and novel THz accelerator R&D supporting an existing Early Career Award. Plans for revitalizing this 25-year-old facility are under development.

The higher-energy Sector 30 Transfer Line (S30XL). The S30XL, now under construction, will connect the LCLS-II SRF linac to End Station A. This beamline will allow parasitic near-CW beams of 4 GeV electrons for test beams, as well as dark sector searches and other precision measurements.

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 get the hands-on experience they need 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 29 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 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.

SLAC scientists partner in this work with Stanford on such initiatives as the Precourt Institute for Energy's StorageX Initiative, 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 of next-generation X-ray facilities such as 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 intrinsic scientific interest, but also essential for designing new materials with properties tailored for technological applications – including 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. For the Background Imaging of Cosmic

Extragalactic Polarization (BICEP) cosmic microwave background (CMB) program, we designed and built detectors and readouts that allowed the project to establish new limits on cosmic inflation. Our goal is to lead and build the ultimate experiment in this field, cosmic microwave background stage 4 (CMB-S4), which will be the world's largest camera for microwaves; it will build on BICEP and other experiments to definitively measure the universe's first detectable light and contribute to studies of cosmic inflation, neutrino masses, gravitational lensing, and the evolution of galaxy clusters.

Large-scale microfabrication of superconducting devices. Our goals for playing a major role in building and directing the CMB-S4 project are supported both by our expertise in designing and building arrays of superconducting devices, and by our experience in managing and engineering large-scale projects like the LSST camera. We are building the Detector Microfabrication Facility (DMF) with Stanford support; it will be a new capability for the DOE complex and allow us to produce superconducting devices on a large scale. In addition to its role in building CMB-S4, the DMF will be used to develop new systems for X-ray applications and to construct advanced quantum devices.

Advanced quantum devices. Our quantum program has several thrusts. "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 future of CMB-S4, quantum information science (QIS), dark matter searches, and 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.

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. 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 NBDB 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 recently took 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 technical design report to follow in about a year.

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 (SC 2, 21, 22, 23, 24, 25, 26, 29).

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 100-Hz 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 a new DOE-FES Early Career Award that supports research into the dynamic evolution of fusion ablator materials and the role of defects and voids in hydrodynamic instability growth.

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 predict that certain types of shocks 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 that are unique to ultrafast studies with X-ray lasers or UED.

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 (SC 2, 24).

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 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
- **Pioneer an internationally leading biosciences program** by applying our state-of-the-art integrative, multi-modal imaging program to advance discovery and innovation in bioenergy, biology, and medical sciences
- **Advance QIS 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 lab'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

Our land, facilities, and utilities serve as the backbone to enable DOE's mission at SLAC. SLAC is located on 426 acres of Stanford leased land in unincorporated San Mateo County on the San Francisco Peninsula. With SLAC supporting six of DOE's core capabilities, our Laboratory has grown along with the science, resulting in leading-edge facilities as well as legacy utility systems built over the span of nearly 60 years.

The land lease agreement between DOE and Stanford has been in place since 1962, and was renewed in 2010 for 33 additional years. As part of this agreement, 25 acres across three separate parcels were identified as opportunities for Stanford to consider removing from the ground lease. Although Stanford has not communicated intentions to pursue development in these areas, they continue to be identified in our land use planning. Stanford has strong academic and mission ties to the SLAC site and continues to show interest in supporting the Laboratory's infrastructure development.

The total real property inventory in the Facilities Information Management System (FIMS) consists of 287 assets: 158 buildings, 102 other structures and facilities (OSFs), and 27 trailers. Most of our properties are mixed-use buildings that include offices, laboratories, research facilities, and support buildings, with approximately one-fourth of the square footage attributable to tunnels and unique experimental facilities. The largest real property asset houses the 2-mile-long accelerator located 25 feet below grade.

The utilities infrastructure supporting SLAC facilities comprises electric, chilled and hot water, domestic and fire water, low-conductivity water (LCW), storm sewer, sanitary sewer, natural gas, fire alarm, telecommunications, and compressed air. SLAC purchases electric power through the DOE Power Purchasing Consortium using Western Area Power Administration rates, and it is delivered through Pacific Gas and Electric's (PG&E's) transmission lines. The primary power feeder is connected to PG&E lines, then delivered to SLAC across a 230-kilovolt (kV), 5.4-mile-long transmission line owned by DOE. A second PG&E transmission line rated at 60 kV provides an alternate power source, but it cannot fully support SLAC's power demand or loads. PG&E also provides natural gas. Water, storm sewer, and sanitary sewer services are provided by the local municipality and districts.

Campus Strategy

Our campus strategy is strongly aligned with the Laboratory's goals and strategic initiatives and ensures that we deliver highly reliable, efficient, and effective infrastructure. To achieve the Laboratory's scientific vision, we have set in motion a plan that includes near-, mid-, and long-term actions. As these are implemented, the results inform and guide our decision making on resources and infrastructure investments. The following sections describe our plan to ensure mission-ready facilities as Laboratory capabilities expand and as infrastructure matures.

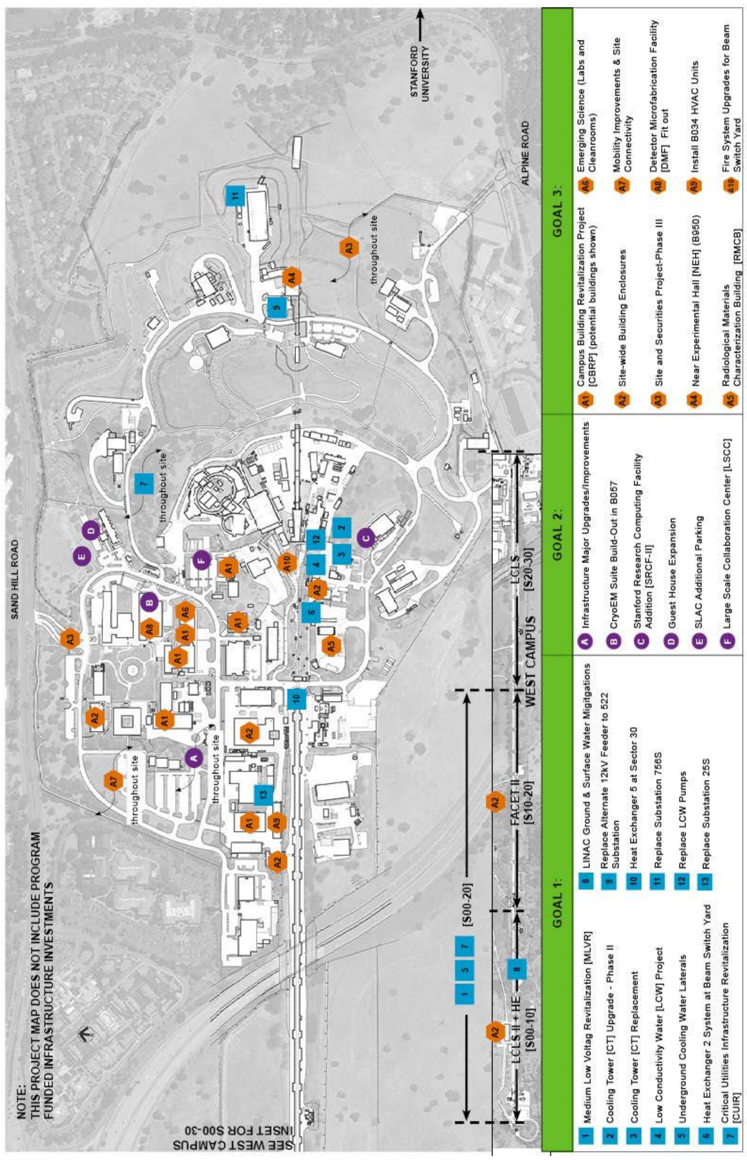


Figure: SLAC's 10-Year Planned Facility and Infrastructure Investments

The SLAC Long Range Vision plan (2015) illustrates our capability to grow the Laboratory's physical infrastructure to support DOE's science mission over the long term, spanning multiple decades. The next update of this document, which will be developed in partnership with Stanford, is scheduled for 2021. The strategy for achieving the long range vision will be to focus on the mid-term outlook of a five-to-ten year window to address existing capability gaps, and to leverage both direct and indirect infrastructure investments to close such gaps to maintain mission ready facilities today and into the future.

SLAC's infrastructure investment strategy focuses on optimizing the use of current assets, modernizing facilities, and synchronizing stewardship of operations and maintenance in support of current and future science missions. Our three campus strategy goals are:

1. Revitalize and modernize our utility infrastructure backbone to ensure resilient delivery of utilities, operational reliability, and mission readiness;
2. Provide a variety of spaces and areas for diverse groups to work collaboratively and explore science opportunities;
3. Modernize existing facilities to enable our strategic initiatives.

Figure 1 is a location map of 10-year planned investments across our site. It depicts how each project meets one of our three campus strategy goals within the unified infrastructure vision.

The following sections articulate how we are currently executing our campus strategy as well as our highest priorities for the future. Through each investment, we integrate sustainable actions to optimize systems for life cycle, systems management, and maintenance.

Revitalize and Modernize our Infrastructure Backbone to Ensure Resilient Delivery of Utilities, Operational Reliability, and Mission Readiness

Resiliency and reliability of utilities are essential in meeting the requirements for user facilities, scientific instruments, laboratories, and experimental equipment. We must continue to revitalize and modernize our aging infrastructure, especially with increased reliance on computing systems for telework and a need to perform research and develop means of addressing emerging threats, as well as the criticality of supporting experimental systems with extreme tolerances and operating parameters. While many of our highest safety risks have been addressed, the most crucial concerns now are electrical power and cooling water systems, both of which directly affect science missions.

Electrical Power

Direct investments in electrical substations – such as DOE's Science Laboratory Infrastructure (SLI) General Plan Projects (GPP) K-Substations (KSubs) and Medium Low Voltage Revitalization (MLVR) – have modernized assets to improve electrical utility delivery and operational reliability for multiple accelerator systems housed in the 2-mile-long linac.

As part of facility operations, we perform rigorous assessments and field inspections that focus our priorities and implementation plan for maintenance and repair actions. As a result of the investments and renewed maintenance strategy, there have been zero electrical faults caused by lack of maintenance since 2016.

We have made significant progress in reducing the fire risk associated with the DOE-owned 5.4-mile 230-kV transmission lines that deliver power to SLAC through dense vegetation, steep terrain, and residential areas outside our leased area. We mitigated these risks by conducting aerial and ground inspections of the transmission line and pursued proactive vegetation management and repairs along the line. We developed a multi-year maintenance strategy that includes inspections, vegetation removal and trimming, and electrical repairs.

In successful partnership, our utility provider PG&E installed fault protection devices on their portion of the power system, and we installed devices at our master substation. PG&E has committed to implementing major upgrades at several of their area substations to provide better automatic and instantaneous fault protection for the community and SLAC. Additionally, our strategy includes installing remote switching and controls in the future to quickly and safely isolate our site in the event of high fire risk.

Cooling Water

Our next highest operational reliability risk is the sustainment of our cooling water systems. An SLI-GPP for LCW systems was recently completed, and an SLI-GPP for replacement of cooling towers will be underway this year. The new LCW skid system provides a reliable and reconfigured system with the ability to isolate heat exchanger loops for maintenance, minimizing disruption to multiple science programs. The cooling tower project replaces aging cooling tower cells that serve critical loads in the Beam Switch Yard, SSRL, LCLS experimental halls, and research end stations. Completion of the LCW project enables the cooling tower system to be optimized from the current oversized 50-megawatt (MW) capacity to a more efficient 12 MW system. These two projects will retire approximately $1.9 million in deferred maintenance (DM).

Through Institutional General Plant Projects (IGPP) investments, we recently completed a project to replace underground cooling water laterals, which included replacing corroded 50-year-old valves and piping along multiple sectors of the Klystron Gallery. This IGPP reduced the overall failure risk for mechanical infrastructure, and improved cooling water reliability for multiple accelerator systems. We have prioritized IGPP funding to modernize original heat exchanger infrastructure that supplies critical LCW throughout several sectors and the Beam Switch Yard for multiple science programs.

Other Utility Project Priorities

Our goal is to continue to demonstrate a strong performance record in the execution of investments that ultimately result in reliable infrastructure supporting our large-scale user facilities, research capabilities, and scientific community. The next major category of capability gaps that contribute to operational risks is our underground utility systems: sanitary sewer, storm drainage, domestic water and fire protection, gas, and lift stations. Most of this infrastructure is degraded and past its service life, and in some cases deterioration and failure have reduced utility service capabilities. In addition to underground utility networks, our computing infrastructure is currently overloaded and should be modernized to support existing requirements as well as the additional requirements brought on by new science projects, such as LCLS-II, LCLS-II-HE, the MEC upgrade, and LSST.

Critical Utilities Infrastructure Revitalization

We plan for the revitalization of our utilities through an SLI line item (LI) request for an infrastructure investment project, the Critical Utilities Infrastructure Revitalization (CUIR) project: $189 million, FY 2021 – FY 2029, CD-0 approved May 2019. The primary objective of this project is to close infrastructure gaps that support multi-program science missions by creating resilient infrastructure for reliable science delivery. Additionally, we will leverage this major infrastructure investment by introducing the application of AI and ML into facilities operations.

The CUIR project addresses degraded infrastructure with critical repairs, replacements, and modernization of underground domestic water and fire protection, sanitary sewer, storm drain, electrical systems site-wide, and compressed air, as confirmed by our specialized assessments and inspections. The current anticipated reduction of repair needs (RN) and DM of this project is approximately $42.5 million and $33.1 million, respectively. This project provides a more robust utility distribution system to science facilities and addresses obsolete parts and equipment. The project provides two new 12-kV feeders and switch installation along the linac, replaces electrical feeders throughout the site, and modernizes electrical switching equipment.

The result is a more resilient electrical grid that is interconnected and configured in a manner that minimizes science disruptions caused by power fluctuations and faults at the local level, and at the regional level due to PG&E's Public Safety Power Shutoff (PSPS) program. This outcome is necessary to address electrical reliability risks to LCLS, the cryoplant, and FACET-II. This project also installs a Supervisory Control and Data Acquisition (SCADA) system for power monitoring of electrical infrastructure for DOE-BES, DOE-HEP, DOE-BER, DOE-FES, DOE-ASCR, and DOE-NP science programs. Additional electrical improvements include replacement of the linac's Motor Control Centers (MCC), variable voltage substation (VVS), low-voltage breakers, and KSubs low-voltage breakers, collectively reducing the risk of beam downtime.

In addition to underground infrastructure and electrical work, this project addresses vital cooling water system revitalization with increased capacity to support multiple programs. Two new 5 MW cooling towers, cooling system controls, and tower piping connecting to the existing underground cooling tower water infrastructure are also included. Timely delivery of this project is essential for current and future success of DOE's science programs.

To manage these investments into the next generation, CUIR provides an opportunity to incorporate data collection devices, control systems, and instrumentation to gather data that will be foundational for future development of AI and ML algorithms. Leveraging AI/ML may: increase operational reliability; optimize systems; enable faster diagnostics and fine tuning; and perform analysis of complex variables. CUIR will enable more efficient and effective means for delivering reliable utilities for research and technology and such operations as computing.

Provide a Variety of Collaboration Spaces

SLAC's campus vision fosters our core values, one of which is emphasizing collaboration. We accomplish this through design and by optimizing campus layout for pedestrian and traffic patterns across the site to help integrate research groups across various science programs. Key to this collaboration is workplace design and the physical location of people and workspaces.

Photon Sciences Laboratory Building

The SLI LI Photon Sciences Laboratory Building (PSLB) / ASC – a joint DOE-Stanford partnership – became operational in 2019 and now hosts metrology and calibration laboratories, laser laboratories, an optics nanofabrication facility, and two SLAC-Stanford joint institutes (PULSE and SIMES). This laboratory facility advanced our campus vision and furthered DOE's sustainability goals by earning a high-performance sustainable building (HPSB) certification in January 2020 and U.S. Green Building Council's LEED Platinum certification in February 2020.

LSCC

The LSCC ($58 million - $92.4 million, FY 2020 – FY 2026, CD-1 ESAAB November 2019) is the next logical step in our campus vision to provide collaborative spaces to exploit new sciences. While ASC delivered multi-mission laboratory spaces, LSCC supports current and future sciences by providing a modern research collaboration facility for large-scale data science, visualization, ML, and user interaction. Extremely large data rates – *e.g.* terabytes per second generated from detectors at LCLS (DOE-BES), LSST (DOE-HEP), FACET-II (DOE-HEP), SSRL (DOE-BES), cryo-EM (DOE-BER, DOE-BES, NIH), DOE-NP, and DOE-ASCR – drive our need for data analytics, visualization, ML, and complex simulation codes using high-performance computing. LSCC will enable collaborations that will catalyze advancements with the use of new imaging tools and software.

SLAC will influence and leverage a wide range of large-scale programs by co-locating teams of X-ray scientists, instrument scientists, computer scientists, and visiting users who develop critical algorithms and data analysis techniques. Early examples of a cross-functional approach have already produced strong results in the ability to interpret complex images in a wide variety of situations through the application of ML and other AI methodologies. Synergies will be realized across all major DOE-sponsored programs at SLAC with a broad spectrum of researchers in materials science, chemical science, cosmology, computational support, AI, ML, exascale applications, Bay Area laboratory partnerships, and industry partnerships. LSCC will co-locate approximately 100 to 150 personnel, enabling a robust collaboration and crossover between major programs to gain insight, innovation, and co-development.

This new building will also serve as a beautification project by removing degraded trailers currently occupying the project site boundary, resulting in a DM reduction of approximately $90,000.

Stanford Collaborative Projects

As demonstrated by the DOE-Stanford partnership on PSLB/ASC, Stanford remains a strong supporter and continues to show interest in creating a "best-in-class" laboratory. We are leveraging this interest to grow the Laboratory with key support facilities that will support both the science and people. While both of these projects were slated for preliminary design in 2020, the COVID-19 pandemic impact will delay this project by at least one year.

ASC 3rd Floor

The Stanford-SLAC-DOE partnership for the construction of the ASC included two floors with 71,500 GSF of laboratory and support space. The remaining 34,000 GSF provides an opportunity for laboratory expansion space that could serve as an additional resource between SLAC and Stanford. Potential major applications include microelectronics, batteries, energy, and sustainability. These laboratory spaces can foster synergy within existing capabilities in advanced characterization at SSRL, LCLS, and cryo-EM, and in addition to advancing the DOE-SC mission, these opportunities can potentially advance partnerships with other federal agencies.

SRCF-II

SRCF-II ($52 million) is an approximately 9,700-square-foot, 3 MW proposed expansion to the existing SRCF. Both SRCF and SRCF-II will provide the Stanford-SLAC research community with computing facilities designed specifically to host high performance computing equipment in a state-of-the-art facility. The scientific computing resources are planned to use 40 percent less energy per square foot than the national average.

Guest House Expansion

The Stanford Guest House expansion ($38 million) is an approximately 47,000-square-foot, 120-room addition to the Guest House. The project also includes interior gathering areas, conference areas, and other guest amenities. This will provide a vital asset to the Laboratory as our science programs continue to grow, with a concomitant need for hosting more visiting scientists.

Modernize Existing Facilities to Support Laboratory Goals

A holistic approach to our campus strategy leverages the strengths and opportunities of our existing infrastructure. Modernization of existing facilities already in an optimal location demonstrates good stewardship of DOE resources and reduces DM. Demolition of obsolete facilities for the clearing of high-value real estate provides opportunities for the construction of new facilities that enable growth. With this growth, we must also have adequate information technology (IT) and security infrastructure to secure our people, science, facilities, and equipment.

Over the last decade, both direct and indirect funding were invested in the modernization of our most critical infrastructure. SLI LI projects supported the conversion of an underutilized warehouse and the renovation of old office space to provide modern administrative spaces to support various mission support functions. More recently, Laboratory indirect funding supported replacement of roofs, construction of laboratory space, and upgrades to fire panels in the linac.

The next phase of building modernization focuses on major renovation of some of our most critical aging laboratory buildings that have become "substandard" – despite best efforts – in terms of providing the capabilities and configurations required by the current mission and future science. To advance, the functionality of these buildings must be modernized.

Campus Building Renovation Project

The Campus Building Renovation Project (CBRP) ($96 million, FY 2023 – FY 2027) will be an SLI LI modernization project to update aging laboratory and office spaces in buildings around the Science Quad for programs supporting existing multi-program missions. This modernization will involve 83,000 to 125,000 GSF of existing space. This project renovates buildings that house infrastructure that supports the full lifecycle of the Laboratory's accelerator systems. Also included are buildings that house engineering and scientific talent in particle and X-ray detector systems, sensors, ASICs, and electronics for a broad range of advanced applications.

Renovation of substandard office and laboratory spaces will modernize workspaces and align them with sustainability requirements.

Recent assessments identified additional requirements for this project, namely end-of-life roofs and building utility infrastructure. Heating, ventilation, and air conditioning (HVAC) units, mechanical utilities, roofing systems, and electrical systems will be replaced or upgraded to align with current mission needs and comply with building codes; these improvements will also enhance sustainability by reducing DM. Current documented DM for this project is approximately $5.3 million. However, condition assessments are scheduled in FY 2020 and FY 2021, and we anticipate the DM associated with the targeted facilities will increase substantially.

Site Security and Access Improvements III

The Site Security and Access Improvements III project ($9.4 million, FY 2023 – FY 2026), with proposed funding by the DOE Safeguards & Security Program, represents the final phase of security projects at SLAC over the past decade. It will complete the protection of DOE assets and enhance science collaboration across our Laboratory. The project will replace the main entrance gate house with a modern guard house and security dispatch center. This will reconfigure SLAC's main entrance and exit at Sand Hill Road to improve safety for security officers and efficiency in access badge verification. The project will also install radiation portal monitoring capability at SLAC's main entry and Alpine Road gates, which reduces the risk of inadvertent off-site transport of activated materials. In addition, the project will secure the remaining 31 buildings and 12 accelerator tunnels by using card key access at entry control points. Providing modern access control at these buildings will improve property and personnel security by providing site lockdown capability for active threat situations that complies with DOE Design Basis Threat requirements. This will also substantially reduce the accelerator gated access area, converting the area around PEP Ring Road into a general access area for improved site-wide collaboration. This project will reduce the Laboratory's DM by approximately $12,000 as a result of the demolition of the current undersized and ill-configured guard house.

Building Enclosures

The site-wide building enclosures ($19.8 million, FY 2022 – FY 2023) is our SLI-GPP request to upgrade and modernize 1960s- and 1970s-era buildings across the site that support mission-critical and mission support functions. These facilities have long supported laboratories, specialized shops, and office spaces, but are now affecting operations because certain major system components are beyond their useful life. Building envelopes are severely degraded, including roofs, doors, windows, and exterior enclosure materials. A number of facilities have been identified that are strategically located for optimal use, however the facility itself is obsolete and cannot adequately support current science requirements. This project will improve overall workforce productivity in these buildings by repairing persistent water leaks, eliminating workarounds, and renovating facility systems.

Asset Management

As stewards of DOE's physical assets, it is important to monitor and maintain infrastructure inventory and provide current and accurate data regarding its mission, use, status, condition, operations, and maintenance. DOE relies on the FIMS extensively for making investment and management decisions for real property. Complete and accurate information on real property assets is critical to DOE for managing facilities and satisfying such external reporting requirements as the Federal Real Property Profile. At the local level, Facilities & Operations staff use this data to assess conditions and address needs for current and future infrastructure.

Described below are our current efforts to ensure data quality in FIMS so that it conveys an accurate depiction of the site environment. We rely on the data quality enforced through annual DOE FIMS data validation conducted in close coordination with our site office. Also discussed are SLAC's most recent DM trends, maintenance index (MI), and replacement plant value (RPV). A discussion of the items is necessary to tie together the full context of our campus strategy.

FIMS Data Accuracy and Geographic Information System

Over the years, our Accelerator Directorate's Metrology Geospatial Mapping Services has taken data from dozens of sources including CAD, aerial and drone surveys, ground surveys, LIDAR, and photogrammetry and converted this information into Geographic Information Systems (GIS) data to offer timely 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. This feature transforms FIMS data elements into visuals that are easier to analyze and match to other GIS data, and serves as a foundation to validate the overall real property asset inventory at SLAC. As a result, we have a number of subsequent endeavors to reconcile our data sets.

In FY 2019, 19 records were added to FIMS. The most prominent addition to the assets portfolio is the ASC, a new 105,340-square-foot multi-mission laboratory building. Other increases in FIMS are not representative of new assets but are a refinement of existing infrastructure that had previously been combined into a single property record. To more acurately capture the Laboratory's overall asset condition, records were categorized into "zones," or locations. For example, all cooling tower piping and LCW piping were previously combined on a single record representing the entire distribution piping network. Because of the decoupling effort, cooling tower piping is now associated with the cooling tower it is connected to, and LCW piping is associated with its LCW support structures. We also assigned new property records to certain electrical substations that were previously accounted for on one property record. This method of structuring property records provides a simplified breakdown for very complex networks and systems. Follow-on efforts for storm water, sewer, and domestic water will occur in 2020. Critical to all these efforts is the ability to see the data in GIS, informing decisions about property records structures in FIMS.

Being able to present the FIMS data in GIS as "layers" allows facilities planners and operators to more easily analyze FIMS data and trends and make more strategic decisions about future planned investments. The FIMS data is also the foundation for segmenting our linear assets to have the ability to isolate areas for utility projects. Our utilities subject matter experts, along with our Mission Readiness team, are currently working on identifying utility deficiencies as documented in conditions assessments to create a visual representation of those utilities in GIS layers. This follow-on effort will identify utility project areas and result in a GIS Master Plan for our SLI LI CUIR project.

Our space planners, who document current space utilization as workforce members are placed or relocated, also use GIS. The ability to capture space used by the Laboratory's population supports important data elements in FIMS. GIS continues to be an integral system for asset management of our facilities and operations.

Maintenance and Repair

In recent years, we have taken an improved approach to ensure reliable FIMS and CAIS data which serves as the foundation of our infrastructure investment plan. Beginning in 2016, a collaboration of DOE-SC laboratories, under the Infrastructure/Mission Readiness Working Group, developed a process to better define Repair Needs (RN) and Deferred Maintenance (DM). Our utility "Stewards," who are the subject matter experts responsible for assessing systems, have used this methodology to validate the classification of deficiencies as either RN or DM. Their efforts have increased the accuracy of our documented infrastructure gaps.

The baselined DM increased from $28.4 million in FY 2016 to a more accurate $80.3 million in FY 2017. As a result of critical infrastructure improvements to substations for our linac Gallery and other indirect projects, we decreased DM to $76.2 million for FY 2018. Although DM remains high, the overall SLAC Facility Condition Index earns a "good" rating by industry standards. Assets identified as high risks are addressed through our campus strategy in our planned infrastructure investments. Investments in our electrical substations, cooling towers, and low conductivity water systems will further reduce our DM. The combination of planned maintenance activities, indirect investment, and the proposed projects discussed in Section 6.2 should result in a decrease of DM by about 40 percent compared to the current trendline through 2026. SLAC will constantly track new and retired DM to accurately monitor this key performance indicator.

In the third quarter of FY 2017 we began to recalculate RPV using DOE models to reflect the uniqueness of our facilities and higher plant replacement costs associated with the San Francisco Bay Area. RPV in the coming years will increase because of this adjustment. Before this change our reported RPV in FY 2017 was $1.92 billion; in FY 2019 our reported RPV increased to $3.15 billion. The increase is a result of recalculating RPV for approximately 550,000 square feet of our underground tunnel facilities, OSFs, and certain older buildings. To date, 66 percent of the facilities have customized RPV calculations. We will continue to update about 25 assets each year until the remaining 98 assets are updated. We will review updates annually and gain concurrence from DOE on the methodology, models, and factors used to adjust RPV. One result of these adjustments is a decrease in the MI for our facilities due to the increase in RPV.

DOE has historically assumed a “rule of thumb” maintenance target of 2 to 4 percent for the Maintenance Investment Index (MII). MII is defined as the percentage of annual actual maintenance (AAM) in relation to RPV (MI=AAM/RPV). For FY 2019, our reported AAM was $16 million and RPV was $3.15 billion, which results in a low MII. However, DOE’s MA-50 now recognizes that this target is typically assumed in commercial industry which might not be representative of the type of industrial infrastructure within the DOE complex. For example, at SLAC there are many high value, low maintenance infrastructure items in our accelerator housing and experimental tunnels. MA-50 is looking to eliminate this 2 to 4 percent target approach and use a more tailored measure for our individual sites. Notwithstanding, we still intend to convey our maintenance investments within the current DOE guidance and have adjusted to more accurately represent our maintenance investment strategies. MII was calculated separately for operational assets by property type: building, OSFs, and trailers. OSFs were then divided into two categories: utilities and other. The results are summarized in the table below. We would like to highlight that we have also provided our Condition Index (CI), represented as the ratio of RN to RPV. While MII is low, our overall CI is relatively good and is also provided to tie maintenance investment to the relative condition of each asset category.

The data illustrates our current largest maintenance investment is in assets with the lowest condition index: OSFs utilities. The majority of the Laboratory’s utility infrastructure is old and inefficient, which escalates overall maintenance costs. Our request for SLI LI CUIR closes infrastructure gaps in various utilities.

The lowest MII is on OSFs (Other). This is typical since many of these facilities are high value and low maintenance, such as concrete tunnels and other support structures around the site. For buildings, SLAC is not investing the typical industry standard, represented by an MI of 2 percent. However, we are managing to keep them in relatively good condition as demonstrated by the average condition index of 90 percent. Mission-critical buildings in “substandard” condition are included in our SLI LI CBRP request.

Maintenance Investment Index and Average Condition Index
by Property Type for Operational Facilities (in $k)

		Buildings		OSFs: Utilities		OSFs: Other		Trailers	
AAM	**MII**	$8,165	0.93%	$5,502	1.51%	$2,111	0.39%	$59	0.91%
RPV		$876,249		$364,004		$534,747		$6,454	
Average CI		90%		66%		91%		86%	

Source: FIMS Year-End Data FY 2019

DM Trends

In 2017, we re-baselined our DM from $28.4 million to $80.3 million by using the 2016 DOE-SC Infrastructure - Mission Readiness Working Group guidance. Our 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 to date. The Mission Readiness team also implemented the use of the “Projects Module” in CAIS to accurately capture RN and DM associated with planned and active projects, and retire such deficiencies when projects are completed. Because of more coordinated efforts and well-managed infrastructure investments, we have stopped the increase in DM and have begun to see a steady decrease, as evidenced by a DM of $75.8 million for FY 2019.

It is important to note that the DM value is subject to many variables in any given year. Each year, deficiencies are both removed as minor and major projects are completed and added due to results from that year's Condition Assessment Surveys (CAS). FY 2019 CAS resulted in the addition of $6.5 million in DM. Additionally, every year MA-50 escalates and applies a geographic adjuster to RN and DM costs. At 1.29, SLAC's geographic adjuster is the highest in the DOE-SC complex, LBNL's is the second highest (1.237), followed by Brookhaven National Laboratory (1.229).

Our DM reduction in recent years included infrastructure investments in our electrical substations, linac 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, and roofing. To reduce DM for maximum impact, we will leverage SLAC 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 discussed in section 6.2 should result in a 59 percent decrease ($45.1 million) of our current DM.

Site Sustainability Plan Summary

Sustainability is embedded within our campus strategy and integrated into designs, new construction, repair projects, facilities operations, and service contracts. Sustainable design to maximize performance while reducing environmental impact are key elements incorporated with modernizations. The guiding principles for HPSB and the California Building Energy Efficiency Standards, Title 24, are firmly established in our capital project design guidelines and performance specifications for both partial renovations and new buildings.

An example of our progressive approach is the build-out of our newest building, the ASC, which was constructed as part of the SLI project that built the PSLB. In February 2020, the facility attained the U.S. Green Building Council's highest certification level – LEED Platinum – for meeting environmentally and socially responsible standards. Strategies for this project included 96 percent of construction waste being sorted for recycling, a design for 41 percent water reduction, and 25 percent less energy use compared to the national average for a laboratory building. Sustainable features include maximizing natural light to illuminate offices and laboratory spaces, and a dashboard monitor and touch screen display of real-time building energy performance for occupants and visitors.

Next steps:

- In 2019, re-commissioning of the energy consuming systems was completed for two buildings: the Operations Support Building (B028, 20,355 square feet) and the Administration & Engineering Support Building (B041, 44,997 square feet). As a result, the energy saved in each building is 25 percent and 7 percent, respectively. An energy tune-up for three additional buildings is planned for 2020.
- The proposed SLI LI CUIR project will develop resilient and efficient cooling water and energy infrastructure system upgrades.
- Improved transportation options for travel between SLAC and Stanford will be explored to meet increased needs of staff and students working at the joint institutes. A site-wide survey will be conducted to identify needs regarding the Marguerite shuttle and alternative transport. In parallel, the Laboratory is developing an easy-checkout GSA fleet vehicle system as well as a safety training to prototype bike-share as an option.

The resumption of accelerator operations and commissioning of LCLS-II is planned to increase energy consumption in terms of Gigawatt hours (GWh) starting in FY 2021 as indicated in the figure below.

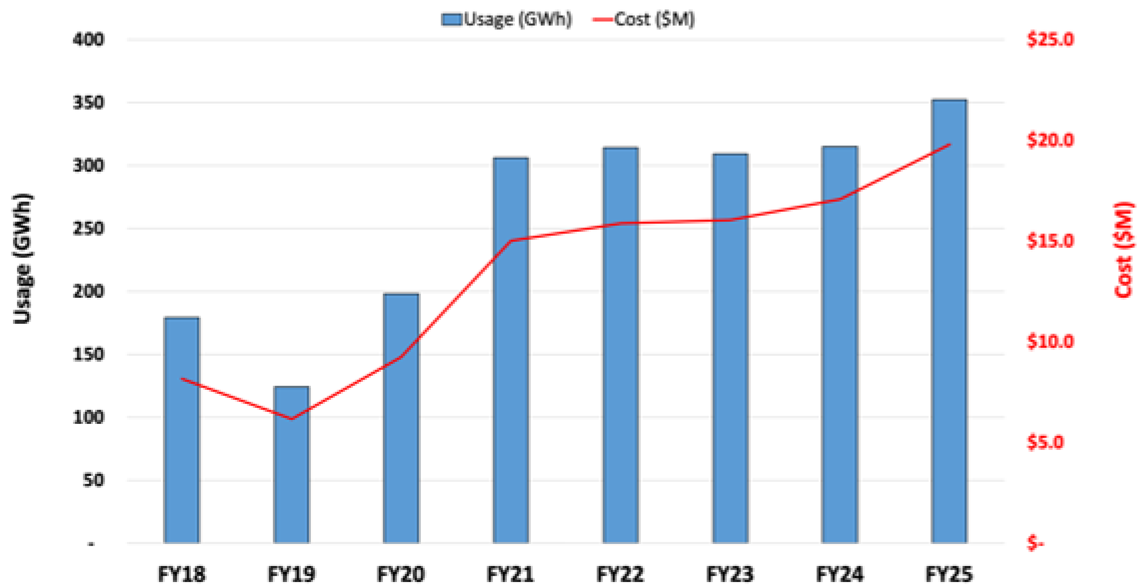


Figure: Electricity Usage & Cost Projections

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 2019 Lab Operating Costs:** $159.9 million
- **FY 2019 DOE/NNSA Costs:** $158.1 million
- **FY 2019 SPP (Non-DOE/Non-DHS) Costs:** $1.8 million
- **FY 2019 DHS Costs:** $0 million

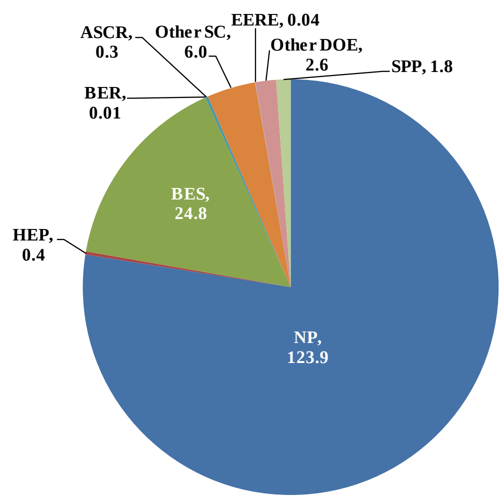
Physical Assets:

- 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:

- 714 Full Time Equivalent Employees (FTEs)
- 24 Joint Faculty
- 30 Postdoctoral Researchers
- 40 Graduate Student
- 33 Undergraduate Students
- 1,691 Facility Users
- 1,552 Visiting Scientists

FY 2019 Costs by Funding Source ($M)



Mission and Overview

The Thomas Jefferson National Accelerator Facility (TJNAF), located in Newport News, Virginia, is a laboratory operated by Jefferson Science Associates, LLC, for the Department of Energy's (DOE) Office of Science (SC). The primary mission of the laboratory is to explore the fundamental nature of confined states of quarks and gluons, including the nucleons that comprise the mass of the visible universe. TJNAF also is a world-leader in the development of the superconducting radio-frequency (SRF) technology utilized for the Continuous Electron Beam Accelerator Facility (CEBAF). This technology is the basis for an increasing array of applications at TJNAF, other DOE labs, and in the international scientific community. The expertise developed in building and operating CEBAF and its experimental equipment has facilitated an upgrade that doubled the maximum beam energy (to 12 GeV (billion electron volts)) and provided a unique facility for nuclear physics research that will ensure continued world leadership in this field for decades. TJNAF's current core capabilities are: Nuclear Physics; Accelerator Science and Technology; and Large Scale User Facilities/Advanced Instrumentation.

The lab supports an international scientific user community of 1,691 researchers whose work has resulted in scientific data from 192 full and 21 partial experiments (including 14 full and 21 partial in the 12 GeV era), 476 Physics Letters and Physical Review Letters publications and 1,618 publications in other refereed journals to-date at the end of fiscal year (FY) 2019. Collectively, there have been more than 182,000 citations for work done at TJNAF.

Research at TJNAF and CEBAF also typically contributes to thesis research material for about one-third of all U.S. Ph.D.s awarded annually in Nuclear Physics (28 in FY 2019; 658 to-date; and 195 more in progress). The lab's outstanding science education programs for K-12 students, undergraduates and teachers build critical knowledge and skills in the physical sciences that are needed to solve many of the nation's future challenges.

Core Capabilities

Nuclear Physics (funded by DOE SC – Nuclear Physics)

TJNAF is a unique world-leading user facility for studies of the structure of nuclear and hadronic matter using continuous beams of high-energy, polarized electrons. The completion of the 12 GeV Upgrade project enables many outstanding new scientific opportunities. 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 Continuous Electron Beam Accelerator Facility (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. With nearly 1,700 users annually, of which roughly two-thirds are domestic, TJNAF supports what is generally considered the largest nuclear physics user community in the world.

The CEBAF science program spans a broad range of topics in modern nuclear physics. Recent 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 and theoretical 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 scientists are heavily engaged in the community effort and its phenomenological studies to help develop the strong science case and unique detection capabilities for a future Electron-Ion Collider (EIC). 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 (funded by DOE SC – Nuclear Physics, High Energy Physics)

TJNAF has world-leading capabilities in technologies required for superconducting linacs; notably, as follows:

- Complete concept-to-delivery of superconducting linear accelerators and associated technologies
- 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

These world-leading capabilities are evidenced by the production of more than 100 cryomodules produced and in continuous operation today. The ability to deliver large projects on time and on budget is evidenced by our involvement in major superconducting projects for SRF and cryogenics, including SNS and LCLS-II, for which TJNAF is responsible for construction of half of the superconducting cryomodules, as well as the two cryogenic refrigerators, and the FRIB helium refrigerator.

Construction of the Upgraded Injector Test Facility (UITF) at building 58 is complete. The UITF provides a means to test important devices for CEBAF, like photocathode guns, the new SRF "booster" cryomodule and the HDice polarized target for Hall B. It is a testbed to evaluate new accelerator technologies, like Nb_3Sn-coated accelerating cavities operating at 4K, and with a new beamline being prepared using LDRD funds, potential accelerator applications of e-beams, like wastewater treatment with electron beams. And although providing only low-energy electron beams (< 10 MeV), the UITF could be used to conduct PAC-approved experiments like the bubble chamber astrophysics experiment to study photodisintegration of oxygen.

In addition, TJNAF has pioneered Energy Recovery Linac (ERL) concepts and technologies, holds the record for recirculated beam power (1.4 MW), and has been a world leader in high-power free electron lasers (FELs) based on ERL technology. TJNAF, through its Center for Advanced Studies of Accelerators, possesses world-leading capabilities in beam dynamics aspects of linear accelerators, ERLs, FELs, and colliders.

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.

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. 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)

As mentioned above, CEBAF has been recently upgraded to provide an electron beam with energy up to 12 GeV, a factor three over the original 4 GeV CEBAF design. In addition to the increase in beam energy, the maximum number of simultaneous experiments that CEBAF is now four, with the completion of a four-laser injector upgrade and the addition of Hall D. With the completion of the 12 GeV Upgrade, TJNAF will continue to be the world's premier experimental QCD facility.

With 418 installed SRF cavities, CEBAF operations provide an important contribution to the worldwide SRF performance data set. Some of the CEBAF SRF cavities have been operating for more than 20 years. The CEBAF data set and operational experience is a valued resource for new or existing SRF-based accelerators. TJNAF has the ability to conceive and design large accelerator facilities, building upon 6 GeV CEBAF operations and augmented with the ongoing 12 GeV Upgrade.

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. 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.

As a result of the development, construction and operation of CEBAF, TJNAF has developed world-leading expertise in superconducting RF linear accelerators, high-intensity electron sources, beam dynamics and instrumentation, and other related technologies. These capabilities have been leveraged to develop new technologies relevant to other disciplines beyond nuclear physics, as well as applications to areas of national security.

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 is responsible for construction of half of the superconducting cryomodules as well as the two cryogenic refrigerators. An upgrade is already 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 seven new high beta cryomodules with 28 new SRF cavities to increase the SNS linac beam energy to 1.3 GeV.

Cryogenics (funded by DOE SC – Nuclear Physics)

Over the last two decades, 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 is presently responsible for designing, specifying, procuring, and commissioning the helium refrigerators for LCLS-II, based on the successful CHL2 design for the 12 GeV Upgrade and designs developed for FRIB. The FRIB refrigerator is complete and commissioning for the LCLS-II refrigerators has begun. Significant CEBAF upgrades in progress include the completion of in-house fabrication of a replacement 2K cold box for CEBAF operations using the latest cold compressor technology. Installation and commissioning of this cold box is to be completed by the end of CY 2020. Work continues on the modification and installation of a surplus SSC refrigerator, ESR-2, to support future CEBAF end station operations. Additionally, project planning is underway to utilize funding received to upgrade the 2K capacity of the Cryogenic Test Facility that supports super conducting 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 has a strong foundation based on the advancement of the U.S. nuclear physics program (as embodied in the 2015 Nuclear Science Advisory Committee (NSAC) Long Range Plan) and the support of other initiatives and thrusts in the Office of Science. TJNAF has developed the FY 2020 Laboratory Agenda to delineate major initiatives associated with strategic objectives in Science and Technology as well as Operations. The Agenda was constructed around a set of four Strategic Outcomes that deliver on the mission of the laboratory, and three of these Strategic Outcomes are related to TJNAF's science and technology activities.

Infrastructure

Overview of Site Facilities and Infrastructure

Thomas Jefferson National Accelerator Facility 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 five-acre parcel owned by the Commonwealth of Virginia and leased by SURA, the managing member of the JSA joint venture, which sub-leases five acres to DOE for use by TJNAF. Also adjacent to the federal reservation is an 11-acre parcel owned by Newport News that contains the Applied Research Center (ARC), within which JSA leases additional office and lab space. SURA owns 37 acres adjacent to the TJNAF site, where it operates a 42-room Residence Facility at no cost to DOE.

The TJNAF complex consists of 69 DOE-owned buildings comprising 882,990 square feet (SF) of office, shop, technical, and storage space. JSA leases an additional 37,643 SF of office and shop space from the Commonwealth of Virginia in the VARC and 11,097 SF of office and lab space from the City of Newport News in the ARC. JSA also leases 17,549 SF of storage space in two offsite storage warehouses within 12 miles of TJNAF. These areas are gross, usable space as summarized in the table below.

The TJNAF complex provides office and workspace for approximately 760 JSA contractor, JSA, and federal government employees along with a transient population of 1,600 users and visiting scientists. Facility space is well utilized with a current asset utilization index of 98.6%. Distribution of space by use is summarized in the table below.

Type of Use	Total Square Feet, Usable Space, 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

The condition of TJNAF facilities is generally good (Table 5). Of the 74 DOE-owned or -leased buildings, 65 are rated adequate, eight substandard, and one inadequate. Of the 36 other structures and facilities (including OSF 3000 series assets) assessed, 33 were rated adequate and three substandard. Only 2,783 SF of space is currently rated as underutilized. There are currently no excess facilities at the Lab and none are expected within the next ten years. In addition to real property assets, there are 49 personal property shipping containers representing 15,160 SF of storage space in use at TJNAF.

Condition		Mission-Unique Facilities		Non-Mission-Unique Facilities		Other Structures and Facilities	
		Number	SF	Number	SF	Number	SF
Rating	Adequate	36	339,976	29	343,444	33	N/A
	Substandard	0	0	8	259,221	3	N/A
	Inadequate	0	0	1	6,638	0	N/A
	TOTAL	36	339,976	38	609,303	36	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 is summarized in Enclosure 1. With the decision not to site the EIC at TJNAF, the Campus Plan and Land Use Plans have been updated to align with this decision. The SURA owned land, as well as Newport News owned land which is reserved for TJNAF interests, adjacent to the Lab site will still play a critical role for preserving expansion opportunities critical to the Lab's strategic plan. This involves constructing a new service road entrance directly connecting the campus with a major public road which will facilitate the future relocation of maintenance and logistics functions. Additionally, it locates a future High Performance Computer Center that is ideally located on the campus. Discussions with SURA are ongoing related to the transfer of the land to DOE to enable development of projects included in the Campus Plan.

The SLI funded CEBAF Renovation and Expansion (CRE project received CD-1 in March 2020. The project includes the acquisition of the Applied Research Center (ARC), renovation of CEBAF Center and 82K to 144K SF building expansion which will eliminate an existing ARC building lease from the City of Newport News Economic Development Authority as well as the lease of the Virginia Applied Research Center (VARC) from the College of William and Mary. The ARC acquisition process is ongoing and is anticipated to be concluded in early FY 2021. An extension of the current 11,097 SF lease in planned 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 <1079.5 hours of total downtime over a 32-week experimental period. To accomplish this Facilities Operations and Maintenance completed 5,206 preventative maintenance tasks and 1,715 corrective tasks in 2019.

The recent failure history suggests 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 remain 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 removal of trees near transmission lines, inspecting overhead lines, coordination of utility PM tasks with Accelerator downtimes, proactively monitoring line voltage variations within tariff limits and meeting regularly to review power reliability. In the third quarter of 2019, Facilities Operations and Maintenance performed Preventative Maintenance (PM) on 46, 15 kV transformers. The tests included oil tests and electrical tests and. Of the 46 transformers serviced, 17 transformers either failed or had less than satisfactory test results. Transformers failing the test were repaired or replaced. In 2019, Facilities Operations and Maintenance completed a major PM of the 40 MVA switchgear.

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. Heat detection in the tunnel failed due to higher radiation levels during 12 GeV beam operations. A project was completed in FY 2019 with a more robust fire heat detection system capable of withstanding higher radiation levels. Replacement of accelerator fire detection and suppression systems is scheduled to start in FY 2020 due to its poor service condition.

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 LHe to the Test Lab to enable the development, production and testing of SRF components and cryomodules, both for use by TJNAF in CEBAF and under WFO projects for other labs.	The Cryogenics Test Facility (CTF) has experienced heavy utilization due to the CEBAF upgrade and large WFO projects. Approximately $4M of system components have reached end-of-life and others require upgrading to maintain adequate capacity for projected workload.	Complete the **Cryogenics Test Facility (CTF) Upgrade.** Funding was provided in FY20 under the SLI-GPP program.
	Provide sufficient storage space for material and tooling needed to design, produce and test SRF components and systems.	18,000 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.	Construct a 15,000 –20,000 SF of Equipment Storage as part of the Large Scale Assemble and testing (LSAT) project to relieve the demand for remote, off-site leased storage for SRF components, tooling, and work in process. Need date is FY24 or sooner if practical.
	Low Energy Recirculator Facility (LERF) for R&D on magnetized high-current beams, characterization of materials using low-energy positrons, and 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.	Execute a **LERF Renovation** to ensure the facility can meet its planned operational use. Need date is FY26 or sooner if practical.
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 >85% 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 a FY 2017 SLI-GPP project scheduled for completion in 2021.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
	Provide 10,152 SF of suitable office and workspace for Cryogenics Engineering staff adjacent to CHL plant.	Current facility is substandard due to aging mechanical systems and worn finishes. Office space is over utilized due to expanding cryogenics staffing.	**Cryogenics Engineering Office Renovation (Building 89)** replaces worn systems and finishes and increases office space capacity. Project is under construction with expected completion in July 2020.
	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 32 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.	Construct 45,000 SF of environmentally controlled high bay and technical work space as part of the **LSAT** project. Need date is FY 2024 if practical.
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 **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 funded was provided in FY20.
	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 over utilized 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.	**CEBAF Center Renovation and Expansion (CRE),** possibly including the acquisition of the ARC, renovates CEBAF Center and provides an additional 82K-144K SF of space. The project consolidates staff and vacates leased space. Need date is FY 2026 or sooner is practical Initial project funding was received in FY20
	The Experimental Equipment Lab (EEL) provides 54,800 SF of technical and lab space for physics, engineering, and facilities staff and is integral to our campus plan.	The EEL mechanical systems are at the end of their service life. Portions of the building need to be brought within code. Exterior cladding is approaching the end of its serviceable life and requires replacement within the	The **LSAT** project provides a midlife renovation of the EEL facility. . Need date is FY 2024 or sooner if practical.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
		next 8-10 years to maintain effective use of this facility.	
Support Facilities and Infrastructure (SC25)	Relocate service entrance road to the TJNAF campus	TJNAF service vehicle traffic flow and facilities maintenance operations and logistics 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 if FY31 or sooner if practical.
	Relocate facilities maintenance & operations functions.	Facilities maintenance and operations functions are primarily located in two substandard (Buildings 13 and 19) located in the administrative core of the campus. Due to insufficient space in these facilities storage of critical spares are inefficiently scattered among numerous service buildings 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 FY23 or sooner if practical.
	Relocate logistics functions	TJNAF logistics functions are primarily located within high bay space within the Experimental Equipment Laboratory (EEL) building which is already oversubscribed and needed to support research and technical operations	The **Integrated Maintenance and Logistics Center (IMLC) Phase 2** provides a fully integrated solution and relocates these functions to the Lab's service corridor. Need date is FY24 or sooner if practical.
	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	Site-wide **Road, Parking, and Sidewalk Improvements** rebuild existing roads and resolve impacts created by both on-site and adjacent off-site construction. Need to align solution with selected option for this project.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
		support vehicle loads and maintain compliance with safety and regulatory requirements.	Need date is FY26 or sooner is practical.
	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.	**Cooling Tower Reuse Water** project develops a 40 Mgal/year alternate water source for use in cooling towers. Project would direct and treat water from off-site retention ponds for use in cooling towers. Need date is FY21.
	Main entrance sign appropriate for a DOE national laboratory and adequate wayfinding signage to safely direct users and visitors	Existing entrance sign was designed and built when TJNAF was first opened and no longer reflects the scope and capabilities of the site or its important technology anchor role in the community	The **Main Entrance and Site Signage** project will replace the main entrance sign and provide needed wayfinding signage across the site. The site circulation plan will be impacted with the CRE project. Need to align solution with selected option for this project. Need date is FY27 or sooner if practical.
	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 be no longer available after FY 30.	**Test Lab Chiller Replacement** includes replacing the existing chillers with a new chiller to be installed in the Central Utility Plant (CUP). Need date is FY27 or sooner if practical.
	Provide 165,000 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 700,000 SF of existing laydown area will be lost due to future building construction.	The **Laydown Area 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 FY21 or sooner if practical.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
	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 and making it more susceptible to storm water flooding. Further, rad waste processing equipment and work in process are currently located in part of the Equipment Storage Building assigned to Physics Division.	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 FY30 or sooner if practical
	Suitable potable water distribution to reliably meet need for 120 Mgal. per 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 **Potable Water Improvements** 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 FY28 or sooner if practical.
	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 **Sanitary Sewer Improvements** project will correct existing deficiencies and add additional capacity to meet expected growth requirements. Need date is FY29 or sooner if practical.

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 Asset Condition Index is 0.95. However, this could drop over time if Facilities Operations and Maintenance funding continues to be limited to 1.4% of replacement value. Modernization projects and construction of new facilities through SLI and GPP funding has enabled TJNAF to maintain a modest deferred maintenance value ($7.2M in FY 2019). Over the next decade, no significant increase in deferred maintenance is expected as JSA implements the capital spending plan.

Site Sustainability Plan Summary

The table below shows Sustainability Project funding for planned actions to meet DOE Sustainability goals.

Category	FY 2019 Actual	FY 2020 Planned/ Request	FY 2021 Projected
Sustainability Projects	153,331	321,229	0
Sustainability Activities other than projects	0	0	0
SPO Funded Projects (SPO funding portion only)	0	0	0
Site Contribution to SPO Funded Project	0	0	0
ESPC/UESC Contract Payments	0	0	0
Renewable Energy Credits (REC) Purchase Costs	23,700	27,000	32,000
Total	177,031	348,229	32,000

Table: Summary of Sustainability Project Funding ($k)

The lab 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/or the use of advanced and distributed energy technologies under the Computer Center Modernization project achieving a PUE of 1.3.

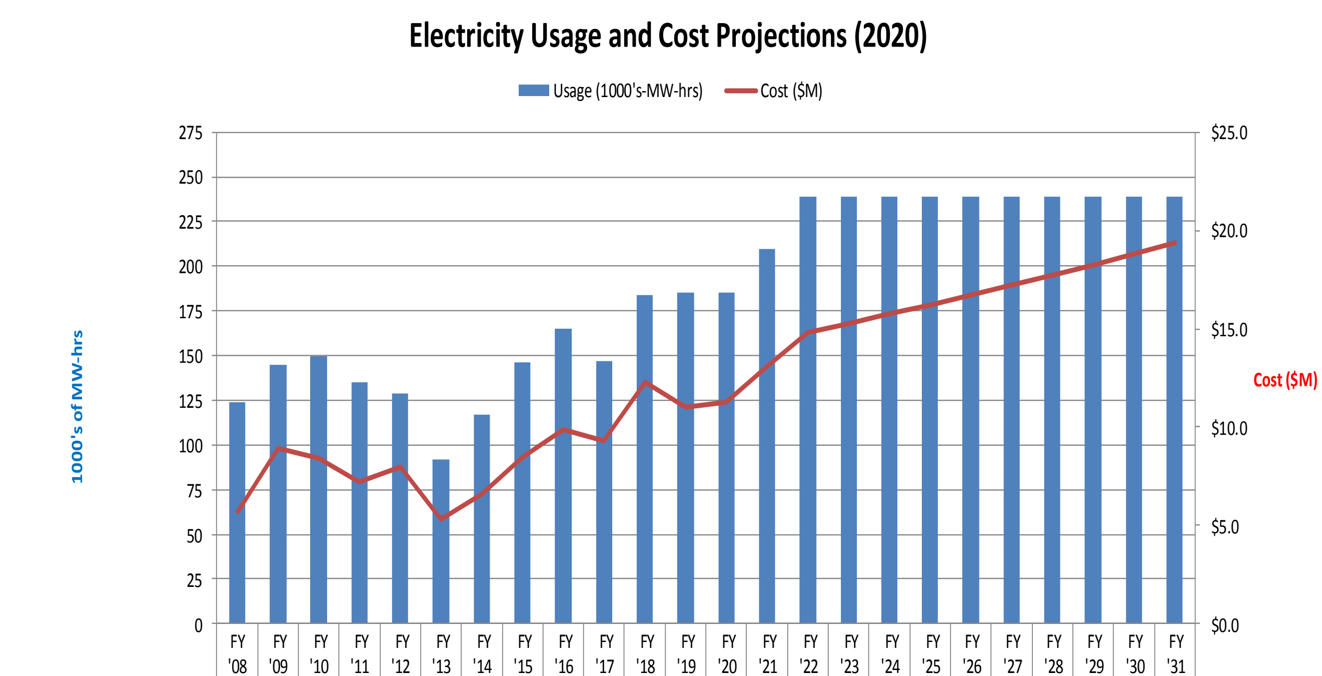
JSA decided against awarding a UESC project totaling about $3.48M addressing lighting, domestic water conservation, Ultra-Pure Water Reuse, and mechanical upgrades, due to operation risk. These elements are being implemented separately by the Lab as part of operations and maintenance efforts or incorporated into planned recapitalization projects. This approach is expected to reduce the risk while delivering the same or better outcome at a lower cost.

All but two sustainability interim target goals were met this year: potable water intensity and sustainable buildings (by building count). While achievement of the water intensity goal remains the most significant challenge for TJNAF due to the large amounts of potable water required for evaporative cooling of high energy mission specific facilities, a water conservation project was completed in FY 2019 which reuses discharged ultra-pure water (UPW) from the Test Lab as a make-up water supply source for a nearby cooling tower. The project is on track to reduce water consumption by 4.5 million gallons per year and reduce water and sewer utility cost by over $60,000 annually. Additional water conservation strategies have been identified and will be implemented in time to meet the sustainability target goal of a 36% reduction in water intensity by FY 2025 relative to the FY 2007 baseline.

Projects and strategies to achieve target goals in other categories have been identified and incorporated into building renovation plans. Energy intensity (BTU/GSF) should realize significant reduction through high-efficiency lighting upgrade in subject buildings. Reduction of domestic water consumption strategies are also included in building renovation plans. The building level energy and water reductions will also contribute to achievement of High Performance Sustainability Building (HPSB) compliance for several additional facilities.

Electricity Usage and Cost Projections

The figure below shows TJNAF's historical electricity usage in 1000's of Megawatt Hours and costs (actual year $M), including future projected electricity usage and costs. Projections are based on scheduled operations for FY 2020 of 22.5 weeks and FY 2021 of 26 weeks. FY 2022 onward include summertime runs at the highest achievable beam energy. From FY 2022 forward, 34 weeks of operations are projected for each year.



	FY '08	FY '09	FY '10	FY '11	FY '12	FY '13	FY '14	FY '15	FY '16	FY '17	FY '18	FY '19	FY '20	FY '21	FY '22	FY '23	FY '24	FY '25	FY '26	FY '27	FY '28	FY '29	FY '30	FY '31
Usage (1000's-MW-hrs)	124	145	150	135	129	92	117	146	165	147	184	185	185	210	239	239	239	239	239	239	239	239	239	239
Cost ($M)	$5.7	$8.9	$8.4	$7.2	$8.0	$5.3	$6.6	$8.5	$9.9	$9.3	$12.3	$11.0	$11.3	$13.1	$14.8	$15.3	$15.7	$16.2	$16.7	$17.2	$17.7	$18.3	$18.8	$19.4

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		✓	✓	✓	✓	✓	✓			
3	Applied Materials Science and Engineering	✓	✓	✓		✓	✓	✓			
4	Applied Mathematics		✓			✓	✓	✓			
5	Biological and Bioprocess Engineering		✓			✓	✓	✓			
6	Biological Systems Science			✓		✓	✓	✓			
7	Chemical and Molecular Science	✓	✓	✓		✓	✓	✓		✓	
8	Chemical Engineering		✓	✓		✓	✓	✓			
9	Climate Change Science and Atmospheric Science		✓	✓		✓	✓	✓			
10	Computational Science		✓	E		✓	✓	✓			
11	Condensed Matter Physics and Materials Science	✓	✓	✓		✓	✓	✓		✓	
12	Cyber and Information Sciences		✓			✓	✓	✓			
13	Decision Science and Analysis		✓			✓	✓	✓			
14	Earth Systems Science and Engineering					✓	✓	✓			
15	Environmental Subsurface Science					✓	✓	✓			

	Core Capabilities	AMES	ANL	BNL	FNAL	LBNL	ORNL	PNNL	PPPL	SLAC	TJNAF
16	Large Scale User Facilities/Advanced Instrumentation		✓	✓	✓	✓	✓	✓	✓	✓	✓
17	Mechanical Design and Engineering					✓	✓		✓		
18	Nuclear and Radio Chemistry		✓	✓		✓	✓	✓			
19	Nuclear Engineering		✓				✓	✓			
20	Nuclear Physics		✓	✓		✓	✓				✓
21	Particle Physics		✓	✓	✓	✓				✓	
22	Plasma and Fusion Energy Science					E	✓		✓	✓	
23	Power Systems and Electrical Engineering					✓	✓	✓	✓		
24	Systems Engineering and Integration		✓	✓		✓	✓	✓	✓		

✓ **=** DOE Endorse Core Capability **E** = Emerging Core Capability

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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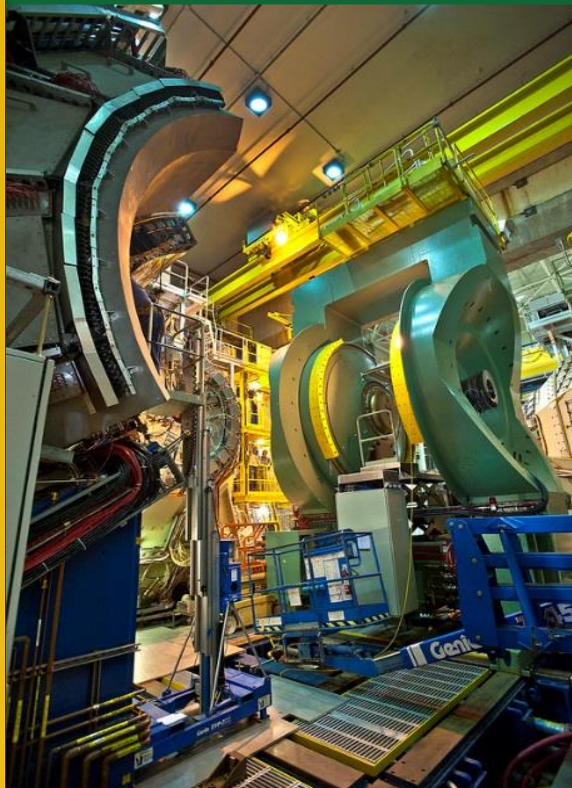

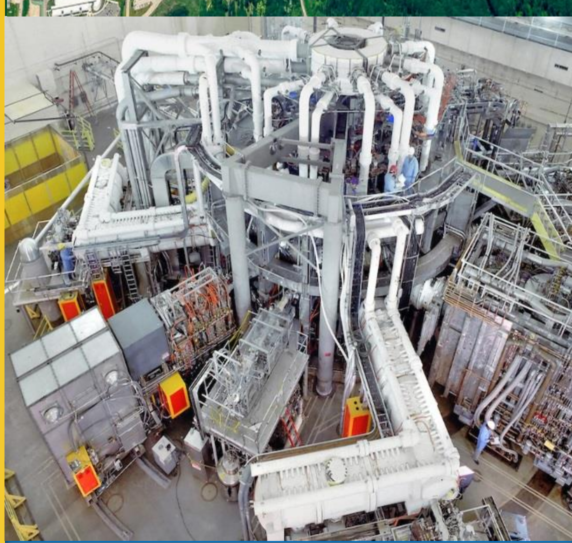

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