U.S. DEPARTMENT OF ENERGY

The U.S. Department of Energy's Ten-Year-Plans for the Office of Science National Laboratories FY 2022

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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 30,000 facility users and more than 8,000 visiting scientists in Fiscal Year (FY) 2021, 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 2022-2032.

[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

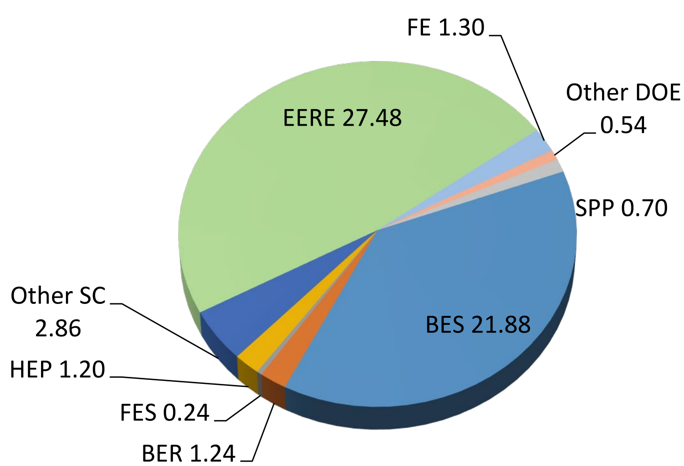
Location: Ames, IA
Type: Single-program Laboratory
Contractor: Iowa State University of Science and Technology
Site Office: Ames Site Office
Website: www.ameslab.gov

- **FY 2021 Lab Operating Costs:** $57.42 million
- **FY 2021 DOE/NNSA Costs:** $56.73 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $0.70 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 1.2%
- **FY 2021 DHS Costs:** $0 million

Physical Assets:
- 10 acres and 13 buildings
- 340,968 GSF in buildings
- Replacement Plant Value: $146 M
- 0 GSF in 0 Excess Facilities
- 0 GSF in 0 Leased Facilities

Human Capital:
- 298 Full Time Equivalent Employees
- 43 Joint Faculty
- 51 Postdoctoral Researchers
- 125 Graduate Student
- 62 Undergraduate Students
- 0 Facility Users
- 7 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Mission and Overview

Ames Laboratory delivers critical materials solutions to the nation. For 75 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 conducts fundamental science addressing critical chemistry and materials challenges, with a focus on three long-term strategic directions: critical materials and upcycling science, atomistic and molecular design and control for energy and chemical conversion, and novel synthesis to manufacturing. Each strategic direction has a particular focus on rare earth elements, sustainable chemistry, alloys, and compounds. Building upon our chemistry, physics, and materials sciences core strengths in the science of interfaces, science of synthesis, science of quantum materials, and science with rare earths, and a proven track record of transitioning basic energy science through early-stage research to licensed technologies and commercialization, Ames Laboratory will lead the nation in translating foundational science for energy and chemical conversion into critical technology innovation. To address these challenges and future unforeseen challenges, the Laboratory focuses 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 transform the way we do science and to create next-generation materials and chemistry, enabling a more sustainable future. Our scientific success results from 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 465+ scientific publications, 150+ inventions, 26 patents awarded, 10 technology licenses, 5 open-source software, 6 R&D 100 Awards. Ames Lab continues to be a leader in development of magnets for clean energy applications, and is currently developing new magnet manufacturing prototyping capabilities that will provide a unique, national capability to enable US magnet manufacturing. Ames is working with an Iowa company to establish ton-level recovery of rare earths from electronic waste.

Advances in our fundamental science has motivated expansion into applied areas, such as catalysts for biofuel production, magnets, alloys for extreme environments, and cooling technologies with caloric materials. 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. 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. This capability is being used for manufacturing materials at extremes, including applications for nuclear and fusion energy.

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 by developing and utilizing electronic structure theory and statistical mechanical and multiscale modeling. An integral component of these efforts is the advancement of computational chemistry codes, especially GAMESS and NWChemEx, and the development of the interoperability between these codes. Our unique competencies include the development of these highly scalable computational chemistry codes suitable for exascale computing.

We are 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. The Ames Laboratory-led Energy Frontier Research

Center, the *Institute for Cooperative Upcycling of Plastics* (iCOUP), is developing new catalytic methods for upcycling hydrocarbon-based polymers and establishing principles of cooperativity in catalytic materials that are specifically designed to interact with macromolecules on multiple length scales.

Atomic-scale characterization of catalysts and surface chemistry 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. A new 14.1T magnet sets the stage for a next-generation DNP-NMR system. 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. We are developing an in-depth understanding of the use of ionic liquids and deep eutectic solvents as separation media. We are examining rare earth interactions in clay-like materials, using unique synthesis, characterization, and computational tools. 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. This now utilized Ames-developed capabilities in AI-optimized molecular synthesis.

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. Ames Laboratory has been at the forefront of research in rare-earth science and novel electronic and magnetic materials since the Laboratory was started. 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 of these materials. 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.

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 innovative synthesis routes for tunable quantum materials with strong spin orbital coupling and non-centrosymmetric symmetry, enabling new studies in new compositional spaces. We reveal mechanisms of 2D growth of nanomaterials, most recently for graphene-protected nanosystems. We have developed several theoretical approaches for predicting ground state crystal structures of complex compounds, and for high-throughput prediction of alloys for harsh conditions.

Quantum materials: Many of our projects are focused on the discovery, control, and applications of quantum and topological materials. The ability to coherently excite materials are 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. Ames Lab 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. We continue to develop the fundamental understanding that underpins extraordinary magnetocaloric, magnetoresistive, and magnetorestrictive materials that owe their functionality to rare earth compounds.

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

Primary Source of Funding: Office of Science

Science and Technology Strategy for the Future/Major Initiatives

Ames Laboratory's mission is to deliver critical materials solutions to the nation. Critical materials are those materials and chemicals that are both currently in short supply and subject to supply chain disruptions, and new materials and chemistry that advance our nation's energy, economic, environmental, and national security. Ames Laboratory is enabling a sustainable future and addressing national challenges facing the country through the discovery, application, and recovery of materials and chemicals that enable critical technologies. Our vision is to lead the nation in foundational science for energy and chemical conversion, and to translate this into innovative energy-relevant technologies. This is reflected in our strategy: *Today's fundamental science for tomorrow's critical chemistry and materials solutions*. Ultimately, our goals are to transform the way we do science, to create next-generation materials and chemistry, and to enable these developments into manufacturing, to achieve a more sustainable future. We accomplish this through three high-priority scientific initiatives, and by utilizing a diverse workforce, modern business systems, safety-focused research and operations, renewed infrastructure and facilities, and a cultural ecosystem unique to Ames Laboratory and Iowa State University.

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

- *Discovery for a Sustainable Future – Critical Materials and Upcycling Science*: Ames Laboratory seeks a sustainable future through efficient separations, chemical transformations, and materials design and synthesis. We are developing novel approaches to better reuse and recover materials, to efficiently convert end-of-life products into useful resources. We are developing alternate materials for use in energy conversion, reducing our dependence on critical minerals. We are developing fundamental science around the needs necessary to create transformative approaches that enable a sustainable future.

- *Making Every Atom Count – Atomistic and molecular design and control for energy and chemical conversion:* Ames Laboratory is understanding and directing novel material behaviors that underpin new quantum technologies, and new optical properties. We study and develop materials that enable energy savings: from caloric materials for reduced energy solid-state cooling technologies, to novel superconductors and topological materials that minimize energy dissipation, to stronger, more conductive wires for a more efficient energy grid. We are providing fundamental insights into the atomic and molecular mechanisms that enable low-energy, highly specific separations.
- *Innovating for Science and Industry – Novel Synthesis to Manufacturing:* Ames Laboratory makes new materials out of compositions never before explored, efficiently predicts materials properties to accelerate their development, and enables additive manufacturing and materials synthesis of components with revolutionary properties. We discover, design, and make magnetic materials that reduce our dependence on critical materials, and that enable efficient energy conversion. We develop new chemical approaches to convert waste and under-utilized materials into value-added resources. Our ability to predict, direct, and control atomic and molecular transformations results in new materials with transformative properties, new approaches to make these materials across length scales, and to transform materials into new resources.

Infrastructure

Overview of Site Facilities and Infrastructure

Ames Laboratory, with a mission to provide critical materials solutions to the nation, is located in Ames, Iowa, on the campus of Iowa State University (ISU). The Laboratory occupies 10 acres of land leased from ISU where 13 DOE-owned buildings reside (see the Ames Laboratory *Land Use Plan*). There are four research buildings, an administrative building, and eight support buildings on the campus. The four research buildings are for general use and support research for all three of our core capabilities: applied materials science and engineering, chemical and molecular science, and condensed matter physics and materials science. The Ames Laboratory campus consists of 340,968 gross square feet (GSF) with a replacement plant value (RPV) of $146M.

In the 2014 DOE Laboratory Operations Board (LOB) infrastructure survey, 10 out of 13 of the DOE-owned buildings were rated as *Adequate* (31.4% of the GSF). The three older research buildings (Harley Wilhelm Hall, Spedding Hall, and Metals Development) were rated *Substandard* (68.6% of the GSF). In 2020, a Facilities Condition Assessment (FCA) was conducted of these three facilities. The FCA rated each of these facilities in below average (Spedding Hall) and poor condition (Harley Wilhelm Hall, Metals Development), highlighting the need for significant renovation investment in major infrastructure systems (electrical, HVAC, plumbing, building envelopes, and elevators). The buildings have good structural integrity, but they were designed for research needs of the mid-1900s. In FY 2020, Ames Laboratory and the Ames Site Office also deemed two maintenance and general storage facilities substandard due to their 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 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. As Ames Laboratory focuses on our three key strategic scientific directions and strives to meet our mission to provide critical materials solutions to the nation, we must also optimize our infrastructure and facilities to accelerate progress. We will continue to maintain our legacy research buildings through infrastructure modernization to provide a safer and more operationally efficient campus while reducing deferred maintenance costs. As we embark on these efforts, the design and planning must include consideration for a Net Zero environment that focuses on the deliberate reduction of carbon emissions and utilization of environmentally friendly energy sources. The Ames Laboratory Director is leading a group exploring opportunities for emissions reduction across the Laboratory complex. 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. Partnering with ISU, the Laboratory has earmarked a site adjacent to Ames Laboratory for a Critical Materials Supply Chain Research Facility (CMSCF).

Rendering of Critical Materials Supply Chain Research Facility (CMSCF).

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

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

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

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

Ames Laboratory utilizes the Mission Readiness process to identify new and review existing facility improvement requests. Projects are prioritized through use of the Capital Asset Management Process (CAMP) and management review. During the FY 2022 Mission Readiness interviews, several common themes were discussed. First, the COVID-19 pandemic has resulted in wider acceptance of the virtual work environment. While the Laboratory has transitioned out of a maximum telework posture, and the COVID-19 Community Status is "low", some team members continue to work nearly 100% from home, some have hybrid schedules with a blend of onsite work and telework time, and others who were working offsite have returned to 100% onsite. As a result, Ames Laboratory did convert a minimum number of spaces to hoteling configurations, allowing for generic desk spaces that can be used by multiple hybrid staff members for short visits to the Laboratory when they need to be onsite. Second, the COVID-19 pandemic has resulted in a majority of business to still be conducted via virtual meetings. Leaders across the Laboratory are assessing small conference rooms' capabilities and looking to improve technology in those spaces through overhead budgets. Technology updates for the larger Laboratory-managed conference rooms are also being considered. Priority will go to updating the Spedding Hall 301 conference center.

Current Gaps

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

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

To address the needs of its aging facilities, the Laboratory recommends advancing the $30M SLI Line-Item project, Ames Infrastructure Modernization (AIM) to the design phase (CD-1). Given current budgetary constraints, DOE has delayed CD-1 for the AIM project. Given this delay, the Laboratory recommends that DOE increase General Plan Project (GPP) capital funding to $3-4M each year for the next 12 years to address critical infrastructure needs; otherwise, critical infrastructure needs will go unattended and the risk of impact to research will increase. 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 exist for all three of our older research buildings and the Laboratory which would benefit from DOE's support to address their deficiencies:

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

Building Envelopes: Building envelopes include roofs, exterior walls, windows, and other exterior building systems. The three general use research buildings require upgrades or repairs to their building envelopes. Future projects will need to add insulation to the roofs of the three primary research buildings to improve energy efficiency and improve each building's ability to protect people and equipment. A new white reflective roof system will increase energy efficiency, eliminate the need for ballast, and add at least 25 years to the life of the buildings. In addition, the Net Zero planning team came forward with a recommendation to add solar panels to the roofs, should funding be available.

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

Plumbing Systems: 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.

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

Helium Recovery System: The Low-Temperature Laboratory (LTL) requires several important upgrades to support the Ames Laboratory mission. Laboratory helium liquefaction and recovery services allows research efforts to obtain liquid helium on demand, at a lower price, and helps in the recycling of this precious natural resource. In-house production makes for 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 was used to upgrade the helium storage tanks ($500K). The Laboratory also received SLI-GPP funding in FY 2020, which is being utilized to upgrade the compressor on the helium recovery system in the LTL ($1.0M). Ames Laboratory is working closely with ISU to ensure the infrastructure in Zaffarano Hall (ISU building) is sufficient to support the updates to the Helium recovery system. The next priority for equipment replacement in the LTL is the Helium liquefier. The LTL is researching several options for the replacement of the liquefier. The initial estimate for a new liquefier is $900K (equipment only). Total project cost for equipment, design, installation, and overhead is expected to be $1.7M.

Telecommunications Infrastructure: Most 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. The Laboratory is creating a new IT room in Spedding Hall, with new telecommunications equipment, cabling, racking, and ventilation utilizing FY 2020 BES-GPP funding. Telecommunication updates are also needed in TASF, Wilhelm Hall, and Metals Development. This scope has been developed during a feasibility study and will be included in the Ames Infrastructure Modernization (AIM) SLI line-item project.

Electronic Access Control: The Laboratory began converting its door access from physical keys to electronic proximity card readers with American Recovery and Reinvestment Act (ARRA) funding. When the ARRA funds were exhausted, the Laboratory allocated GPP funds to continue progress. The exterior doors for all buildings, the property protection areas for the site, and the interior doors for two buildings were completed. This electronic system provides the operations staff a greater amount of control for different access situations and helps to provide better safety, security, and accountability for room use. We have used this capability to secure exterior doors during the pandemic to control access. With the electronic access control system, it would only take one command to lock down all Laboratory exterior and interior doors in the case of an active shooter. However, most of the interior doors in Spedding Hall and Metals Development are still physical key access only and require conversion to electronic card access. The Laboratory received $3M in FY 2021 SLI-GPP funding for this gap. The Laboratory completed a conceptual design for access control upgrades in FY 2021. The Laboratory is currently in design development and plans to begin construction on this project in FY 2023.

Heating, Ventilation, and Air Conditioning (HVAC) Systems: The FY 2020 Facilities Condition Assessments (FCAs) completed for Harley Wilhelm Hall, Spedding Hall, and Metals Development identified some significant deficiencies in their HVAC systems. Though some HVAC updates have been completed by the Laboratory over the last 12 years utilizing GPP funds, the aging systems still require more resources to better support current and future research. The building automation systems need updated as the current Metatsys hardware and software systems are close to obsolete and will not be supported by Johnson Controls International (JCI) in the future (ROM $3M). Multiple air handlers in each of the three older research buildings are nearing the end of their life expectancy and need replaced (ROM $10M). The FCAs also identified a significant amount of HVAC distribution ductwork that is nearing the end of its life expectancy and needs replaced. Legacy contamination concerns will also have to be addressed as a part of the efforts to replace the ductwork (ROM $20M). The Laboratory completed a conceptual design in FY 2022 for the proposed HVAC upgrades in Wilhelm Hall. The total project cost for the Wilhelm Hall HVAC upgrades is estimated to be $6M. The Laboratory is working with the Ames Site Office on potential funding solutions for this project. The rough estimate for the Spedding Hall HVAC upgrades is $12M. The rough estimate for the Metals Development HVAC upgrades is $8M. The Net Zero planning team has identified HVAC systems as the highest priority to reduce Scope 2 emissions.

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

Spedding Hall
Existing Built-Up Roof
(circa 1985)

Harley Wilhelm Hall
Backup/Emergency Generator
(circa 1970)

Harley Wilhelm Hall
Poor Condition Lab Space
(circa 1950)

Spedding Hall
Deteriorating Sewer Piping
(circa 1953)

Spedding Hall
Deteriorating Brick/Limestone Exterior
(circa 1953)

Investment Summary

The Laboratory made significant progress in FY 2021, completing the installation of the new helium recovery system storage tanks, and completing the Metals Development freight elevator safety upgrades.

The Laboratory continues construction efforts in FY 2022 for the fire alarm system upgrades project, the new telecommunications room in Spedding Hall, Building Automation System (BAS) updates in Spedding Hall and Wilhelm Hall, and the installation of a new helium recovery system compressor.

Ames Laboratory developed a project plan, *Ames Infrastructure Modernization (*AIM), to address facilities gaps primarily in Harley Wilhelm Hall, Spedding Hall, and Metals Development. Gaps that will be addressed with this project include plumbing systems, building envelopes, UPS and emergency power systems, telecommunication systems, and deteriorating research laboratory spaces. This project is focused on major infrastructure systems whereas SLI GPP investments are targeted at ancillary projects, renovations and other minor facility modifications that work to improve the physical work environment along with the safety and security of personnel, equipment, and facilities. The AIM Mission Need was approved by the Office of Science on September 9, 2019, followed by the approval of CD-0 on September 16. The Total Project Cost (TPC) range for the preliminary alternatives identified during Mission Need is $10M to $90M (target $30M). Ames Laboratory is currently working toward achieving CD-1 and starting the design effort for this project. Due to budgetary constraints, DOE has delayed pursuit of CD-1 for this project. Delays will result in addressing critical infrastructure needs in the Laboratory's three primary research facilities and increase the risk for impacts to scientific research. Pre CD-1 activities completed so far by the Laboratory include: Facilities Condition Assessments (FY 2020), IT Feasibility Study (FY 2020), and conceptual designs for the plumbing, electrical and building envelope gaps (FY 2021). The Laboratory also completed the Analysis of Alternatives (AoA) in FY 2021 and conducted a CD-1 Director's Review in January 2022. Based on feedback from the Director's Review, the Laboratory is currently finalizing the Conceptual Design Report (CDR), the Acquisition Strategy (AS), and Preliminary Project Execution Project Plan (PPEP). Ames Laboratory plans to fund maintenance and repair activities through overhead at 2.0%-2.4% of RPV for the duration of this plan. Support of this investment strategy will result in the three older research buildings moving from "Sub-Standard" to "Adequate" for their Overall Asset Condition and contribute to the success of the Laboratory's mission. Deferred Maintenance (DM) was re-baselined in FY 2020 as result of the updated guidance from the Office of Science DM Working Group. DM at Ames Laboratory is $4.4M, and will increase with continued delays to the AIM project.

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

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

Objective 2: Provide infrastructure that supports mission readiness. The Laboratory replaced one of the main HVAC air handlers in Metals Development in FY 2020 ($1M). Design was completed in FY 2020, and the construction contract awarded in early FY 2021 for the replacement of the fire alarm system across the complex ($1.5M). The Laboratory received $3M of SLI-GPP funding in FY 2021 for upgrading the access control systems in Spedding Hall and Metals Development. The Laboratory recommends advancing the $30M SLI Line-Item project, AIM, to the design phase in FY 2022 (Note: $2.150M is currently appropriated for AIM). The Laboratory requests sustained funding of $1M per year (BES-GPP), and $3M per year (SLI-GPP) from FY 2022 to FY 2032 to focus on critical mission readiness and infrastructure updates.

Objective 3: Pursue opportunities for future scientific capabilities. The Laboratory completed the conceptual design in FY 2021 for a proposed new research building, the Critical Materials Supply Chain Research Facility (CMSCF). The conceptual design explored the possibilities of a 75,000 SF to 120,000 SF new facility. Discussions during Strategic Planning and Mission Readiness have also 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 2021 Lab Operating Costs:** $871 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $86 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 11%
- **FY 2021 DHS Costs:** $24 million

Physical Assets:

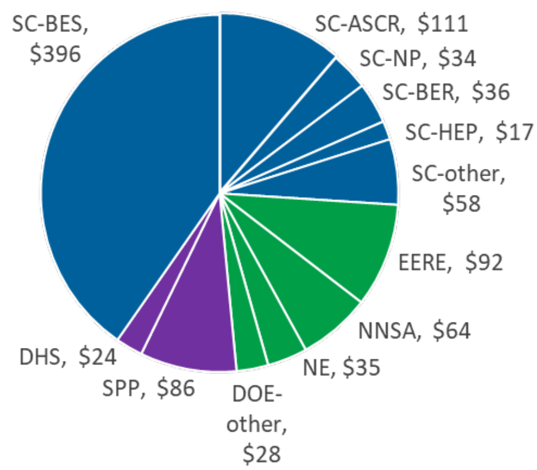
- 1,517 acres and 153 buildings
- 3.9 million GSF in buildings
- 5.1 million GSF in buildings
- Replacement Plant Value: $3.9B
- 0.5 million GSF in leased facilities
- 0.02 million GSF in 13 Excess Facilities

Human Capital:

- 3,523 Full Time Equivalent Employees (FTEs)
- 473 Joint Faculty
- 325 Postdoctoral Researchers
- 205 Graduate Students
- 291 Undergraduate Students
- 5,995 Facility Users of 6 research facilities*
- 1,640 Visiting Scientists

**Five of these facilities are supported by the DOE Office of Science and the sixth by the DOE Office of Nuclear Energy*

FY 2021 Costs by Funding Source ($981 million total)



Mission and Overview

For more than 75 years, Argonne National Laboratory has accelerated science and technology to drive American prosperity and security. We are recognized internationally for pioneering discoveries in multiple fields of research and for technology innovations that have changed the world.

We support the U.S. Department of Energy (DOE) mission through four signature contributions:

- Our ***scientific discoveries*** solve the deepest mysteries in the physical, environmental, and biological sciences, laying the foundation for new technologies that improve the quality of life
- We build on our discovery science to create ***energy and climate solutions*** that we transfer to the Midwest, the nation, and the world for near- and long-term impact
- Our ***global security advances*** help protect society from diverse natural and anthropogenic threats to health, supply chains, and physical and cyber infrastructure
- We design and operate ***cutting-edge research facilities*** that provide unmatched capabilities in discovery science, engineering research, and computing to the second largest user community in the DOE complex.

Argonne's impact is amplified by our extensive collaborations, across the full spectrum of basic science to technology deployment, with universities, businesses, other national laboratories, and government agencies at home and abroad. We are an active partner in the U.S. government's Net Zero World initiative to accelerate global energy system decarbonization, and we play a key support role in Li-Bridge, a public-private alliance focused on strengthening the U.S. supply chain for lithium-based batteries. Argonne also is proud to be a member of the DOE Isotope Program and to direct five multi-institution DOE research centers that are focused on battery development and recycling, materials for energy conversion and water treatment, and quantum science.

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

Our main campus is in the Chicago suburbs, with satellite research and collaboration centers in Washington, D.C., and Chicago. Our Chicago location supports our growing role as a regional convener to drive economic growth and broaden STEM outreach to disadvantaged communities to build the workforce of the future.

Core Capabilities

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

UChicago Argonne, LLC, enables Argonne to effectively use our capabilities by providing guidance, advocacy, and oversight. Led by UChicago, the Joint Task Force Initiative (JTFI) identifies and pursues opportunities for Argonne, UChicago, and Fermilab to drive breakthroughs in research, engage with sponsors, and boost the efficiency of operations.

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

- Advanced Photon Source (APS)
- Argonne Leadership Computing Facility (ALCF)
- Argonne Tandem-Linac Accelerator System (ATLAS)
- Atmospheric Radiation Measurement (ARM) User Facility observatories
- Center for Nanoscale Materials (CNM)

- Intermediate Voltage Electron Microscope (IVEM)

The first five facilities are supported by DOE's Office of Science and the sixth by DOE's Office of Nuclear Energy.

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

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 large-scale user facilities at Argonne and across the DOE complex. Activities among facilities are coordinated and communicated via the Argonne Accelerator Institute. We also broaden our expertise and outreach with joint faculty appointments with accelerator groups at Chicago-area universities.

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

- *Modeling, design, and operation of photon sources, electron accelerators and storage rings, X-ray free electron laser seeding and oscillators, and insertion devices, particularly superconducting undulators.*
  We have complementary expertise in beam diagnostics and feedback systems and in vacuum system engineering. These capabilities underlie the APS Upgrade (APS-U) project as well as future X-ray sources at Argonne and elsewhere in the DOE complex.
- *Generation, acceleration, and reliable delivery of stable- and rare-isotope ion beams serving nuclear physics research at ATLAS.* We support several DOE and worldwide accelerator initiatives using expertise gained at ATLAS over the past 40 years in linear accelerator design and modeling and in the design and development of state-of-the-art superconducting radio-frequency cavity systems, especially for ion accelerators. We are drawing on our unique expertise and infrastructure for superconducting cavity production, testing, cleaning, and processing to support four major efforts. Those efforts are R&D for the future electron ion collider at Brookhaven National Laboratory, the APS-U bunch lengthening system, the

superconducting electron gun for the SLAC National Accelerator Laboratory's Coherent Light Source II, and the Proton Improvement Plan II project at Fermilab.

- *Advancements in high-gradient, two-beam acceleration using dielectrically loaded structures,* in support of high-energy physics research. This work is centered at the AWA, a unique facility combining the world's highest electron bunch charge produced by a photocathode gun with a state-of-the-art linear accelerator and beam instrumentation. Using the AWA, we are working to evaluate emittance manipulation techniques in support of future capabilities in photon science. The AWA also is open to the user community for general accelerator R&D in structure and plasma wakefield acceleration, radiation generation, and electron source development.
- *Areas vital to future accelerators and colliders,* including high-power radio frequency sources; generation and preservation of high-brightness beams; photo-injectors; magnetic systems, including design and characterization of accelerator lattices and novel insertion devices; collective beam instabilities; and two-beam acceleration with high transformer ratios. This research is synergistic with our work to improve the performance of light sources and colliders and address national security applications.
- *State-of-the-art accelerator modeling and controls:* our advanced accelerator modeling codes *elegant* and TRACK are used worldwide, and we develop EPICS software tools and applications for distributed control systems for accelerators.
- *Support for accelerator outreach, training, and education* via the U.S. Particle Accelerator School based at Fermilab, the summer undergraduate Lee Teng Fellowship in collaboration with Fermilab, and the DOE-funded graduate accelerator education program led by Michigan State University.

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

Advanced computer science, visualization, and data

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

- Foundational computing software and algorithms for quantum and neuromorphic computing, with a focus on software and methods for science
- Automation of scientific discovery through machine learning (ML), cloud computing, and high-performance computing; this includes platforms to support the basic and applied sciences
- Concepts and strategies that capitalize on our work in data visualization, analysis, and management for the capture, transport, reduction, transformation, storage, and understanding of DOE application data
- 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, the Argonne-led RAPIDS2 SciDAC Institute for Computer Science and Data is enhancing computer science and data analysis capabilities in these strategic areas:

- In hard X-ray science: data transfer from APS to ALCF, real-time analysis, and parallel algorithms
- In earth system science: coupled data analysis across multiple models
- In high-energy physics: multivariate functional approximations of short-baseline neutrino experimental data
- In fusion energy: use of ML to develop low-cost, energy-conserving 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, with sensors deployed in Chicago and around the U.S.
- A quantum simulation capability for understanding quantum architectures, quantum compilation, quantum networks, and quantum sensors
- The Data and Learning Hub (DLHub), a self-service platform for publishing, applying, and creating new ML and deep learning models, helps researchers benefit from advances in those technologies
- Application of artificial intelligence (AI) to screen potential COVID-19 pharmaceuticals: We build infrastructure to integrate AI/ML tools with physics-based tools to screen orders-of-magnitude more compounds than is possible with traditional drug-screening workflows (Argonne was part of the team that won the first ACM Gordon Bell Special Prize for HPC-Based COVID-19 Research at SC20 and part of two of the finalist teams at SC20 and part of two of the finalist teams at SC21)
- New co-design microelectronics efforts that explore relationships from materials to applications focused on energy-efficient memories, neuromorphic devices, and THz terahertz interconnects
- AI-guided experiments: We are developing methods and software for rapid coupling of experimental facilities, AI methods, and leadership computing, enabling AI-guided steering.

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. Production supercomputer systems worldwide use Argonne's research software tools, such as MPICH, and we are highly regarded for our development of operating system and runtime software for extreme-scale computing. 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. Argonne and Fermilab are exploring metro-scale quantum networking over deployed optical fiber via the Illinois Express Quantum Network project. Argonne staff continue to receive recognitions, such as the DOE Ernest Orlando Lawrence Award and designation as DOE/SC Distinguished Scientist Fellows and Fellows of IEEE, ACM, and AAAS.

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

Applied materials science and engineering

Argonne applies internationally recognized expertise in materials design, development, synthesis, processing, and scale-up to drive advances in materials science and technology. Applied and basic science teams from across the Laboratory execute research using a broad suite of resources.

These resources include the APS and CNM, used for materials characterization; ATLAS, IVEM and APS, used for nuclear materials development; the ALCF, used for computational materials science; the joint Argonne-UChicago Center for Molecular Engineering; and our Materials Engineering Research Facility (MERF).

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

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

The integration of basic and applied materials science at Argonne has produced more-efficient batteries, high-performance sorbents, nanofiber magnets, heat exchangers for extreme applications, and design methods for materials used for nuclear reactors and solar receivers. Ongoing work shows promise for more-efficient nuclear fuel reprocessing, lighter-weight transportation alloys, advanced building materials, and higher-performance superconducting materials for use in detectors, accelerators, and energy transmission. Argonne’s extensive experience in energy storage materials R&D positions us to make significant contributions to future storage solutions for stationary and mobile applications.

The MERF enables scientists and engineers to bridge the gap between bench-scale science and industrial implementation through synthesis, process R&D, scale up of materials, and fabrication/testing of components and devices. Capabilities at the MERF are especially well suited to advancing research focused on decarbonization across the energy economy.

At the MERF, researchers develop scalable, energy-efficient, and precisely controlled processes to produce quantities of innovative materials sufficient to enable industrial testing and techno-economic modeling that reduce commercialization risks. For example, capabilities at the MERF allow integration of new nanostructured and soft matter materials developed at Argonne into state-of-the-art, flexible microelectronic sensors and detectors. We advance process science by using artificial intelligence, data science, and *in situ* and *operando* hard X-ray and nanomaterial characterization tools in collaboration with ALCF, APS, and CNM. For example, we have used flame spray pyrolysis to synthesize solid state battery cathode materials and microfluidic techniques to produce core-shell fuel cell catalysts.

In 2021, we established the Materials Manufacturing Innovation Center to enhance partnerships in the scale-up and manufacturing of advanced materials, with the MERF as a key facility for near-term collaborative research. Longer-term, we anticipate a need for additional collaborative space. Partnerships include workforce development efforts with an emphasis on underserved communities.

Argonne’s applied materials science and engineering capability complements additional, diverse collaborative research efforts. These efforts include the Joint Center for Energy Storage Research, a DOE/SC Energy Innovation Hub that creates transformative battery materials, and the Argonne Collaborative Center for Energy Storage Science, which facilitates deployment of novel battery materials to industry. We develop materials technologies to solve global water challenges through the Advanced

Materials for Energy-Water Systems Center, a DOE/SC Energy Frontier Research Center, and the Collaborative Water-Energy Research Center, an international consortium supported by DOE and Israel.

We partner with industry through multiple DOE/EERE initiatives, including Chain Reaction Innovations, Argonne's Lab Embedded Entrepreneurship Program; several Manufacturing USA institutes; and many DOE/EERE consortia, including Chemical Catalysis for Bioenergy (ChemCatBio) and Lightweight Materials (LightMat).

This capability supports the missions of DOE and other sponsors in the areas of nuclear energy, energy efficiency, renewable energy, energy storage, and environmental stewardship. It builds on discoveries in our core capabilities in condensed matter physics, materials science and engineering, and chemical engineering, with the goal of enhanced impact from moving those discoveries to market.

Applied mathematics

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

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

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

- Scalable frameworks for modeling and solving large-scale-optimization-under-uncertainty problems by using high-performance computing for the planning, design, and control of networked systems such as electrical, gas, transportation, and water networks
- Multimodal ML and statistical modelling for analyzing experimental, observational, and simulation data, including ALCF, APS, and ARM data
- Fast algebra for high-order element-based discretization to enable extreme-scale simulation of atmospheric boundary layer flow and its interactions with wind turbines
- Automated ML, multi-objective optimization, and differentiation algorithms applied to post-Moore architectural concepts and deployed for applications such as transportation modeling, supercomputing performance, and self-driving laboratories

Our advances in applied mathematics are captured in state-of-the-art software, including:

- The Nek5000, NekRS, 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 and dozens of other toolkits, which provides scalable linear solvers, nonlinear solvers, and time integration methods for solving discretized PDEs
- AD solutions, including the Enzyme and Tapenade tools, C++ header-only libraries, and Julia modules
- DSP and MINOTAUR, which solve optimization problems with both discrete and continuous variables
- Scalable solvers, such as TAO and PIPS, for optimization problems with billions of variables and constraints

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

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

Biological and bioprocess engineering

Argonne's approach to biological and bioprocess engineering incorporates methods from synthetic biology and synthetic chemistry to create biological systems and biomaterials with tuned functionalities. We apply understanding of complex biological systems to design, test, and validate process components, technologies, and systems relevant to bioenergy production, environmental contaminants processing, and global carbon cycling and biosequestration. We also apply biochemical engineering principles to develop scalable new processes for biofuels and bioproducts. Further, we leverage our computational expertise and resources as leaders in developing bioinformatic tools for the larger research community and incorporating artificial intelligence strategies for data analysis and biodesign. Primary supporting disciplines include biology, chemistry, chemical engineering, materials science and engineering, environmental and agricultural science, microbiology, computational sciences, and systems science.

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

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

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

Current research directions and investments focus on:

- *Synthetic biology for biosystems design.* We analyze and model microbial and microbiome systems to enable predictive design of strains and communities and develop an ecological understanding of them. We are a major contributor to the development of the DOE/SC-BER Systems Biology Knowledgebase, which integrates metabolic modeling with cheminformatics, omics, and meta-omics in support of bioengineering of microbes, plants, and microbial communities. We also develop methods to rapidly design and engineer novel microorganisms and collaborate with Northwestern University and UChicago on automated laboratories to support this effort.
- *Global carbon cycle and environmental chemical cycling.* Argonne research seeks to understand elemental cycling in the biosphere in a variety of environmental contexts. One focus area is the biogeochemical processes that affect iron, carbon, and contaminant speciation within natural environments and wetland sediment, rhizosphere, and stream environments. We also work to discover the plant genes important for adaptation and sustainability in the face of environmental change.
- *Bioprocesses and biomanufacturing.* As the lead laboratory for the DOE/EERE Bioprocessing Separations Consortium, Argonne has developed technologies to separate and recover organic acids and terpenes produced during fermentation and worked with industry to overcome separation issues in biofuels and bioproducts production. We scale up bioprocesses; for example, we have successfully scaled up a bioprocess for organic acid production from a 14-liter (about 3.7-gal) fermenter to a 100-gal fermenter to provide feedstock for sustainable aviation fuel production. We contribute to the development of biomanufacturing technologies as part of two DOE/EERE efforts, the Agile Biofoundry Project and the Feedstock Conversion Interface Consortium. In addition, we have core competencies in lifecycle, techno-economic, and environmental risk analyses of bioenergy-related processes and assessments of the impacts of bioenergy system deployment on soil carbon, water footprint, water quality, and landscape design.

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

Chemical and molecular science

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

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

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

Other relevant facilities include Argonne's unique High-Throughput Research Laboratory, atomic layer deposition laboratories, and Advanced Electron Paramagnetic Resonance Facility. In addition, our DOE/SC-BES programs in heavy-element chemistry and separations science are based in state-of-the-art radiological facilities in the Materials Design Laboratory, a location that fosters interdisciplinary science.

Argonne's our core capability in condensed matter physics and materials science complements these strengths through materials design and synthesis and functional material development. We advance our DOE/SC-BES discoveries in chemical and molecular science through collaborations with industry and in conjunction with our core capabilities in chemical engineering and applied materials science, underpinning our collaboration and leadership of JCESR. We lead the Energy Frontier Research Center on Advanced Materials for Energy-Water Systems (AMEWS), which, in collaboration with UChicago and Northwestern University, continues to deliver breakthroughs in scientific understanding of water/solid interfaces.

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

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

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

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

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

Chemical engineering

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

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

Our multidisciplinary efforts also develop advanced membranes, electrodes, and electrocatalysts to reduce the cost and improve the durability of fuel cells based on solid-oxide and polymer-electrolyte membrane technologies. Recent work is advancing rail, marine, and aviation applications of fuel cells. Our expertise in gas-phase chemistry and chemical and material scale-up is leading to new engine designs and pathways for translating DOE/SC discoveries and DOE/EERE foundational research to meet industry and consumer needs.

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

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

- *Cell Analysis, Modeling and Prototyping Facility*. Cells manufactured in this facility enable realistic, consistent, and timely evaluation of candidate battery-cell chemistries in a close-to-realistic industrial format.
- *Electrochemical Analysis and Diagnostics Laboratory.* This laboratory provides battery developers with performance evaluation of cells, modules, and battery packs, allowing

diagnostic analysis of battery components after use to identify mechanisms that limit battery life.
- *Post-Test Facility.* This facility is designed to understand failure modes in batteries with air-sensitive materials, such as those from lithium-based or sodium-based battery technologies.
- *High-Throughput Research Laboratory.* This laboratory provides robotic tools and reactor systems for fast, automated, and parallel approaches to chemical synthesis and materials development, thereby accelerating optimization of new materials for catalysis, energy storage, fuel cells, solar energy, and nanoscale chemistry.
- *Materials Engineering Research Facility.* This facility allows researchers to scale up innovative materials and chemical processes to move them to the marketplace. It is described in more detail under our applied materials science and engineering capability.

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

Climate change sciences and atmospheric science

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

Argonne's strengths in atmospheric science are grounded in our ability to make sophisticated atmospheric measurements at an unprecedented scale and under challenging circumstances. We are actively involved in the DOE/SC-BER ARM User Facility. We oversee operational activities for all ARM observatories and manage two of them: the 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 – and the ARM Mobile Facility 3 (AMF3).

We are pioneering edge computing that uses artificial intelligence (AI) and advanced wireless technology (5G and beyond) for agile sensing to measure at spatial and temporal scales optimized for the science question being asked. We have deployed edge computing to ARM-SGP, an ARM site in Texas, multiple locations in Chicago and adjacent suburbs, and the main Argonne campus.

Our computational and domain scientists develop AI applications to improve the predictability, speed, and efficiency of earth system models. These competencies enable our strong participation in DOE/SC-BER's AI for Earth System Predictability (AI4ESP) visioning and leadership.

Argonne provides the global scientific community with unique expertise and software for retrieving geophysical variables from atmospheric remote sensing instruments. Our pioneering suite of open-source software codes is internationally recognized and supports the science in hundreds of published scientific articles.

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

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

Argonne is a global leader in downscaling earth system models to project possible local climate conditions. Our 12-km-resolution climate projections for North America support quantitative analysis of risks from extreme weather. We collaborate with DOE/EERE-WETO and NOAA to improve the accuracy of numerical weather prediction models over complex terrain, in support of wind-energy production. We are completing North American continental-scale simulations at a 4-km resolution that fully accounts for convection physics. We finely model drought, fire, and coastal systems in the Great Lakes, including interactions with the Chicago urban region.

Our soil and biogeochemical scientists develop deep predictive understanding of soil response to environmental change, from the molecular to the regional scale. We collaborate with the broader scientific community to develop novel syntheses of regional carbon dioxide flows from arctic and boreal soils, producing the first high-resolution, spatially explicit estimate of organic carbon stocks in permafrost soils. We advance knowledge of soil processes and develop novel sensors and technologies to characterize soil properties by leveraging our plant and microbial ecology expertise and by developing and applying novel synchrotron-based techniques to biogeochemical studies. We use geospatial analytics to extend field measurements. Our rapid mid-infrared spectroscopy technique enables researchers to quickly assess soil properties that are vital for predicting carbon and water cycling through terrestrial ecosystems.

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

Computational science

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

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

- Leverage our computational science division and data science and learning division to build strong collaborative projects with scientists and engineers across Argonne in modeling, simulation, data-intensive applications, and artificial intelligence (AI) and machine learning (ML). We facilitate crosscutting Laboratory-wide engagement in computing and foster multidisciplinary teams for conducting leading-edge computational science.
- Through our computing divisions, provide computational scientists and engineers with ready access to broad, deep expertise in traditional and emerging scientific computing methods and

tools. These methods include modeling, simulation, data science, ML, 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 AI/ML.
- Take advantage of the co-location of hardware and staff expertise to strengthen proposals of both internal and external computational science groups as they apply for DOE's *Innovative and Novel Computational Impact on Theory and Experiment* and *ASCR Leadership Computing Challenge* awards.

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

- We have performed some of the world's largest high-resolution cosmological simulations with Argonne's HACC code, modeling the universe over billions of years. HACC plays an important role in benchmarks for future DOE computing systems and is a significant part of two major efforts within DOE's Exascale Computing Project (ECP).
- We have developed and implemented algorithms and toolkits for analysis of large datasets from Argonne's APS, the Large Hadron Collider in Switzerland, and the Legacy Survey of Space and Time carried out at the Vera C. Rubin Observatory in Chile.
- Our peers have recognized the computational science enabled by our PETSc library with multiple Gordon Bell prizes and the joint prize in Computational Science and Engineering awarded by the Society for Industrial and Applied Mathematics and the Association for Computing Machinery.
- We develop applications in support of fusion energy science programs. This includes simulation (DIII-D plasma-material interaction and Monte Carlo particle transport in fusion device components) and AI/ML to predict tokamak disruptions and model collisions in kinetic plasma simulations.
- Our NekCEM/NEK5000 code has been used in applications including fluid flow, thermal convection, magnetohydrodynamics, electromagnetics, and combustion. It is used in two ECP application projects.
- Argonne staff engage in development of community codes such as NAMD, QMCPACK, and LAMMPS.
- Argonne's computational COVID-19 research has included AI-driven study of viral reproduction using our Balsam workflow software and the Cerebras CS-1 wafer scale engine hardware in the ALCF AI Testbed.
- 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 and electron tomographic analysis), and QMCPACK studies of the electronic and structural properties of semiconductors.
- Argonne is a member of a multi-laboratory partnership under the auspices of the High Energy Physics Center for Computational Excellence, which works to employ exascale computing resources for simulation and data analysis for high energy physics experiments.

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

Condensed matter physics and materials science

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

Our programmatic strategy rests on understanding and exploiting the science of defects and interfaces in quantum materials, including materials for quantum information science (QIS) and microelectronics, materials to enable interface- and defect-directed energy and information transduction, and soft materials under static and dynamic order. Our expertise and capabilities together make Argonne's portfolio unique, positioning us to deliver scientific breakthroughs in these fields of materials discovery. For example, our experimental and computational research is seeking to explore fundamental behavior driven by the interplay of order parameters, such as magnetism and charge, and behavior at the interfaces between soft and hard matter.

We support our core themes with crosscutting and enabling strategies in precision synthesis and *in situ* and *operando* coherent X-ray and electron studies coupled to modeling and theory. Artificial intelligence (AI) and data-driven science underpin all areas of our research. Argonne, through its Center for Molecular Engineering, leverages joint appointments with UChicago to enhance our expertise in soft matter, semiconductor-based QIS materials platforms, and computational materials science.

Collaboration across Argonne and externally enriches our strategy. Our materials science strengths are complemented by Argonne's core capability in chemical and molecular science, particularly in interfacial- and electro-chemistry. Our activities are synergistic with Argonne's efforts in clean energy and sustainability, AI for science, autonomous discovery, hard X-ray sciences, and microelectronics. We lead the Midwest Integrated Center for Computational Materials, a collaboration with UChicago and four other universities. Our core materials science complements the work of the Argonne-led Joint Center for Energy Storage Research and Q-NEXT center, and we play a principal role in several other materials-focused multi-institution projects funded by DOE/SC-BES. Across our portfolio, we seek to transfer our fundamental materials discoveries to applied Argonne research that can leverage them for development and deployment.

Argonne's materials research has had recent impact at frontier areas of science, including understanding the origins of polar state memory in active soft matter, using AI approaches to enable functional imaging of magnetic materials at high spatial resolution, observing dynamically stable active sites on oxide surfaces, and predicting the structure and behavior of strongly correlated materials and opto-electronic platforms.

Looking ahead, we will build on our materials discovery expertise to elucidate hidden order in soft and hard matter, explore ion motion and dynamics across materials systems, and make fundamental contributions to novel materials and phenomena that can be exploited for QIS and for microelectronics, in part with a view toward energy efficiency. We will explore new approaches to autonomous discovery that capitalize on our expertise in AI and extend beyond our current efforts on polymers and electrolytes. Our coherent imaging approaches will encompass both X-rays and electrons, and we will develop regenerative synthesis approaches that allow function to be restored to degraded surfaces and interfaces.

We will capitalize on upgrades at Argonne's major facilities. We are developing exascale-ready codes in preparation for using ALCF's exascale computer Aurora, to expand our data- and AI-driven materials design and discovery efforts. A particular focus will be on simulating heterogeneity in hard and soft matter. To help shape the scientific mission of the APS-U, we will develop new X-ray-based approaches for extracting hidden order in condensed matter, for designing and controlling defects and nanomaterials for QIS platforms, and for exploring ultrafast responses across electronic and structural phase transitions. We will probe ultrafast dynamics using CNM's ultrafast electron microscope, and we will capitalize on other upgrades at CNM such as the new probe-corrected scanning transmission electron microscope.

We will develop autonomous discovery approaches to guide these experiments and to facilitate analysis of the complex datasets they will produce. In addition, condensed matter physics and materials science will play a key role in developing and executing on the planned Sensing and Imaging at Argonne building.

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

Our cyber and information sciences research supports critical national missions: it strengthens the overall cybersecurity of national infrastructure in a proactive way, including the electric grid, water systems, transportation assets, and supply chains; and enhances national efforts in nonproliferation and counterproliferation of weapons of mass destruction, military decision support, and radiological response and recovery. We are a trusted partner to federal, state, and local agencies in developing and deploying innovative solutions to manage both current and emerging information threats. Our research protects, analyzes, and disseminates information from information systems to defend U.S. critical infrastructure from cyber attacks.

We take a collaborative cross-disciplinary approach to address emerging problems and deliver results with national impact. Our cyber and information sciences programs leverage Argonne's discovery sciences and advanced computing and engineering capabilities including the APS and ALCF. Our external partners include Iowa State University, UChicago, additional universities and businesses, and other national laboratories.

We help protect the nation through our research into the resiliency of information assets, the security of cyber-physical systems, and the collection and dissemination of intelligence needed to defend against cyber threats. For example, we:

- Conduct proactive cybersecurity research in critical infrastructure resilience; autonomous, proactive, and moving target defenses; autonomous vehicle security; applications of machine learning and artificial intelligence; risk quantification; modeling and management; and other technologies to improve national security
- Partner with DOE/CESER and DOE/SC-ASCR to develop the cybersecurity workforce, including hosting the annual CyberForce Competition™ to increase college students' understanding of the challenges of cyber-physical systems and high-performance computing environments, to drive interest in related careers
- Design tools and testbeds, such as the SECURE testbed, to evaluate resiliency, dependencies, and defenses of computer systems that operate critical infrastructure and industrial control systems, as well as the consequences of cyber-attacks on systems
- Explore implications of quantum cryptography, communication and sensor technologies on critical infrastructure and nonproliferation missions
- Share cyber threat information using real-time, machine-to-machine methods for energy sector defense using the CyberFed Model, while also working to define next-generation automated

information sharing tools and protocols to enable coordinated cyber threat discovery and and mitigation
- Investigate the use of differential privacy and secure enclaves to support federated learning on sensitive data through DOE's PALISADE-X project
- Explore the challenges that will emerge when heterogeneous and complex systems (those composed of a continuum of compute and storage resources connected through high-speed networks and that expand multiple domains) are fully integrated into distributed science ecosystems and used to support autonomous science
- Collaborate with industry and academia to develop and evaluate algorithms to monitor the physics of the smart grid and distribution energy resources to detect and mitigate cyber attacks
- Develop structured knowledge representations based on information extracted from internet sources, including the darknet, using machine learning and natural language processing to better understand proliferation patterns
- Provide a fully reconfigurable platform with thousands of cores for computer science and security research at scale
- Develop edge-computing platforms for detection of moving objects such as birds and unmanned aerial systems
- Integrate cutting-edge research into complex models for analysis of military transportation, disaster response and recovery, storage and transportation of spent nuclear fuel, and supply chains

Facilities that support this capability include enterprise data centers hosting a multi-agency, secure private cloud and testbeds to model physical and cyber dependencies.

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

Decision science and analysis

Argonne is recognized for developing and applying novel decision science and analysis approaches to inform decision makers as they address pressing national, cross-border, and global challenges in rapidly changing environments with incomplete and imperfect data. These approaches include agent-based modeling, complex adaptive system modeling, system dynamics, life-cycle analysis, and network analyses that model parameters of dynamic, complex systems.

We are an international leader in the development of high-performance computing software tools, including their use in extreme-scale agent-based modeling applications; these tools include the Recursive Porous Agent Simulation Toolkit (Repast) and the Extreme-scale Model Exploration with Swift (EMEWS). This core capability – linked with Argonne's core capabilities in cyber and information sciences; applied mathematics; advanced computer science, visualization, and data; and systems engineering – positions us to deliver impactful solutions to complex, multidisciplinary problems.

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

Argonne continued to leverage many aspects of this core capability during the ongoing U.S. response to COVID-19. For example, we engaged with the City of Chicago and the State of Illinois with the CityCOVID agent-based model, which we used to forecast the spread of COVID-19 and test the effects of potential mitigation measures.

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

- Apply decision science principles and techniques to create assessment frameworks for use across critical infrastructure systems, to enable subject matter experts to make cost-benefit tradeoffs for different security and resilience features
- Assess the intricate interactions of infrastructure interdependencies in local, regional, national, and international systems to identify potential cascading and escalating failures and inform resilience-enhancement decisions
- Develop optimization models that enable decision-makers to prioritize transport routes that support disaster relief supply chains and identify pre-disaster planning and mitigation measures to protect them
- Model and analyze global supply chains to inform decisions affecting the U.S. stockpile of critical materials that support national security and energy technologies
- Develop decision support resources for the valuation and performance of energy projects to help policymakers evaluate the ability of prospective international energy projects to meet established guidelines and support U.S. priorities
- Use agent-based modeling and high-performance computing to understand the resilience of companies and market indices to targeted disinformation campaigns, informing the development of a new construct for characterizing how disinformation can affect financial markets
- Continually upgrade our Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model, and use it to support planning and investment decisions by government and industry about a wide range of new energy technologies, by projecting the associated energy and water use and emissions impacts throughout the life cycle of technologies, from material supply chains to final use in the marketplace; GREET currently has more than 48,000 registered users worldwide

In the future, our research will concentrate on model coupling, ensemble modeling, and uncertainty propagation to support decision making in dynamic hazard and policy environments. A near-term focus will be integrating our decision science capabilities with environmental and infrastructure science expertise to help communities evaluate adaptation strategies that will enhance their resilience to climate change.

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.

Large-scale user facilities/advanced instrumentation

Argonne is at the forefront in the design, construction, and operation of world-leading scientific user facilities and innovative instrumentation. These assets are strongly integrated with our research programs and reflect our commitment to nurture a diverse and vibrant user community. The six facilities described here are part of the DOE/SC and DOE/NE portfolios of user facilities. This capability supports the DOE mission to provide the highly advanced research tools needed to address the greatest challenges in science and technology. In addition to DOE support to operate these facilities, specific capabilities at individual facilities are also supported by DOE/NNSA, DOE/OE, NIH, NSF, and industry.

Advanced Photon Source (APS)

Funded primarily by DOE/SC-BES, the APS is an internationally leading source of high-energy X-rays for scattering, spectroscopy, and imaging studies over a wide range of length and time scales. Capabilities include *in situ* and *operando* measurements of materials and systems in real conditions; 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 advanced electron microscopy in the planned Sensing and Imaging at Argonne building.

Argonne Leadership Computing Facility (ALCF)

Funded by DOE/SC-ASCR, the ALCF provides petascale open-science computing capabilities and support services that enable the researchers to run the largest and most complex calculations, including Theta/ThetaGPU, a 15.6-petaflop system, and Polaris, a 44-petaflop system that ranked as the 12th fastest machine in the world on the current Top500 list. ALCF also hosts the *Joint Laboratory for System Evaluation*, which gives staff and collaborators access to the latest production and prototype computing resources, and the *ALCF AI Testbed*, a testbed of AI-accelerated systems, opening to the DOE community in 2022. In 2023, we will begin user testing of the Aurora exascale computer.

Argonne Tandem Linear Accelerator System (ATLAS)

Funded by DOE/SC-NP, ATLAS is a superconducting linear accelerator and one of two DOE user facilities 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

We manage two observatories within the DOE/SC-BER ARM User Facility: The Southern Great Plains site and Mobile Facility 3, which will begin operations in the southeastern U.S. in 2023. The former, based near Lamont, Oklahoma, is the world's largest and most extensive field site for climate research, with instruments arrayed across 9,000 square miles. Argonne also oversees operations and instrumentation and provides instrument and measurement expertise to all ARM sites. Scientists from Argonne and other institutions use ARM data to advance scientific understanding of cloud, aerosol, and atmospheric processes, which supports improvements in models of the earth's climate.

Center for Nanoscale Materials (CNM)

The CNM, funded by DOE/SC-BES, supports interdisciplinary nanoscience research, with emphasis on quantum materials and sensing, manipulation of nanoscale interactions, and nanoscale dynamics. Its capabilities include autonomous synthesis and characterization through integration of AI and machine learning methods, ultrafast electron microscopy, broadband ultrafast optical spectroscopy, nanofabrication, and first-generation user tools for quantum information science. A hard X-ray nanoprobe is one of many joint capabilities and collaborations with the APS. New, dedicated space to house equipment is needed to expand CNM's electron microscopy capabilities; the proposed Sensing and Imaging at Argonne building would provide such space.

Intermediate Voltage Electron Microscope (IVEM)

Argonne's IVEM is one of the Nuclear Science User Facilities funded by DOE/NE. It is used for *in situ* transmission electron microscopy studies of defect structures in materials under controlled ion irradiation and extreme sample environments. It uses an ion-beam accelerator to produce high-dose ion damage to materials in hours, rather than the years that would be required to produce the same damage in an operating nuclear reactor. The IVEM enables real-time observation of defect formation and evolution. New capabilities being developed include automated defect detection and deep learning for real-time imaging, analysis, and prediction.

Nuclear and radio chemistry

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

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

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

- APS, ATLAS, and ALCF
- Electron microscopy tools including the Intermediate Voltage Electron Microscope
- Two co-located radiological facilities: the Low-Energy Accelerator Facility (LEAF) and a chemical separations system for radioisotope recovery and purification
- Radiological laboratories that enable development and testing of advanced electrochemical and aqueous separation processes and nuclear fuels, to support development of innovative nuclear fuel cycle and safeguards technologies

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

Within the context of minimizing the quantities of weapons-usable nuclear material in reactor applications worldwide, we are a leader in research, development, and demonstration of the use of low-enriched uranium fuel 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 have developed and demonstrated new accelerator-based production channels, as well as chemical separation and purification methods, to facilitate domestic molybdenum-99 production without the use of weapons-usable materials.

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

We also conduct sensor and detector research for national programs in border, cargo, and transportation security, as well as chemical, biological, radiological, and nuclear incident mitigation. Our focus includes domain awareness technologies for detectors and detection equipment testing and analysis, as well as forensics to identify sources of nuclear and biological materials.

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

Nuclear engineering

Argonne pioneered nuclear energy systems and continues to be a world leader in advancing nuclear energy science and technology. We are recognized for ground-breaking research in nuclear energy development and nuclear materials security. Our nuclear engineering capability supports national goals in advancing civilian nuclear reactor and fuel cycle design and safety, nuclear nonproliferation and peaceful uses of nuclear technology, and isotope research and production. 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 the APS, ALCF, ATLAS, and Intermediate Voltage Electron Microscopy-Tandem Facility, which has unique capabilities to image changes in materials during irradiation. An activated materials laboratory is being built in the APS Long Beamline Building to enable use of the upgraded APS for X-ray analyses of radioactive samples. Using the ALCF, Argonne has made major advances in exploiting high-performance computing (HPC) for multiphysics analysis of nuclear-reactor behavior. We use specialized laboratories to study nuclear reactor materials and components under extreme conditions like those encountered in nuclear energy systems. Throughout our history, we have enhanced the efficiency and benefits of our research through national and international collaboration with research and industrial partners.

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.

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 Advanced Nuclear Security, Waste and Energy Research initiative, working with DOE, Idaho National Laboratory, and Oak Ridge National Laboratory, to position the U.S. as the enduring leader in global deployment of advanced civilian nuclear energy systems through a coordinated focus on science, technology, and policy.
- Advance technologies for next-generation reactor and fuel cycle systems, including micro-reactors, in partnership with industry and other DOE national laboratories. This includes working on industry-led projects awarded under the DOE Advanced Reactor Demonstration Program.
- Lead the core design and safety analysis efforts for the Versatile Test Reactor, one of the priority projects of DOE’s Office of Nuclear Energy.
- Increase fundamental understanding of nuclear energy materials, processes, and systems to enable their optimal application and development. Argonne is exploring the use of artificial intelligence (AI) and machine learning (ML) techniques to correlate neutron damage in reactors to ion damage measurements in accelerator facilities such as ATLAS.
- Develop and validate advanced, mechanistic modeling and simulation capabilities to better predict the performance characteristics and safety behavior of nuclear energy systems, leveraging our broader capabilities in AI/ML and HPC.
- 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, and enhancing the proliferation resistance of advanced nuclear processes and facilities.
- Enable technological advances that can reduce construction, operating, and maintenance costs for advanced nuclear energy systems.

Argonne’s nuclear engineering 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 components; and enhance the security of nuclear technology applications worldwide. Current sponsors include DOE/ARPA-E, DOE/NE, DOE/NNSA, DOE/OCED, DOE/SC-NP, DOD, DHS, NRC, the nuclear power industry, and international organizations.

Nuclear physics

Argonne is a global leader of research in nuclear structure, nuclear astrophysics, fundamental interactions, and hadron physics as well as in the enabling areas of nuclear instrumentation and accelerator development. Our ATLAS user facility is at the cutting edge of discovery science with recent upgrades to deliver a unique capability set. Capabilities include beams of stable isotopes at energies up to 20 MeV/nucleon, radioactive ion beams from the californium rare isotope breeder upgrade (CARIBU), and state-of-the-art instruments such as the helical orbital spectrometer (HELIOS). The recent addition of a radioactive ion separator (RAISOR) 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.

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

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

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

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

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

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

Particle physics

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

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

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

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

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

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

We also play key roles in the construction of Fermilab's muon-to-electron-conversion experiment, in parallel with our work on providing the most precise magnetic field map for the muon g-2 experiment. For Fermilab's Long-Baseline Neutrino Facility/Deep Underground Neutrino Experiment (LBNF/DUNE), we are, among other things, the lead institution for design and engineering of the high-voltage system and for production and installation of the cathode-plane assemblies for the DUNE Far-Detector. We have delivered a half-wave cryomodule for Fermilab's Proton Improvement Plan-II project, which aims to produce the most intense high-energy neutrino beam for LBNF/DUNE.

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

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

Systems engineering

We bring together multiple engineering disciplines to integrate scientific discoveries into technological solutions to national challenges. Through systems engineering research, we drive improvements in the reliability and efficiency of energy-distribution and transportation systems, in environmental sustainability, in economic competitiveness, and in energy justice.

Using Argonne's specialized experimental facilities, systems engineering expertise, and analytical tools, we advance understanding of complex systems such as urban environments, communications, transportation, critical infrastructure, and other large-scale systems. Our work draws on Argonne's core capabilities in decision science and nuclear energy and uses the ALCF for advanced modeling and the APS for characterization of advanced materials for energy systems.

We develop advanced analytical and computational tools, including artificial intelligence and machine learning, to drive engineering improvements in our nation's critical infrastructure in partnership with industry, academia, and government agencies. Argonne's electric grid research focuses on improving the grid's reliability, resilience, affordability, and sustainability. This work builds on our strengths in power systems analysis, cross-sectoral analysis and economics, and emergency readiness and response analysis. Our portfolio of system engineering methods also enables us to model security, risk, and resilience for critical infrastructure systems beyond the electric grid and evaluate their increasingly complex interdependencies.

For example, we apply our broad energy systems perspective to:

- Improve understanding of the impacts of energy policies on electricity markets, the value of nuclear flexibility for grid integration of renewables, and the role of enhanced wind power forecasting in power system operations
- Advance energy storage through our leadership of Li-Bridge, the public private partnership focused on creating a U.S.-based ecosystem for lithium battery manufacturing, supply chains, and recycling

We also lead efforts to use "system of systems" analyses to quantify system interdependencies beyond critical infrastructure. For example:

- Our SMART (Systems and Modeling for Accelerated Research in Transportation) Mobility workflow allows the simultaneous assessment of multiple metrics for advanced transportation technologies, including mobility, energy use, emissions, cost, and energy and environmental justice.
- Our BEnefit ANalysis (BEAN) tool enables stakeholders to quantify the impact of individual component technology choices on the full lifecycle cost of light-duty passenger cars and commercial vehicles.

We are widely recognized for our long-standing leadership in applying systems engineering to advanced transportation systems. Examples of the goals of Argonne's current work in transportation systems are to:

- Improve the cost-effectiveness of hydrogen technologies such as automotive fuel cells and hydrogen storage systems, including production, transmission, and dehydrogenation of hydrogen carriers
- Quantify the energy consumption, performance, and cost impacts of millions of propulsion and vehicle technologies, using our Autonomie simulation tool and experimental validation at our Advanced Mobility Technology Laboratory
- Develop sustainable aviation fuels, electrical aviation technologies, and tools to evaluate aviation performance requirements, such as our Aeronomie tool that simulates energy consumption and performance in planes and drones
- Advance vehicle electrification and grid integration at the Argonne EV-Smart Grid Interoperability Center
- Perform lifecycle analysis of the energy, emissions, and water use impacts of advanced vehicle technologies, using our Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies (GREET) model

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

Science Strategy for the Future / Major Initiatives

Throughout Argonne's history, our research capabilities have grown to enhance our service to science and society. Our strategy for the future charts critical new directions in that service. We will execute this strategy through our major initiatives, core research programs, and the multi-institution partnerships we lead. Our initiatives will extend our four signature contributions to science and technology, as shown in the figure below Argonne's portfolio of initiatives has evolved over the last year and now includes nine efforts:

- Three major initiatives -- in **hard X-ray sciences, artificial intelligence (AI) for science,** and **autonomous discovery --** that are building a powerful suite of capabilities in our research facilities and driving progress across our entire science and technology enterprise
- Six major and emerging initiatives that position Argonne for greater impact in discovery science and for expanded contributions to global security challenges in areas ranging from physical and cyber infrastructure to supply chains to human health. Two of these initiatives also build our capabilities to deliver energy and climate solutions.
    - Two initiatives, in **climate action** and **clean energy and sustainability** – that represent a reshaping of our FY21 initiatives in these areas

- Two continuing initiatives in **quantum information science** and **radioisotope discovery**
- An initiative in **detection and imaging of signatures** with a new global security component and continuation of detector development work that began under our “universe as our laboratory” (ULab) initiative; other ULab components have transitioned to sponsor funding
- A new emerging initiative in **microelectronics**

Together, these initiatives represent bold steps in our ongoing efforts to expand our scientific leadership and impact. Our initiatives both draw on and contribute to one another. We are investing internal resources to advance them and identifying opportunities for direct funding from DOE, other government sponsors, and the private sector. UChicago Argonne, LLC, will continue to support our strategy through seed funding of new research directions.

We remain committed to the vision we expressed in our FY21 Annual Laboratory Plan: Revolutionizing the conduct of research by bringing together massive computational power, modeling, AI, machine learning (ML), robotics, and advanced characterization methods. Six DOE user facilities – the first five sponsored by the Office of Science and the sixth by the Office of Nuclear Energy -- are integral to our overall strategy:

- APS: Advanced Photon Source
- ALCF: Argonne Leadership Computing Facility
- ATLAS: Argonne Tandem Linac Accelerator System
- ARM (Atmospheric Radiation Measurement) User Facility observatories in the southern Great Plains and southeastern U.S.
- CNM: Center for Nanoscale Materials
- IVEM: Intermediate Voltage Electron Microscope

Together with our rich and diversified research expertise, our user facilities position us for continued leadership in expanding human knowledge and taking on the nation’s energy, climate, and security challenges.

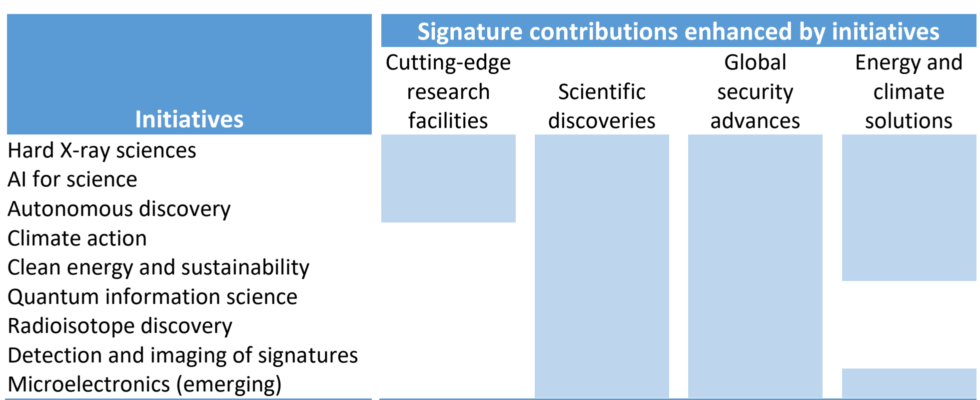


Figure: Relationships of research initiatives to Argonne’s signature contributions

Infrastructure

Argonne Facilities and Infrastructure

Argonne's campus in Lemont, Illinois, a suburb of Chicago, is stewarded by DOE/SC. The average age of Argonne-operated facilities and infrastructure is 50 years, with 57% of the buildings being more than 50 years old. Our facilities are roughly 86% occupied.

In addition to buildings operated by Argonne, our campus includes the Howard T. Ricketts Regional Biocontainment Laboratory, operated by UChicago, and the Theory and Computing Sciences Building, a privately operated building in which we lease space. In FY21, we entered into a new lease of 18,000 sq ft of space near our main campus to support the Radiological Assistance Program. We also continue to lease or license off-campus space for other purposes, such as the APS Upgrade and the work we carry out in Chicago and Washington, D.C.

We reduce operational risks by focusing investments on substandard support infrastructure and utilities, which account for most of our deferred maintenance (DM). Despite steady investments in infrastructure, we carried $109 million in DM costs in FY20 and $110 million in FY21. In FY20, we completed a full five-year cycle of Condition Assessment Surveys (CAS) for all of our facilities. We expect to begin seeing a reduction in DM for FY22 compared to FY21, because of targeted investments aligned with our campus strategy.

Meaningful, large-scale investments such as the Argonne Utilities Upgrade (AU2) project are crucial to our strategy for significantly reducing DM. Further, by executing Argonne's Excess Facilities Plan and reinvesting the savings associated with nuclear facility and waste reductions, we could decrease current and future DM by an estimated 98%. We identify these risk-reduction measures in our ten-year campus modernization plan, *Facility and Infrastructure Strategic Investment Plan*, which aligns with the Annual Laboratory Plan and details our intended facility operations funding portfolio and future campus vision.

Campus Strategy

Overview of 10-year modernization plan

Our vision for the future is driven by a foundational goal of resilient, sustainable facilities and infrastructure to enable mission readiness during any operational circumstance, while supporting federal goals for net-zero carbon emissions ("net-zero"). The 10-year modernization plan establishes a roadmap for achieving this vision, with investments aligned to support key research program drivers and position Argonne to prepare for, adapt to, withstand, and recover rapidly from events that affect our facilities and infrastructure.

We saw the positive impact of our infrastructure planning during the COVID-19 pandemic, as we smoothly transitioned from minimum safe operations in March 2020 to limited operations in June 2020 and continued construction projects without interruption. The unprecedented levels of telecommuting by our workforce during the COVID-19 pandemic led us to investigate the interest in and potential campus impacts of long-term telework. Through Laboratory-wide preference surveys and working groups, we identified a few office buildings in which to explore more-flexible workspaces when our workforce returned. When Argonne reopened to full capacity in March 2022, we piloted different workstation options to accommodate our hybrid workforce. For example, one-day reservable desks and offices were created within existing space in primary office use buildings.

The reduction in daily, on-site work creates a need to identify modern space planning opportunities within buildings and further evaluate vacant and inadequate facilities for shutdown, removal, or reuse. The Argonne 2050 vision, completed just before the pandemic, calls for facilities to operate at net-zero carbon emissions and for flexible facilities suited for in-person and remote workers. Our 10-year modernization plan further explores these emerging workforce trends. Planned building renovations will provide collaborative spaces and technology to support the hybrid work experience.

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

Our resilience planning will establish campus-specific performance goals for our infrastructure portfolio and mitigate gaps in performance and event recovery time with planned investments to prepare for a climate-resilient future. We are investing in artificial intelligence (AI) and machine learning (ML) to drive resilience by optimizing and automating utility, facility, and maintenance operations where feasible. This investment will help us reduce DM by making the most effective use of limited resources for maintenance. Execution of the 10-year modernization plan will contribute to our sustainable and resilient campus of the future. That plan provides a strategy to reduce DM while improving the resilience of facilities and infrastructure.

Our integrated campus sustainability strategy is described in Sec. 6.4. We intend to build on our sustainability accomplishments to date to move Argonne toward net-zero carbon emissions in alignment with the federal sustainability plan.

To meet Argonne's science strategy and support foundational investments, we take an integrated planning approach to establish a comprehensive portfolio of facility needs, align necessary investments, and complete projects within specific timeframes. Our 10-year infrastructure investment plan includes estimated total capital investments in buildings and utility systems across the Argonne campus of $978 million between FY22 and FY33, consisting of:

- $304 million in Argonne indirect funds
- $375 million in DOE funds (line items, program funds, scientific laboratories infrastructure [SLI], and general plant projects [GPP])
- $184 million in DOE/EM clean-up funds
- $115 million in State of Illinois funding

We will also maintain our robust operations maintenance and repair program with planned spending of $659 million during that period.

Site Sustainability Plan Summary

As noted in Argonne's annual site sustainability plan, our sustainability program is an integral part of our campus strategy, leading efforts to meet DOE's sustainability and resilience goals. We realigned our sustainability plan and program over the last year to address key federal sustainability requirements: the Energy Act of 2020, Guiding Principles for Sustainable Federal Buildings 2020, Executive Order 14008 - Tackling the Climate Crisis at Home and Abroad, and Executive Order 14057 - Catalyzing Clean Energy Industries and Jobs through Federal Sustainability. We are taking a Laboratory-wide approach to reduce greenhouse gas (GHG) emissions and improve resilience. We have incorporated these goals into our long-range plans while also dramatically increasing our near-term efforts for energy-reducing facility and infrastructure renovations, green fleet management, and sustainable product acquisitions in commercial contracts and construction.

We developed a strategy for achieving net-zero carbon emissions to meet federal goals and identified the key associated, necessary near-term and long-term activities. Leveraging our digital twin (a computer model of energy use by our buildings and utilities), we determined that 34% of our building emissions reduction will come from deep energy retrofits of heating and cooling systems, with seven facilities having the largest potential for energy savings. As noted in Section 6.2, we propose a new SLI-GPP project, under our ongoing Smart Labs Assessment Program, to enable deep energy retrofits in Buildings 202 and 203 to optimize the heating and cooling systems. At Building 362, the Smart Labs Energy Retrofit project will complement Laboratory internal funding used to modernize office and collaboration space in that building. The Smart Labs Energy Retrofit project for the three buildings will require $12 million in SLI-GPP support in FY23-24, which would result in an estimated reduction of 5,000 metric tons of carbon dioxide equivalent ($MTCO_2e$) per year.

Our net-zero carbon emissions strategy also includes waste-heat recovery systems to reduce campus heating load on the central steam plant, which currently uses natural gas and represents 28% of our carbon emissions. We propose two new SLI-GPP projects that would install waste-heat recovery systems, based on conceptual designs completed in FY20, for the 200 and 400 Areas of the campus, at a cost of $3.8 million in FY23 and $6.9 million in FY24. The 400 Area system would save about $240,000 per year in energy costs and provide nearly 55% of the annual APS heating load, reducing our carbon emissions 24% below current levels, or 1,416 $MTCO_2e$ per year. The 200 Area system would support Buildings 223, 241, and 242, resulting in $250,000 in annual energy savings and a 36% reduction in carbon emissions of 1,364 $MTCO_2e$ from current emission levels.

Over the next year, we will develop an implementation plan that outlines the sequence of activities and funding needed to successfully carry out our net-zero strategy, beyond the three GPP-SLI projects at $42.3 million already described in this plan. Argonne's diverse building stock, energy-intensive research facilities, and central utility systems, all within a three-square-mile secure campus, provide an ideal setting to pilot local decarbonization solutions and serve as a model for place-based solutions.

Our sustainability efforts reach every corner of the campus. FY21 accomplishments included the following:

- *Increased resilience with project planning and implementation*. We launched a formal resilience planning effort leveraging technical assistance and support from the DOE/EERE Federal Energy Management Program and Pacific Northwest National Laboratory. We also made significant progress on key infrastructure projects that support resilience, including the ECDC Project ($60 million, SLI) and Site Chilled Water Capacity Upgrades ($5.3 million, IGPP).
- *Improved implementation of Guiding Principles (GPs) for Sustainable Federal Buildings.* We developed a comprehensive tool to evaluate and track progress for meeting GPs within new construction, major renovations, and existing buildings, incorporating best practices with input from the DOE complex-wide sustainability and environmental subgroup of the safety working group of the Energy Facility Contractors Group (EFCOG).
- *Reduced cost of operating and maintaining facilities.* We completed 12 energy- and water-savings projects, adding $166,000 in annual savings to Argonne's portfolio of internally funded efficiency projects. We continue to use energy-savings performance contracts (ESPCs) to improve infrastructure efficiency and resilience, with ESPC payments totaling $3.9 million in FY21. Efficiency measures were also incorporated into Argonne-funded modernization, maintenance, and repair projects. We provided a total of $5.4 million in FY21 for sustainability projects.

- *Completed maintenance and planning for electric vehicles*. We completed maintenance on our electric vehicle (EV) charging equipment, which includes 29 Level 2 (240-volt) and two quick charge (500-volt) stations. We also completed a 10-year modernization plan to upgrade and expand our EV charging stations to meet anticipated growth for fleet vehicles and employee vehicle charging.
- *Recognized for sustainability excellence.* DOE recognized Argonne's Energy and Water Reinvest Program with a Sustainability Award in the Outstanding Sustainability Program/Project category. Since the program's inception in 2008, Argonne has implemented more than $10 million of energy and water conservation projects using savings generated from completed projects.

Argonne's sustainability program plays an integral role in our AI-Ops initiative. We are using operational-efficiency-software analytic tools to identify facility system improvements and predict maintenance needs and savings achieved from completed efficiency projects. Our 10-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 Assessment Program. Next steps include developing machine-learning algorithms and leveraging other data to automate system optimization and maintenance efforts. Our AI-Ops initiative will improve system resilience and support long-term sustainment of our building efficiency investments.

BROOKHAVEN NATIONAL LABORATORY

Lab-at-a-Glance

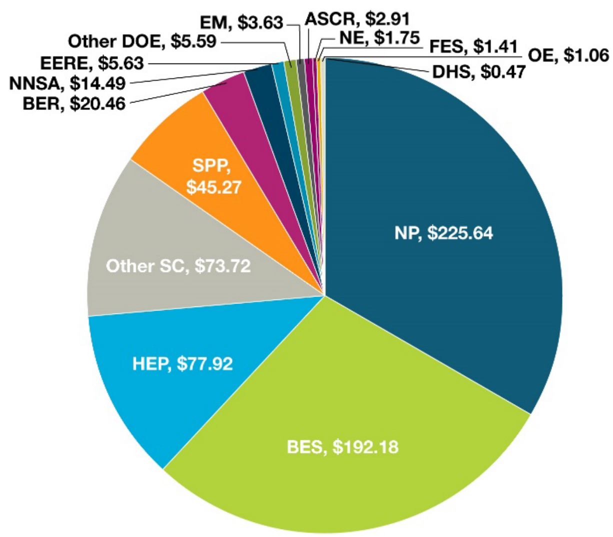
Location: Upton, New York
Type: Multi-program Laboratory
Contractor: Brookhaven Science Associates
Site Office: Brookhaven Site Office
Website: www.bnl.gov

- **FY 2021 Lab Operating Costs:** $672.1 million
- **FY 2021 DOE/NNSA Costs:** $626.4 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $45.3 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 6.8%
- **FY 2021 DHS Costs:** $0.5 million

Physical Assets:
- 5,322 acres and 314 buildings
- 4.8 million GSF in buildings
- Replacement Plant Value: $6.13 B
- 195,102 GSF in 28 Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:
- 2,609 Full Time Equivalent Employees (FTEs)
- 138 Joint Faculty
- 173 Postdoctoral Researchers
- 214 Graduate Student
- 266 Undergraduate Students
- 2,972 Facility Users
- 1,468 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Mission and Overview

Brookhaven National Lab (BNL) is a multi-program laboratory with seven Nobel Prize-winning discoveries and 75 years of pioneering research. Established in 1947, BNL brings unique strengths and capabilities to the DOE laboratory system.

The Lab's 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. BNL carries out its mission safely, securely, and environmentally responsibly, with a commitment to diversity, equity, and inclusion, and with the cooperation and involvement of local, state, national, and international communities.

As a U.S. Department of Energy (DOE) Office of Science laboratory, BNL has a strong focus on fundamental science. Included among the challenges the Lab is taking on in the next ten years are: uncovering the structure of visible matter in nuclear physics; helping enable a net-zero U.S. economy in clean energy and climate; enabling the quantum information science revolution; integrating artificial intelligence into all the Lab's facilities for discovery science; helping ensure the Nation's isotope supply; continuing to deliver accelerator science and technology for the Nation's future; and continuing to understand the origins of space and time in high energy physics. These initiatives are enabled by BNL's unique suite of powerful facilities and capabilities, and by its remarkable staff. BNL's facilities serve DOE's basic research needs and reflect BNL/DOE stewardship of national research infrastructure critical for university, industry, and government researchers. Despite the pandemic, they all continued to operate in FY 2021, serving close to 3000 users in FY 2021.

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

Core Capabilities

Fifteen existing and two emerging core technical capabilities underpin all activities at Brookhaven National Laboratory. 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 chemical, materials, biological, environmental, and data sciences with applications to today's problems; in developing and operating major user facilities; and in targeted applications in national security. These core capabilities enable BNL to deliver transformative science and technology that is relevant to the Department of Energy (DOE)/Department of Homeland Security (DHS) missions.

BNL has updated and condensed its core capabilities to reflect recent efforts in each capability area. The revisions are not major changes in focus. In FY 2020, BNL was assigned two new core capabilities in Computational Science and Applied Mathematics that were previously "emerging." Last year, BNL proposed two additional emerging core capabilities in Nuclear Engineering and in Power Systems and Electrical Engineering. BNL still considers both as "emerging."

Accelerator Science and Technology

BNL has been a center for accelerator science and technology development since the construction of the Cosmotron in 1948 to the current project to deploy the next cutting-edge capability for nuclear physics, the Electron-Ion Collider (EIC). The Laboratory operates three DOE Office of Science User Facilities based on its accelerator capabilities – the Relativistic Heavy Ion collider (RHIC), the National Synchrotron Light Source II (NSLS-II), and the Accelerator Test Facility (ATF) – and several smaller accelerators for other users and applications. With this portfolio, BNL has expertise in electron and hadron beams, and the associated technologies, over wide parameter ranges. Core areas of expertise include the design and construction of magnets (from permanent to superconducting), including the unique direct-wind technology for complex field profiles developed in the Magnet Division; high-intensity high-brightness electron and hadron beam sources (unpolarized and polarized); high-power mid- and long-wave infrared laser systems; development of radio frequency (RF) and superconducting RF components and systems; beam instrumentation; beam vacuum systems (including coating capabilities); power supply systems; cryogenic systems; and control systems. Expertise in beam dynamics ranges from low-emittance beams at NSLS-II that produce some of the brightest X-ray beams in the world, to the unique electron and laser interactions at the ATF, to multiple hadron beam cooling techniques implemented in RHIC. This expertise drives critical advances for accelerator-based science in the U.S. and around the world. The most important accelerator resource at BNL, given its wide range of accelerator capabilities, is a talented and engaged staff that can support the research and capability needs for the nation. DOE support for BNL's core accelerator capabilities comes from the Offices of Nuclear Physics (NP), Basic Energy Sciences (BES), High Energy Physics (HEP), and Accelerator R&D and Production (ARDAP), and Laboratory Discretionary Funds.

Advanced Computer Science, Visualization & Data

BNL has long-standing research, development, and operational programs in advanced computer and data science methods, applied mathematics, algorithms, tools, and infrastructures — particularly in support of experimental facilities - making it one of the largest data science Labs in the DOE complex. Scientists have 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., the Exascale Computing Project (ECP) ExaLearn, the Office of Advanced Scientific Computing Research (ASCR)-funded extreme scale spatio-temporal learning, and the Scientific Discovery through Advanced Computing (SciDAC) Institute for Computer Science and Data - called RAPIDS); Objective-Driven Data Reduction for Scientific Workflows; and 5G-enabled Reliable and Decentralized IoT Framework with Blockchain. The technologies developed are applied to projects in other DOE offices, such as the Office of Biological and Environmental Research (BER) RadBio, and the BES Automated Sorting of High Repetition Rate Coherent Diffraction Data from X-ray Free Electron Lasers. This program is complemented by research into AI explainability and reproducibility and supported by research into programming models (e.g., ECP SOLLVE), runtime systems for ML, and new performance portability approaches that provide a capability to enable the effective use of novel architectures. Advanced workflow management tool concepts (ECP ExaWorks) are used to create high throughput workflows that can effectively leverage Exascale systems in projects, such as ECP CANDLE and ExaLearn, and the BER National Virtual Biotechnology Laboratory project Medical Therapeutics. The research is supported by a new state-of-the-art data center, which began operation in FY 2021. BNL operates one of the top ten archives in the world, with over 220 PB of actively managed data and 1.1 EB analyzed in 2021. Data traffic has reached up to 180 PB/year. The primary sources of funding are from ASCR, HEP, NP, BES, BER, the Office of Electricity (OE), the Office of Energy Efficiency and Renewable Energy (EERE), the National Nuclear Security Administration (NNSA), New York State, Other Government Agencies (OGA), and Laboratory Discretionary Funds.

Applied Materials Science and Engineering

BNL capabilities in applied materials encompass a broad range of activities related to energy storage and growing capabilities for studies of materials in extreme environments for nuclear applications. Capabilities in energy storage include materials synthesis, characterization and functional electrochemical evaluation, high energy density cell technology, evaluation of thermal stability and functional limits of battery materials, fundamental studies of charge and discharge mechanisms and the associated material-structure evolution. BNL has established expertise and capabilities for in situ characterization of energy storage materials by X-ray methods and electron microscopy, including new approaches for spatio-temporal measurements of mechanisms with enhanced resolution under operando conditions. BNL is applying its expertise and capabilities as a partner in the Battery 500 consortium. BNL continues to build its portfolio of electric grid research projects and has become an important player in performing research to enable grid modernization. BNL's research focuses on the deployment and grid integration of renewable energy systems and the development of new technologies. BNL has capabilities to study materials in extreme environments for nuclear applications. This includes a specialized robotic system at NSLS-II for the rapid characterization of radioactive materials, a unique suite of environmental cells for the in situ characterization of reactor materials and molten salt samples that are highly corrosive, and X-ray diffraction computed tomography, which enables three-dimensional (3D) imaging of the microstructure of engineering-scale samples. The 200 MeV proton beam of the Linac and the Brookhaven Linac Isotope Producer (BLIP) target facility allow for the investigation radiation damage by of beam collimators, beam windows, and high-power targets, and have been used by the RaDIATE collaboration. The primary sources of funding are: BES, the EERE Vehicle Technologies Program, OE, the Office of Nuclear Energy (NE), New York State, and Laboratory Discretionary Funds.

Applied Mathematics

Over BNL's long history, its mathematics research traditionally has focused on areas distinctly relevant to HEP, NP, synchrotron science (BES), and accelerator physics. Today BNL is emphasizing: 1) optimal experimental design under uncertainty and broader optimization of complex systems under uncertainty. The Lab is a partner in ASCR's Mathematical Multifaceted Integrated Capabilities Center, called Advances in Experimental Design, Optimal Control, and Learning for Uncertain Complex Systems (AEOLUS) and in the BER Optimal Experimental Design of Biological Systems project, and with the Center for Functional Nanomaterials (CFN) and NSLS-II in a Laboratory Directed Research and Development (LDRD) project, which develops new optimal experimental design concepts in autonomous systems; 2) multiscale modeling that addresses the bridging of scales and integration of data from experiments/observations and from simulations. Initial focus areas are nuclear physics, climate, and chemical processes; and 3) applied math for scalable AI and ML that will provide key foundations needed for BNL's AI research program. An added focus involves exploring how to achieve AI explainability through foundational applied mathematics work. BNL's new ASCR-funded Noether Fellowship in Applied Mathematics supports work in optimization and uncertainty quantification in rational therapeutics design. Additional work is being carried out on the development of numerical methods for solving functional renormalization group equations for strongly coupled physics problems. Support comes primarily from ASCR, BER, New York State, and Laboratory Discretionary Funds.

Biological Systems Science

The goal of BNL's program is to develop a systems-level understanding of complex biological processes relevant to the DOE mission with respect to energy and the environment. This involves generating and testing hypotheses using approaches that include genomics, molecular biology, biochemistry, structural biology, computation, imaging, and biosystems design. This work will lay the foundation for desired manipulations of growth rates, biomass accumulation, resistance to stresses, and the accumulation in organisms relevant to the BER mission of desired products that constitute feedstocks for bioenergy and bioproduct production. This program is synergistic with programs in physical biosciences (funded by BES, Core Capability (CC) 6). BNL's Quantitative Plant Science Initiative (QPSI) Science Focus Area addresses the grand challenge of "Enabling predictive biology" by accelerating the discovery of gene and protein function in metal homeostasis with present focus on micronutrient acquisition, transfer, and utilization. BNL also contributes to three Bioenergy Research Centers - the Center for Advanced Bioenergy and Bioproducts Innovation (CABBI), the Joint BioEnergy Institute (JBEI), and the Center for Bioenergy Innovation (CBI). Efforts within CABBI are directed at engineering the accumulation of energy-dense oils in perennial grass crops; those in JBEI and CBI are directed at reducing or modifying lignin in biomass to optimize their saccharification efficiency. BNL also participates in three Biosystem Design projects undertaking foundational studies to facilitate the engineering of terrestrial and aquatic species as sources of renewable oil. Biological Systems Science research at BNL integrates with and contributes to the expansion of biomolecular characterization and imaging user facilities, including capabilities at NSLS-II and a cryo-Electron Microscopy (EM) facility. BNL's biological systems science activities are supported by: BER, the Joint Genome Institute Community Science Programs, the Environmental Molecular Sciences Laboratory's user program, Facilities Integrating Collaborations for User Science (aka FICUS), ASCR, the NNSA/Advanced Scientific Computing ECP, New York State, the National Institutes of Health (NIH), a Cooperative Research and Development Agreement (CRADA), and Laboratory Discretionary Funds.

Chemical and Molecular Science

BNL's chemical and molecular sciences conduct fundamental research to support rational design of chemical and biological processes for DOE mission goals. Sustainable energy research is focused 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 for application in future nuclear energy systems. The research utilizes BNL user facilities (NSLS-II and CFN) and the divisional Accelerator Center for Energy Research (ACER).

BNL expertise in thermal heterogeneous catalysis is being applied to improve understanding of catalysts for conversion of difficult-to-activate small molecule feedstocks like CO_2 to synthesize fuels and chemical intermediates. The research, including that through the Synchrotron Catalysis Consortium, combines operando studies of powder catalysts, in situ studies of model nanocatalysts, both at NSLS-II and CFN, and quantum chemical computation. 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. BNL's program in solar photochemistry has 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. The radiation chemistry program develops and applies advanced pulse radiolysis capabilities at ACER, which is also a foundation for growing BNL capabilities in chemistry of extreme environments. The Molten Salts in Extreme Environments Energy Frontier Research Center (EFRC) builds on these. Fundamental chemistry and physical biosciences programs are funded by BES and Laboratory Discretionary Funds.

Chemical Engineering

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

Climate Change Sciences and Atmospheric Science

BNL's atmospheric and terrestrial ecosystem science efforts develop process-level insight into the role of aerosols, clouds, and ecosystems in a changing climate through its long-standing expertise in measurement science and climate theory. BNL researchers are advancing the understanding of interactions along the aerosol-cloud-precipitation continuum and their impacts on climate for the Atmospheric Systems Research (ASR) Program through a joint Science Focus Area with Argonne National Laboratory "Process-level AdvancementS of Climate through Cloud and Aerosol Lifecycle Studies." Scientific staff support the Atmospheric Radiation Measurement (ARM) User Facility and data archive as instrument mentors and as data science specialists and contribute to the design and interpretation of ARM measurements. Ecosystem understanding is being advanced through participation in the Next Generation Ecosystem Experiments in the Arctic and Tropics under support from the Environmental System Science (ESS) Program. Climate modeling scientists support the Energy Exascale Earth System Model (E3SM) and the Large Eddy Simulation (LES) ARM Symbiotic Simulation and Observation (LASSO) project. As computing resources grow and models achieve higher resolution, observations must also push current resolution boundaries. BNL staff are bringing novel measurement methodologies, instrumentation, and Laboratory facilities to bear on this problem through collaborations with BNL's Instrumentation Division. In partnership with the Computational Science Initiative (CSI), BNL's climate scientists are building capabilities for very high-resolution and data-driven simulations of the atmosphere and climate that will be developed through the insights gained from new high-resolution measurements. BNL has developed new capabilities in support of BER's needs in environmental data analysis, development of innovative measurement platforms and instrumentation, uncertainty quantification, and high-resolution atmospheric modeling. Through the Center for Multiscale Applied Sensing (CMAS), BNL has also established a mobile remote-sensing platform to support research in characterization of renewable energy resources, urban system studies, and national security applications. The application of BNL's long-standing Perfluorocarbon Tracer (PFT) technology is also coordinated through CMAS and used to conduct urban dispersion studies. Funding comes from BER, EERE, DHS, and Laboratory Discretionary Funds with projects also supported by the New York Police Department, the New York State Energy Research and Development Authority (NYSERDA), the National Aeronautics and Space Administration (NASA), and the Defense Advanced Research Projects Agency (DARPA).

Computational Science

Computational science, both numerical modeling and data analytics, is essential to enabling advanced scientific discovery at BNL's facilities – RHIC and EIC (NP), the BLIP (Isotope R&D and Production); ATLAS and Belle II (HEP); the ATF (ARDAP); NSLS-II and CFN (BES); cryo-EM and ARM (BER) - and supporting science programs. Collaborations around numerical modeling applications benefit 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 Quantum Chromodynamics (QCD), computational chemistry (NWChemEx), and the HEP Center for Computational Excellence that supports the ATLAS and Deep Underground Neutrino Experiment (DUNE) experiments. 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. In collaboration with the Instrumentation Division, the Scientific Data and Computing Center (SDCC), and facilities such as NSLS-II, cryo-EM, and CFN, BNL's new Center for Advanced Technologies for Artificial Intelligence (CAT-AI) co-designs new experimental capabilities that integrate advanced imaging technologies with high powered edge computing devices and streaming ML and AI. New efforts will focus on the development of digital twins as part of the Discovery Science Driven by the Human-AI-Facility Integration (HAI-FI) initiative, where advanced modeling and simulation capabilities will be employed to help design, guide, and improve experimental setups and workflows. A digital twin that simulates the physical experiments will be able to respond to environmental changes quickly and learn from past experiments. This will require the integration of High Performance Computing and AI, as well as advanced mathematical modeling methods. The primary sources of funding come from ASCR, HEP, NP, BES, BER, New York State, OGA, EERE, OE, and Laboratory Discretionary Funds.

Condensed Matter Physics and Materials Science

BNL conducts frontier research in Condensed Matter Physics and Materials Science, focusing on new and improved complex, nanostructured, and correlated-electron materials. The research is increasingly focused on quantum materials for quantum information science, building on strengths in high T_c superconductivity and chiral materials. Ongoing research also addresses renewable energy, energy storage, and energy efficiency. Research is pursued 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), 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). OASIS capabilities have been applied to study strongly correlated cuprates and new research directions including 2D materials and heterostructures that can support topological excitations. Abhay Pasupathy now leads the OASIS effort. The Condensed Matter Physics and Materials Science groups are all engaged in NSLS-II activities, including developing new capabilities that have led several proposals for new NSLS-II beamlines. A new complementary ultrafast X-ray research program also focuses on unique science that can be performed at ultrafast X-ray Free Electron Laser facilities. The BNL MeV Ultrafast Electron Diffraction (UED) facility is in operation, which is complemented with a laser-free electron pulser device capable of “tabletop” UED. BNL’s Center for Computational Design of Functional Strongly Correlated Materials and Theoretical Spectroscopy (COMSCOPE) develops 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. BES and Laboratory Discretionary Funds are the primary sources of funding for these ongoing efforts.

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

BNL’s large scale user facilities and advanced instrumentation are extending the frontiers of knowledge and enabling studies of important scientific challenges. In FY 2021, BNL served nearly 3000 users at its DOE designated user facilities, RHIC, NSLS-II, CFN, and the ATF and at the NASA Space Radiation Laboratory (NSRL), the Tandems, RHIC-ATLAS Computing Facility (RACF) and U.S. ATLAS Analysis Support Center. BNL continues to invest in detector and accelerator upgrades for its community of more than 900 **RHIC** users. **RHIC** completed Runs 2021 and 2022 with the upgraded STAR detector and reached the lowest Au-Au collision energy enabled by the Low-Energy RHIC electron Cooling. The sPHENIX upgrade, which will enable precision measurements on hard probes, is nearly complete. BNL will host the **EIC**, a facility that builds on **RHIC**, that will provide high-energy electron-ion collisions for studies of cold nuclear matter at extreme gluon densities and precision measurements of the structure and properties of protons and complex nuclei at the quark-gluon level. **NSLS-II** has strengths in imaging and dynamics and world-leading R&D programs in nano-focusing optics and nano-precision engineering. **NSLS-II** hosted over 1000 users in FY 2021. **NSLS-II** is executing the NEXT-II beamline project and proposed NEXT-III to complement the existing suite and provide needed capabilities in high throughput scattering, spectroscopy, and imaging. The **CFN** supported the research of 571 unique users in FY 2021. **CFN** continues to upgrade its portfolio to maintain leading-edge status, in instruments for synthesis and characterization of nanomaterials created by assembly, and tools for in situ and operando nanoscience. BNL leads the Nanoscale Science Research Centers (NSRC)-Recap project. The **ATF** supports a unique suite of advanced accelerator and laser experiments as part of the Accelerator Stewardship Program managed by the Office of Accelerator R&D and Production. BNL makes key contributions to i**nternational** facilities – the **Large Hadron Collider (LHC)**, **SuperKEKB**, and future facilities such as a **Long Baseline Neutrino Facility (LBNF)/DUNE** and the **Rubin Observatory**. BNL plays a significant role in the globally deployed **ARM** User Facility for climate research, which serves more than 1000 users annually. BNL scientists lead the five-year **ARM** deployment to the Southeast U.S. BNL's new **cryo-EM facility** is up and running as a non-designated user facility, with funding from BER, supporting BER users and the General user community, including BES-funded researchers. BNL hosts the **Long Island Solar Farm (LISF)**, a privately owned 32-megawatt solar photovoltaic power plant. BNL's **Northeast Solar Energy Research Center (NSERC)** enables field tests of solar technologies under actual northeastern weather conditions. From concept through construction, the **Instrumentation Division** makes major contributions to instruments and experiments at BNL and other accelerator- and reactor-based facilities worldwide. Major sources of funding are: BES, NP, HEP, BER, NASA, New York State, NIH, and BNL Discretionary Funds.

Nuclear & Radio Chemistry

BNL's nuclear science programs span the range from applications in medicine to national security. The BLIP uses the 200 MeV Linac and target processing facilities for the production of isotopes not commercially available, mostly for nuclear medicine. BNL participates in a collaboration with Los Alamos National Laboratory and Oak Ridge National Laboratory to produce Ac-225 in sufficient quantities to support clinical trials for cancer. Ac-225 is an alpha emitter that has demonstrated reduced toxicity and improved cure rates in clinical trials. Work is ongoing to refurbish and upgrade facilities, including doubling of the 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. BNL hosts the Nuclear and Radiochemistry summer school that provides twelve undergraduates with hands-on experience. BNL's expertise has led to a patent for a Rapid Cycling Medical Synchrotron and for low-mass beam delivery gantries, technologies for the next generation of proton- and ion-based cancer therapy. The effects of ionizing radiation on living systems are studied at NSRL, a flagship international user facility supported by NASA. BNL is home to the NNSA Radiological Assistance Program's Region 1 team as well as a United States Agency for International Development (USAID)-funded international radiological/nuclear crisis operations and consequence-management events response capability. BNL supports NNSA's Defense Nuclear Nonproliferation programs by using its unique facilities, such as NSLS-II, and expertise in instrument development, chemistry, data science, safeguards, and nuclear data analysis. 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. Brookhaven also develops curricula and provides safeguards implementation training for international IAEA inspectors and officials. Funding comes from sources that include NP, Isotope R&D and Production (IP), BES, BER, the Department of State, NASA, NNSA, DHS, and a CRADA.

Nuclear Physics

BNL conducts pioneering explorations of the most fundamental aspects of matter governed by the strong nuclear force. RHIC is a unique facility allowing for heavy ion collisions and polarized proton-proton collisions. RHIC experiments discovered that quark-gluon plasma, which existed microseconds after the Big Bang, is a nearly perfect liquid and gluons' spins have a nonnegligible role in making up the proton spin. The success of the RHIC program benefits from BNL's strong program of advanced accelerator R&D, and the support of the BNL Physics Department and the Instrumentation Division. The successful completion of the RHIC science mission relies on the recently completed upgrades – RHIC electron cooling, STAR iTPC, STAR forward upgrade, and the soon-to-be-completed sPHENIX. As a DOE user facility, RHIC has more than 900 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 continue to contribute to the success of the RHIC program, including BNL's role as the lead institution in two Topical Collaborations in Nuclear Theory. Experimental, theoretical, computational research and nuclear science workforce development are enhanced by the presence of the RIKEN BNL Research Center. BNL develops advanced software and computing facilities for applications in nuclear physics experiments and theory, including lattice QCD simulations. Key expertise has been developed in the management and processing of petabyte-scale data sets generated at high rates and distributed computing for analysis, facilitated by the RHIC Computing Facility, a component of BNL's SDCC. RHIC will be transformed into the EIC through the addition of an electron accelerator and storage ring. The EIC will facilitate a rich science program based on collisions of high-energy electrons with heavy ion and polarized proton beams to precisely image the quark-gluon structure of the proton and atomic nuclei. BNL and the Thomas Jefferson National Accelerator Facility are the two DOE host labs for the EIC project. BNL operates the National Nuclear Data Center (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 program also addresses gaps in the data, through targeted experimental studies and the use of theoretical models. Last year, there were over five million data retrievals from the NNDC websites. Support is provided by NP as well as RIKEN and Laboratory Discretionary Funds.

Particle Physics

BNL has key roles in developing and operating particle physics experiments that seek answers to seminal questions about the composition and evolution of the universe, i.e., understanding the source of the elementary particles' mass, the nature of dark matter and dark energy, and the origin of the matter-antimatter asymmetry in the universe. BNL's major activities 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 project and construction and testing of the high field quadrupole magnets for the LHC accelerator upgrade; leadership in neutrino oscillation experiments, including a leading role in the DUNE Technical Coordination and second module design and construction; leading roles in the short-baseline experiments at Fermi National Accelerator Laboratory (MicroBooNE, ICARUS, and the Short Baseline Near Detector); leading the U.S. Belle II experiment for the KEK Operations Program, including computing facilities; commissioning, and operations; data analysis of the Rubin Observatory cosmological survey; and design and construction of the Lunar Surface Electromagnetics Experiment (LuSEE) night program and coordination of its operations and science programs. 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 in distributed computing for data analysis. Development of new instrumentation technologies for elementary particles and data collection and storage systems provides the foundation for present and future particle physics experiments. These roles are enhanced by BNL high energy physics theory efforts and by BNL's leadership in advanced accelerator research and development, which is critical for the next generation of high energy physics experiments and accelerator facilities. Funding for this work comes from HEP, RIKEN, and Laboratory Discretionary Funds.

Systems Engineering and Integration

BNL designs, constructs, and operates large-scale facilities and advanced instrumentation to address some of the most challenging questions in fundamental science, applied science, and national security, underpinned by a highly trained, multidisciplinary, and internationally recognized workforce. Building on the highly successful construction of NSLS-II and its initial X-ray beam lines, high impact science is now being delivered at a world-leading level. State-of-the-art technologies integrated into NSLS-II include novel RF and X-ray beam position monitors; high heat-load front-end components; and novel X-ray optics and detectors. In addition, NSLS-II staff share their beamline and accelerator expertise with the Advanced Light Source, Advanced Photon Source, and Linear Coherent Light Source upgrade projects. Another example is the RHIC accelerator complex that includes the only collider in the U.S. Technologies developed and employed include high-intensity ion sources; high-power proton targets for medical isotopes; rapid cycling synchrotrons; advanced beam cooling; and superconducting accelerators to produce high luminosity ion and polarized proton collisions. The EIC requires strong systems engineering and integration, which includes all of the above as well as high intensity polarized electron beams. BNL developed noble liquid detectors and cold electronics, from concept to implementation, for particle physics experiments. R&D continues aimed at developing very large liquid argon Time Projection Chambers (TPC) for the DUNE experiment and the TPC for the proposed next Enriched Xenon Observatory (nEXO). Developments include complex combinations of cryogenics, power supplies, microelectronics, readout electronics, and computing. Further, BNL's nuclear energy experts conduct research in support of sustainment of the current nuclear reactor fleet as well as development of next-generation reactors through research on alternative fuel cycles, materials in extreme environments, nuclear data, and safeguards. BNL staff also analyze nuclear reactor performance and safety as well as fuel cycle designs for DOE, the Nuclear Regulatory Commission (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 BNL Discretionary Funds.

Nuclear Engineering (Emerging)

BNL's nuclear engineering capability encompasses three major areas: Materials for Nuclear Energy Applications, Nuclear Systems and Structural Analysis, and Nuclear Data. In the area of materials for nuclear energy applications, BNL researchers develop synchrotron characterization techniques explicitly for the investigation of materials for nuclear energy systems, including using robots for handling radioactive samples, X-ray diffraction tomography to investigate material degradation, and high temperature in situ experiments for the annealing, corrosion, and molten salts. BNL is developing designs for a new dedicated synchrotron facility, the Materials in a Radiation Environment (MRE) Facility, to provide the nuclear research community with a secure, separate, and shielded beamline at NSLS-II to examine radioactive materials. In the area of nuclear systems and structural analysis, BNL has experience with all phases of the design and assessment/evaluation of advanced nuclear systems, such as reactors and accelerator-driven-systems (ADS) and fuel cycles, resulting from decades of support to the NRC and the DOE. State-of-the-art NRC and DOE-developed computational tools are utilized for the full scope neutronics and thermal hydraulics analyses of reactor performance and safety characteristics. In the area of nuclear data, BNL hosts the National Nuclear Data Center (CC 13), which is also the lead unit of the USNDP and BNL chairs the Cross Section Evaluation Working Group (CSEWG). BNL's NNDC is a DOE Office of Science Public Reusable Research Data Resource. BNL's nuclear data research supports a variety of national and international efforts in reactor physics, the nuclear fuel cycle, defense, nuclear non-proliferation, and isotope production. The NNDC has decades of experience in performing high-precision gamma-ray spectroscopy experiments. U.S. major spectrometers Gammasphere and Gamma-Ray Energy Tracking In-beam Nuclear Array (known as GRETINA) as well as new dedicated in-house measuring capabilities are used to improve decay data relevant to isotope production, non-proliferation, and reactor applications. The programs within this core capability are funded by NE, NP, NNSA, NRC, and Laboratory Discretionary Funds.

Power Systems and Electrical Engineering (Emerging)

BNL focuses on research to advance the deployment and grid integration of renewable energy systems and the development of new technologies to enable the next generation smart grid. BNL has significant expertise in power system modeling and simulation, and in transmission and distribution system design, operation, and planning, that can be used to analyze the systems and determine their appropriate use as solutions for grid integration of renewable generation. BNL also has capabilities in the development of control algorithms that can be applied to the operation of energy storage systems for applications to renewable integration. BNL has developed a portfolio of grid modernization research projects and will continue to build capabilities in this area. Previous and ongoing R&D projects at BNL that are related to the research areas funded by the DOE Office of Electricity include the development of a probabilistic technique for sizing energy storage systems, development of probabilistic techniques for transmission system planning, formal analysis for dynamic stability assessment, and a deep learning based online platform for critical anomaly detection and emergency control to enhance grid reliability and resiliency. BNL has invested LDRD funds for investigation of the use of energy storage systems to improve grid inertial response that are broadening these efforts. As evidence of regional importance and interest, programs are also funded by New York State, including the evaluation of grid impacts from utility scale solar generation on sub-transmission and distribution systems and the use of Radar in real-time damage forecasting and response for restoration of electric utility systems. In addition to expanding its research portfolio, BNL will continue to pursue the establishment of the Center for Grid Innovation (CGI) on the BNL campus. This new facility will provide a venue for collaboration with New York stakeholders on grid modernization research, including energy storage systems and increasing the deployment of clean energy generation, including wind and solar. The CGI will enable simulation and validation of innovative new technologies to address the challenges for integrating renewables and energy storage systems on the grid and reduce the risk to utilities of deploying these new technologies. New York State, OE, and Laboratory Discretionary Funds are the primary sources of funding.

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

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

- Discovery Science and Technology to address national needs
    - Nuclear and particle physics to gain a deeper understanding of matter, energy, space, and time
    - Recognized strengths in advanced materials, catalysis, bioenergy, environmental systems, and climate to put the U.S. on a path to a net-zero economy.
    - Advanced computer science, applied math, data science, and computational science to transform scientific discovery at BNL's facilities and enhance its science programs
    - Advanced and emerging technology with demonstrated strengths in instrumentation, magnet, accelerator, and laser S&T

- Transformational user facilities that position the Laboratory and the Nation for continued leadership roles in science and technology. These facilities are enabled by advanced accelerator science and technology.
- Application of the results of BNL' s discovery science to address emerging opportunities, including clean energy solutions, isotopes, national security solutions, and national emergencies.

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

Infrastructure

Overview of Site Facilities and Infrastructure

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

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

At the end of FY 2021, there were 2,653 BNL staff assigned on site in 314 buildings totaling 4,795,149 square feet (sf) and 9,220 sf in 20 real property trailers. BNL does not lease any facilities and the average age of all non-excess buildings is 47.5 years with 60 buildings (712,241 sf) used by the Army during World War II (WW-II) 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 the 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 Science Laboratories Infrastructure (SLI) projects completed in 2013 and 2015, respectively. The Core Facility Revitalization (CFR) Project achieved beneficial occupancy in FY 2021.

The CFR project re-tasked 48,500 sf of underutilized space in FY 2019. In the last two years, over 90,000 sf of underutilized space was 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 (ISOMF), which will further reduce Inadequate space. At the end of FY 2021, there were 28 excess buildings and trailers, comprising 195,102 sf, and 28 buildings and trailers totaling 274,152 sf in Standby status.

Subject to availability of funds, the Office of Environmental Management (EM) will remain responsible for the decontamination and decommissioning (D&D) of contaminated excess facilities, including Building 491 (Brookhaven Medical Research Reactor (BMRR)), Building 701 (Brookhaven Graphite Research Reactor (BGRR)), and Building 750 (High Flux Beam Reactor (HFBR)) as identified in the EM-1 memorandum to SC-1 “EM Transfer Decisions for SC Excess Facilities and Materials,” dated February 20, 2009 and in accordance with the HFBR Record of Decision (ROD). On April 14, 2022, DOE was formally notified by the U.S. Environmental Protection Agency (USEPA) that the Final Closeout Report for the HFBR Stack Decommissioning and Demolition was deemed acceptable. This represents the completion of a major milestone in the ROD between the NY State Department of Environmental Conservation (NYSDEC), the USEPA, and DOE. The demolition of Office of Science (SC) asset Building 650 (known as the “Hot Laundry”) was funded in FY 2021 and demolition is complete. This demolition also represents the retirement of a significant Environment, Safety & Health (ES&H) risk at BNL. EM funded the removal of the Stack associated with the former BMRR outside of building 491, which will be completed in FY 2022.

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

Campus Strategy

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

The planned infrastructure investments will promote and support the scientific initiatives and the wide range of facilities that enable BNL’s core capabilities. Special emphasis is placed on projects “critical to sustain operations” while recognizing future projects “desirable to enhance mission readiness.” BNL recognizes that a commitment to a sustained overhead investment in both areas is critical to assure routine maintenance and infrastructure stewardship is effectively practiced.

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 and mission readiness through targeted investments in buildings and utility infrastructure
4. Ensure critical infrastructure and buildings are sustainable, energy efficient, and resilient against environmental and climate-change, and robust to endure severe weather conditions and events
5. Support the laboratory mission and growing population of scientific users through an innovative concept called “Discovery Park.”

Element 1 - Investment in Critical Core Buildings and Infrastructure

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

One of the most significant infrastructure issues facing the scientific organizations relates to computing and data management. Near-term computing needs are projected to quickly eclipse the existing computing infrastructure and the completion of the CFR project in FY 2022 provides a contemporary computing facility and infrastructure that will meet current Laboratory needs. This investment makes cost-effective use of existing infrastructure by repurposing most of Building 725 (the former NSLS). The facility was designed to accommodate BNL's future computing needs as they are realized. Provisions for the deployment of incremental power and cooling upgrades were considered in the initial planning and design of the facility and can be implemented with little to no disruption to on-going computing activities.

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

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 ISOMF, is proposed for an FY 2027 start.

In addition, significant World War II-era housing remains that impedes operations, reduces efficiency, and impacts employee morale, health, and safety. A New Net-Zero Guest Housing Facility project, to be constructed in Discovery Park, is proposed for an FY 2030 start.

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Element 2 – Optimizing the Campus Footprint

An important element of the overall infrastructure strategy is elimination of excess facilities and footprint reduction to realize operational efficiencies, improved facility safety, and improved utilization and quality of space. BNL is committed to reduce the Lab's building footprint by more than 5% over the planning period. The Infrastructure Investment Table and Integrated Facilities and Infrastructure (IFI) crosscut (Enclosure 4) indicate the annual overhead investments needed to eliminate existing or anticipated future non-contaminated excess facilities, albeit over an extended period, and the requests for direct DOE funding for the costlier contaminated facility projects. An FY 2026 request for direct funds to accelerate the removal of noncontaminated facilities is also included in the Table. Over the planning period, the BNL Demolition Plan estimates that ~322,215 sf of net excess space will be eliminated, the majority of which are WW-II-era buildings. However, an additional 250,000 sf could be eliminated with the assistance of direct funds, which are requested in the Investment Table.

To meet these infrastructure challenges, BNL has formulated a strategy to address the mission and operational needs based on the constraints and strengths of the various funding sources. Capital projects and other requested funding are shown in the Infrastructure Investment Table and indirect expensed projects, such as DMR, are reflected in funding plans shown on the IFI Crosscut. 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 based on mission need.

As part of the continuing consolidation planning to right size the campus, two buildings totaling 10,840 sf were demolished in FY 2020. In FY 2021, a multi-year project to demolish Building 197 (51,988 sf) was started and the demolition of Building 650 (6,453 sf) and Building 421 (5,977 sf) was completed.

Element 3 - Targeted Investment in Building and Utility Infrastructure

While BNL's utilities are currently reliable, they are aging and issues impacting reliability and capacity are increasing. In FY 2011, BNL completed a baseline study, which evaluated its utilities and recommended strategies to address critical needs. The study identified significant short-term needs confirming that the aging water, electric, chilled water, and steam distribution system components need replacement. Recapitalization resources to renew and replace BNL's utility infrastructure have been limited by historically tight operating budgets. In recent years, as the Laboratory growth strategy has begun to take effect, additional overhead resources were gradually provided to operating budgets. 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. Another project, completed in FY 2018, replaces the 28-year-old wood cooling tower at the CCWF. The CURP SLI line-item, which is underway, addresses replacement of one of the three 1,200 Ton electric centrifugal chillers, original to the central plant and beyond its useful life. The project also includes two critical potable water projects: one to rebuild Potable Water Well No. 12, completed in FY 2022, and another to replace the WWII-era 300,000-gallon elevated water storage tank with an upgraded 500,000-gallon tank, expected to be completed in FY 2023.

The aging utility distribution systems present additional utility needs. Sections of the central steam distribution system date back to the late 1940s. 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 by the CURE project.

Element 4 – Resiliency and Sustainability

BNL has been executing its resiliency and sustainability efforts through the execution of the Site Sustainability Plan. To enhance that effort, a cross-Lab team was established to focus on the climate impacts to critical infrastructure and to prioritize investments to increasing resiliency at these facilities.

The utility-related projects and 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 multi-pronged and does not solely rely on maintenance investment, which was 1.2% of Replacement Plant Value for 2021 for non-excess and non-OSF 3000 assets. Continuing to consolidate out of assets not worth maintaining, followed by cold and dark, and ultimately by their demolition is key to BNL's strategy. Continued space consolidation efforts will be enabled by renovation and alteration of underutilized buildings and through new proposed buildings, such as the SUSC and the proposed ISOMF, allowing a major consolidation from Inadequate WW-II-era buildings. There are also proposed GPP projects that would help jumpstart recapitalization of key mission critical building systems, such as HVAC, electrical, potable water piping, and roofing, in mission critical assets and through mission-enabling renovation of key laboratories.

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

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

The Discovery Park concept is a key component of BNL's infrastructure renewal plans and continues to make 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. Discovery Park includes two distinct districts; one for federally owned facilities, referred to as Upton Square, and the other for privately financed facilities. Upton Square currently includes the SUSC, proposed housing, and the proposed Northeast Center for Grid Innovation Center (CGI). The CGI will potentially be a New York State funded/DOE owned partnership facility as the initial focus of development. Initial occupancy of SUSC is planned in the FY 2024 timeframe.

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 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. BNL's projects have been prioritized to ensure they support mission critical infrastructure needs.

- **Science and User Support Center (SUSC)** (TEC $85.0, 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 serve as a magnet for further development. This building (see Figure) will enhance operational efficiency by consolidating approximately 200 BNL support division staff, currently dispersed in several buildings, into a single, modern office building meeting DOE sustainability goals. It will also enable further consolidation of other staff, ultimately allowing the demolition of ~43,000 sf of WW-II-era space with a combined backlog of maintenance and modernization needs of $7M. In addition to the efficiency gained by co-located staff, the facility's location at the BNL main entrance will enhance public access for education and commercial outreach for BNL outward facing organizations (such as Stakeholder and Community Relations, Human Resources, and the Guest, User, Visitor Center, among others), while supporting BNL core functions. A new visitor center, designed as a highly efficient one-stop user access portal, will be the front door of the SUSC structure and will enhance BNL's role as a major user facility laboratory. Scientific collaboration will also be enhanced through a new highly configurable and accessible conference center, the third major element of the SUSC facility. The project received CD-0 in 2016, CD-1 in 2018, and CD-2/3 in FY 2021. Notice to

Proceed construction mobilization was given 2/11/22 and construction 4/4/22. The CD-4 completion date is 2026.

- **Critical Utilities Rehabilitation Project (CURP)** (TEC $92.0M, FY 2020 start) will replace and rehabilitate key utility systems required for operation of mission critical research facilities. Significant portions of the utility systems are well beyond their useful life with some in service since WW-II, including portions of the sanitary system. This project will: 1) Replace central chilled water system(s), constructed in 1990, that are beyond their useful life and no longer reliably serving critical facilities, such as CFN, ISB, SDCC, NSLS-II, and the Collider-Accelerator Department (C-AD); 2) Replace portions of the underground steam and condensate piping system and select manholes, some dating back to the 1940s that are failing due to extensive corrosion, leaks, and deterioration; 3) Refurbish equipment in the central steam facility, first constructed in 1949, which will assure reliable steam service to the site; 4) Replace, repair, or reline the old asbestos water main first constructed in 1941, rebuild the facility housing Well 12, and replace the Elevated Water Storage Tank, constructed in 1941; 5) Repair and refurbish deteriorated sanitary lift stations and sanitary lines; and 6) Refurbish and replace electrical feeders and switchgear with modern, safe, reliable electric equipment and systems that will reduce arc-flash hazards. The project received CD-0 in 2018, CD-1/3A in 2020, and CD-2/3 is planned for FY 2022.
- **Critical Utilities Revitalization and Enhancement (CURE)** (TEC Estimated Range $200-$350M, FY 2025 start) will replace and rehabilitate additional key utility systems required for operation of mission critical research facilities. Some, such as portions of the sanitary system, are over 100 years old. The project will: 1) Replace the remaining original 1200 Ton electric chillers in the CCWF; 2) Replace portions of the old underground steam and condensate piping system, first constructed in 1941, and select manholes that are failing due to extensive corrosion, leaks, and deterioration; 3) Replace, repair, or reline the old asbestos water main, some dating back to 1941; 4) Replace, repair, and refurbish deteriorated sanitary lift stations and reline or replace sanitary piping and associated manholes; 5) Refurbish and replace electrical feeders and switchgear with modern, safe, reliable electric equipment and systems that will reduce arc-flash hazards; and 6) Replace key utility plant infrastructure to ensure operational control, efficiency, and reliability including electrical system and instrumentation components. This project is scalable to match available funding profiles.
- **Integrated Site Operations & Maintenance Facility (ISOMF)** (TEC Estimated Range $70-$95M FY 2027 start) will replace and demolish approximately 107,000 sf of Substandard or Inadequate buildings, trailers, and OSF assets. The project (see Figure) will co-locate maintenance and operation resources that are spread out across 16 buildings and 19 trailers, located in five separate areas of the site, increasing operational efficiency. Most of the buildings are WW-II era wood buildings, which have an Overall Asset Condition of Inadequate. It is anticipated the project will reduce at least 20% of administrative and shops space and 30% of storage space, and significant amount of common space, such as bath and locker rooms, breakrooms, and training space. The facility will also enable enhanced operations by centralizing the control areas for the computerized maintenance management and building management control systems. Due to co-location, the use of shared facilities will allow more effective staffing and supervision, improved communications (e.g., lessons learned and staff feedback), and greater building energy efficiency, resulting in an increase in operational efficiency. The building will include a central location for Facilities and Operations (F&O) stock and material kitting, which will enable workers to receive their assignments and work kits in one location. The facility will improve workforce development by having dedicated space that will be used to develop the next generation of craft, and the co-location of Subject Matter Experts to provide technical guidance. Included will be space for training and for modern remote conferencing with external vendors to support staff development, troubleshooting, and remote instruction. The facility will also

provide testing and assembly space for hands on mockups, such as for electrical protective device maintenance and safety, fire alarm systems, and value maintenance. The building will contain a center for real-time operations performance monitoring to allow issues and improvement opportunities to be identified and implemented efficiently.

- **New Net-Zero Guest Housing Facility** (TEC Estimated Range of $42.3M-$51.7M, FY 2030 start) will create a new, highly energy efficient, sustainable, resilient, and effective user housing facility at Discovery Park. This facility will create modern housing options for the scientific users, conducting research in BNL's major scientific user facilities. The project will address BNL's site sustainability goals and the administration's expectations for federal facilities related to decarbonization and the Net-Zero policy. It will provide a publicly accessible, proof-of-concept that can inform the residential and commercial construction industry and serve as a testbed for future demonstration of cutting-edge energy saving building technologies and systems. The project will provide approximately 64 housing units, replacing an equal amount of 75+ year old housing, eliminating substantial deferred maintenance costs and significant ES&H, and building code deficiencies.

Other DOE Line Items: As part of the Lab's mission readiness effort, BNL is executing an FY 2021 Notable Outcome to articulate and document the Laboratory's ten-year vision for the DOE Isotope Program. An element of that effort is a concept for a Radiochemical Processing Facility (titled Clinical Alpha Radionuclide Producer (CARP)) with a pre-conceptual point estimate of ~$73M). Under this approach, BNL would repurpose Building 870 to support dedicated radiochemical processing of accelerator targets to provide Curies of radionuclides to meet the growing unmet demand for clinical evaluation of drugs containing Ac-225.

GPP (DOE SLI) via the Infrastructure Crosscut: BNL continues to evaluate where DOE GPP level investment will complement and accelerate BNL indirect investment. Several major recapitalizations and other needs to provide mission ready facilities and infrastructure were identified and prioritized. These cover several requested improvements to address the most urgent gaps. Details of cost and request year can be found in the Investment Table. The highest priority projects include the following:

- Mission Critical Buildings, Upgrade HVAC Systems II ($9M, FY 2023)
- Upgrade Interior Potable Water (PW) Systems
- Mission Critical Buildings, Upgrade Interior PW Distribution
- Mission Critical Buildings, Replace Roofing
- Building 463 Revitalize Biology Labs
- Mission Critical Buildings, Upgrade Electrical Distribution Systems.

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. BNL also seeks direct DOE support to accelerate the demolition of the growing list of excess facilities with a proposed project ($9.3M, FY 2026). Additional facilities will be excessed as a direct result of the ISOMF; eliminating more than $21.5M in DMR, repair and modernization costs. EM committed to incorporating several SC assets including Building 491 (BMRR) and Building 701 (BGRR) into its cleanup program. The demolition of the Building 491 Stack is now EM funded and scheduled to be complete this year ($3.5M, FY 2022) and EM is partially funding the Building 197 demolition by supporting the removal of the mercury contaminated soil ($1M, FY 2022) EM funded the D&D of Building 650 in FY 2021 and the demolition is complete.

Indirect Funding: The Laboratory anticipates marginal increases to overall infrastructure spending over the ten-year period. Infrastructure funds include routine maintenance, dedicated DMR projects, IGPP, and OIP. OIP projects are not part of the Investment Table but fund alterations, non-capitalized betterment projects, demolition, and infrastructure studies. These OIP projects totaled ~$7.16M in 2021 (69% of the overall indirect infrastructure project budget, known as the Consolidated Unfunded Requirement List (CURL)) and are forecast at ~$13.8M (74%) in 2022.

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

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

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

Discovery Park will repurpose the existing BNL Apartment Complex and adjacent area into a publicly accessible research park. This area is contiguous to BNL's federal research core but is easily configured to be outside the security area. Its location, which is adjacent to the Laboratory entrance and the William Floyd Parkway, presents a unique opportunity for public/private development in the interest of the DOE. The initial development in Discovery Park is comprised of the SUSC, guest housing, and the potential CGI. The SUSC, housing at Upton Square, and CGI will become an entry portal, a user housing community, and a location for scientific collaboration. The balance of Discovery 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 housing facilities
- An enhanced guest and user portal for growth and sustainment of the scientific user community and user facilities
- Unique facilities for energy science, education, technology transfer, and Discovery to Deployment industrial partnerships.

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

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

Brookhaven's plan for the EIC is a cost-effective, low-risk strategy based on adding an electron ring and other components to the existing RHIC complex. These modifications are critical to ensuring success for the EIC. Infrastructure modifications will be covered by a $100M grant from New York State and will comprise civil construction to prepare the site, provision of support buildings, and the creation of access roads for the development and operation of the new facility.

Site Sustainability Plan Summary

BNL's energy management program continues to be the centerpiece of the Lab's sustainability program. BNL continues to maintain solid relationships with local utility providers ensuring cost effective power rates for operating the energy intensive user facilities and general infrastructure. BNL collaborates with the local utilities to leverage purchasing power and assist in renewable energy production to jointly support the goals of BNL and New York State.

BNL continues to host the Long Island Solar Farm (LISF), a solar photovoltaic power plant, developed through a collaboration that included BP Solar, the Long Island Power Authority (LIPA), and DOE. The LISF, began delivering power to the LIPA grid in 2011. The LISF can produce up to 32 MW of electricity: enough for approximately 4,500 households.

The Laboratory has also developed the Northeast Solar Energy Research Center (NSERC) on its campus, with a full capacity output of approximately 1 MW, that serves as a solar energy research and test facility for the solar industry. The mission of the NSERC is to support the expansion of solar power by providing high-quality data, field-testing, analyses, and solar energy expertise to address technical, economic, environmental, and policy issues facing solar power deployment in northeastern climates.

The Laboratory continues to evaluate leveraging investment approaches, such as UESCs to achieve the goals and create a reasonable return on investment. BNL completed its first UESC in 2015. An investment grade energy audit to form the basis of a second UESC project was completed. However, due to marginal economics and some concerns about the potential Energy Service Company, this effort was put on hold, while BSA evaluated other options. The finance charges and 15-year payback were deemed excessive for this scope and BSA has proposed an alternate financial model for this work. The payments for the first UESC will be completed in FY2023 and BSA will continue using this annual allocation to complete energy efficiency projects without engaging the use of a UESC. As the new sustainability and resiliency requirements are evaluated, BSA will look at all funding options for the completion of projects to help the Lab achieve its goals.

In the coming years, BNL will maintain focus on those areas that are performing well and look to make improvements in areas, such as zero emission buildings, GHG emissions, and data center efficiencies. BSA will replace its government fleet with zero emission vehicle (ZEV) acquisitions on the General Services Administration (GSA) annual replacement cycle, as outlined by Executive Order 14057. Additional charging stations to support ZEV acquisitions will be added, as needed.

BNL's current High Energy Mission Specific Facilities (HEMSF) include C-AD, NSLS-II, the CFN, and eventually the SDCC as it comes fully online. Figure 1 shows projected and historical electricity use.

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 2021 Lab Operating Costs:** $587.87 million
- **FY 2021 DOE/NNSA Costs:** $586.57 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $1,3 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 0.2%

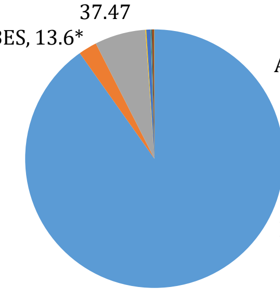
Physical Assets:

- 6,800 acres and 370 buildings
- 3.501 million GSF in buildings
- Replacement Plant Value: $2.66 B
- 28,913 GSF in 10 Excess Facilities
- 25,005 GSF in Leased Facilities

Human Capital:

- 1,917 Full Time Equivalent Employees (FTEs)
- 30 Joint Faculty
- 114 Postdoctoral Researchers
- 273 Graduate Student
- 52 Undergraduate Students
- 1,681 Facility Users
- 975 Visiting Scientists

FY 2020 Costs by Funding Source ($M)



*BES number reflects funding of $1.684M provided by SLAC for LCLS-II work and $11.673M for LCLS-II HE work

Mission and Overview

Fermilab's mission is to be the frontier laboratory for particle physics discovery. Thousands of scientists, engineers, technicians, users, and students from around the globe contribute their expertise to push the boundaries of particle physics knowledge. Fermilab hosts a range of cutting-edge experiments and develops and builds technologies that support research at locations around the world, including the Large Hadron Collider (LHC) in Europe and the South Pole Telescope. Fermilab aims to be the worldwide leader in accelerator-based discovery neutrino science, a goal endorsed by the 2014 Particle Physics Project Prioritization Panel (P5). The new Long-Baseline Neutrino Facility (LBNF) will send the world's most intense neutrino beam to massive Deep Underground Neutrino Experiment (DUNE) detectors at Fermilab in Illinois and at Sanford Underground Research Facility (SURF) in South Dakota. This is made possible by the Proton Improvement Plan II (PIP-II), the first particle accelerator on U.S. soil built with significant contributions from international partners. Through DUNE and a suite of short-baseline neutrino experiments, Fermilab has brought the world together to unlock the mysteries of neutrinos.

The Fermilab Accelerator Complex produces both low- and high-energy neutrino beams for experiments like NOvA and enables precision science experiments such as Muon g-2 and Mu2e. Its unique infrastructure and expertise make Fermilab a world leader in particle accelerator and detector technologies, enabling new particle accelerators for discovery science in many fields, including the Linac

Coherent Light Source II High Energy (LCLS-II HE) project, ensuring continued U.S. leadership in photon science. Additionally, Fermilab's collider science program plays a leading role in the LHC upgrade projects and in the Compact Muon Solenoid (CMS) experiment. Fermilab hosts several world-leading cosmic science efforts exploring the mysteries of dark matter and dark energy. Fermilab is the host of one of five national quantum information science (QIS) research centers, the Superconducting Quantum Materials and Systems Center (SQMS), which has the goal to develop new and unique facilities for quantum computing and sensing. The laboratory's renowned theory division performs research at the confluence of these science themes. Emerging initiatives in QIS, artificial intelligence and microelectronics enhance the fundamental science mission and set the stage for high-impact partnerships, supported by technology transfer programs which leverage this expertise to apply particle physics technologies to problems of national importance in energy and the environment, national security and industry.

Fermi Research Alliance, LLC (FRA), an alliance of the University of Chicago (UChicago) and the Universities Research Association, Inc. (URA), manages and operates Fermilab for the DOE and provides guidance, advocacy and oversight. The corporate parents bring considerable operational and intellectual assets to the governance and oversight of the laboratory. To achieve its ambitious goals, FRA and the laboratory are committed to modernizing business systems and infrastructure, including moving toward net-zero operations, and remaining focused on equity, diversity and inclusion.

Core Capabilities

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

Particle Physics

Particle physics is the heart of Fermilab's science mission. It is defined by five main science themes—neutrino science, collider science, precision science, cosmic science, and detector R&D. Fermilab is the only laboratory in the world that operates two accelerator-based neutrino beams simultaneously. These intense neutrino sources illuminate an important collection of experiments studying neutrinos over both short and long distances, allowing Fermilab to address questions such as whether additional (sterile) neutrinos exist and whether neutrinos violate matter-antimatter (CP) symmetry. The NOvA experiment explores the parameters of neutrino flavor transformation. This exploration will become comprehensive with the operation of the Deep Underground Neutrino Experiment (DUNE) in a new beamline created as part of the Long-Baseline Neutrino Facility (LBNF) and powered by the Proton Improvement Plan II (PIP-

II) accelerator upgrades. The Short Baseline Neutrino (SBN) program searches for sterile neutrinos through a suite of three experiments.

The Large Hadron Collider (LHC) at CERN, the European center for particle physics, is the world's highest energy particle accelerator/collider. Fermilab is the leading U.S. center for LHC science and second-largest world center after CERN. 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 including dark matter. Fermilab also leads the HL-LHC CMS Detector Upgrade Project, the HL-LHC Accelerator Upgrade Project, and U.S. CMS operations. Researchers using Fermilab's CMS facilities played leading roles in the 2012 Higgs boson discovery, and ongoing research promises to further revolutionize our understanding of the universe.

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

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

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 South Pole Telescope data sets have shown correlation of cosmic voids in the DES data with regions of reduced lensing of the CMB. Development of new quantum sensors is enabling rapid progress in direct dark matter searches and simultaneously driving progress in QIS. Over the coming decades, Fermilab will act as a central platform and host for understanding cosmic science data, maximizing the scientific output of experiments across the field.

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

The Fermilab workforce benefits considerably from support provided by UChicago and the Joint Task Force Initiative (JTFI). For example, UChicago provides the Strategic Laboratory Leadership Program (SLLP) through the Booth School of Business, Strategic Program for Innovation at the National Laboratories (SPIN) and Laboratory Innovation Fellows (LIF) in conjunction with Booth and the Polsky Center, as well as other professional development opportunities including the Leadership Academy for

Women in Science and Engineering. The Fermilab community benefits from three awards given annually by Universities Research Association (URA) to recognize superior academic achievements and to encourage young scientists. URA also sponsors a visiting scholars program and hosts and supports the annual Fermilab users' trip to Washington D.C.

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.

Large-Scale User Facilities and Advanced Instrumentation

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

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

For almost two decades, Fermilab has served as the host laboratory for the more than 800 scientists and students from approximately 50 U.S. universities who work on the CMS experiment at the LHC in Geneva, Switzerland. CMS at Fermilab consists of the LHC Physics Center (LPC), CMS Remote Operations Center and the U.S. CMS Computing Facility. The LPC is designed to engage members of U.S. CMS institutions distributed across the country in physics analyses of LHC data and in CMS detector upgrades. The LPC creates a thriving environment for collaboration among participating institutions by facilitating remote participation, conferences, classes and providing visit opportunities. Through the Distinguished Researcher, Guest and Visitor programs, collaborators are supported to spend significant time at the LPC, and the CMS Data Analysis School draws more than 100 participants each year. The Remote Operations Center enables physicist participation in remote operations and monitoring of the CMS detector and keeps scientists, students and technicians connected to operations activities at CERN without the time and expense of European travel. The U.S. CMS Computing Facility at Fermilab is the largest and most reliable Tier-1 computing facility (after the CERN Tier-0 center). As part of a worldwide grid computing capability, this facility is available to qualified CMS researchers around the world.

The LPC enables close communication between CMS scientists and members of the Fermilab theory group. The theory group is deeply involved in advancing LHC new physics phenomenology and improving modeling of Standard Model processes through precision QCD and electroweak calculations. Fermilab theorists participate in LPC events, share new ideas with the experimental colleagues, and collaborate on analysis projects. Several new ideas leading to CMS and phenomenology publications originated through these close interactions.

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

Large-Scale User Facilities/Advanced Instrumentation is funded primarily by DOE/HEP (and DOE/SLI for infrastructure), and advances DOE's Scientific Discovery and Innovation mission.

Accelerator Science and Technology

Fermilab's core capability in accelerator science and technology enables particle physics discoveries and beyond, making significant contributions to research in other scientific disciplines such as photon science, nuclear physics, QIS, industrial applications and more. The critical areas within accelerator science and technology that are key to Fermilab's mission are: superconducting radio-frequency (SRF) acceleration technology, high-field superconducting magnets, accelerator and beam physics (ABP), AI/ML, and high-power targetry. The laboratory's 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.

Results from Fermilab accelerator R&D support the flagship neutrino science program and influence how U.S. and international accelerators are designed, constructed and operated. Fermilab has achieved more than 700 kW beam power to the NOvA experiment through PIP and is running approximately $2x10^{17}$ protons per hour from the proton source to support the SBN program and the Muon g-2 experiment. Fermilab operates three high-power target stations: the 700+ kW NuMI beam (now capable of accepting 1 MW); the BNB; and the muon-production target station for the Muon g-2 experiment. A fourth target station is under construction for the Mu2e experiment. A fifth target station is under design for DUNE, capable of 1.2 MW and upgradeable to 2.4+ MW.

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. 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 enabled 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 and TJNAF 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 projects like PIP-II.

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 and was recognized by the 2018 GARD review as the country's only "Tier-1" facility for ABP. As the world's only facility focused on intensity-frontier R&D in storage rings, the FAST research program will address key technological and scientific challenges in the realization of next-generation, high-power accelerator facilities. The FAST facility also houses a state-of-the-art, high-brightness SRF electron injector, which principally serves the IOTA program but also facilitates a range of R&D programs with outside collaborators. Furthermore, as the only operational SRF accelerator at Fermilab, the FAST injector also comprises a valuable R&D platform for SRF systems integration and operations.

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.

Advanced Computer Science, Visualization, and Data

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

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

The laboratory is a leader in active mass storage and distributed computing, which has evolved to satisfy the rapidly expanding data and computational needs of energy frontier and intensity frontier experiments. Fermilab scientific computing facilities provide active access to exabyte-scale data storage. In addition, Fermilab developed and is operating the HEPCloud platform, which provides a unified portal technology for accessing and sharing resources for data processing, storage and analysis across heterogeneous facilities and platforms. HEPCloud capabilities provide Fermilab computing users [cost] optimized access to DOE/ASCR HPC centers, internationally partnered facilities, university-supported computing clusters and commercial cloud resources. HEP Experiments including CMS, DUNE, Mu2e and NOvA are exploiting Fermilab's HEPCloud capabilities to accelerate their scientific discoveries. Near-term quantum computing systems could be deployed in larger scale scientific calculations as part of hybrid computing systems the way graphics processing units (GPUs) and field-programmable gate arrays (FPGAs) are used today. Fermilab's expertise in developing sophisticated workflows will be essential to leveraging and further developing this technology. HEPCloud is being evolved to assign resources with "quantum co-processors."

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 the Korean Institute of Science and Technology Information, to work on projects that include accelerator modeling, computational cosmology and particle physics simulations. Fermilab's strategy is to leverage DOE/ASCR expertise where appropriate to respond to computational challenges presented by the DOE/HEP program through the judicious use of partnership programs such as DOE's Scientific Discovery through Advanced Computing (SciDAC) program, as well as periodic DOE/ASCR calls for proposals.

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

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.

Science and Technology Strategy for the Future/Major Initiatives

As America's premier particle physics and accelerator laboratory, Fermilab is moving forward with experiments, international engagements and R&D programs that support all science drivers identified by the U.S. particle physics community in the consensus Particle Physics Project Prioritization Panel (P5) report. The Muon g-2 experiment's incredible science impact and media coverage is a major success of the P5 roadmap. Fermilab started with a compelling science question, used its unique capabilities to deploy a definitive experiment and hosted an international collaboration to test the Standard Model's predictions. Using these same building blocks and sustained DOE support, Fermilab will deliver the Deep Underground Neutrino Experiment (DUNE).

Serving as the host laboratory for DUNE is one of Fermilab's major initiatives in the coming years. DUNE will be installed in the Long-Baseline Neutrino Facility (LBNF), which will produce the world's most intense neutrino beam, powered by megawatt beams from an upgraded and modernized accelerator complex made possible by the Proton Improvement Plan II (PIP-II) project. Fermilab also continues to focus on its contributions to the High-Luminosity Large Hadron Collider (HL-LHC) and Compact Muon Solenoid (CMS) detector upgrades and serves as the U.S. host for the CMS experiment. Additional key initiatives include advancing accelerator, detector and quantum science and technology. The laboratory aims to transform its business systems and execute a sustainable campus strategy integrated with its scientific vision. Fermilab's scientific vision builds on six strategic goals:

- Be the international hub for neutrino science
- Advance particle physics discovery across P5 science drivers
- Be a world leader in accelerator science and technology
- Drive innovation in particle detector technology and microelectronics
- Advance the forefront of large-scale data analytics, storage, and real-time AI/ML
- Host national facilities for quantum computing, sensing and communication

Infrastructure

Overview of Site Facilities and Infrastructure

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

All Fermilab real property in Batavia, Illinois is used and owned by DOE, and much dates from the 1960s and 1970s. In addition to the Illinois campus, DOE has a 25,005 gross square footage (GSF) real-property lease with the South Dakota Science and Technology Authority (SDSTA) at the Sanford Underground Research Facility (SURF) in Lead, South Dakota. In FY 2021, there were no new real estate actions, leases, renewed leases, leased disposals, gifts, or third party financed projects. The total Replacement Plant Value (RPV) for conventional facilities is $1.43B. The total RPV including programmatic accelerator and tunnel assets (OSF 3000) is $2.66B. Property use predominantly serves R&D and administrative functions. Other land is preserved for future science by maintaining it as restored prairie, tilled agriculture, or woodland.

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

The Fermilab Campus Master Plan[2] supports the laboratory's strategic plan and major initiatives and requires investment in demolitions to reduce the laboratory's excess facility operating burden. While there are no demolitions scheduled in FY 2022, the laboratory has projects ready for execution if funds become available and has prioritized demolitions as part of its strategic infrastructure plan.

Fermilab's facility strategy is built on the FY 2014 Laboratory Operations Board (LOB) infrastructure assessment. In FY 2019, Fermilab revised its infrastructure planning process to better align and prioritize infrastructure investments with the science strategy. This process matured in FY 2020 and FY 2021 to create an integrated prioritized list of infrastructure projects for execution as funding becomes available. The list includes over 129 infrastructure projects, some with multiple subprojects, that directly support and/or enhance the laboratory's scientific mission, lifeline infrastructure (e.g., water, sewer, and electrical distribution) reliability, workspace modernization, and laboratory security.

During FY 2021, the laboratory made progress in implementing several new initiatives including:

- Fully implemented Fermilab's program of centralized facility management (CFM)
- Completed a CD-1 review for the $314M Utilities Infrastructure Project (UIP); CD-1 was awarded in early FY 2022
- Advanced a project to completely replace the accelerator controls system and associated infrastructure supporting the campus' central experimental neural controls network (ACORN)
- Wilson Hall safety and functional needs have been defined

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

- Matured facilities condition assessment, planning, design, construction, maintenance, resiliency, and disposition procedures
- Completed a Strategic Facility Assessment to provide detailed information regarding facility capability gaps and modernization and demolition needs

Types and Conditions of Facilities

Fermilab has increased both the number of facilities onsite and the utilization of all facilities, while slightly reducing the number of "substandard" and "inadequate" facilities. A labwide facility assessment, contracted to gather comprehensive condition data, is now two-thirds complete. The result, as anticipated, is a marked increase in deferred maintenance, from $41M in FY 2020, to $116M in FY 2021. The FIMS evaluation, utilization, and maintenance cost of existing facilities as of the end of FY 2020 is shown in the snapshot table below.

	Structures				Utilization				Maintenance	
Types of Facility (Usage Codes)	Adequate	Inadequate	Substandard	Total	90-100%	75-89%	50-74%	0-49%	Deferred	Annual
Laboratory/Experiment Buildings (711, 721, 723)	20	9	3	32	32				$19,711,141	$2,009,659
Accelerator (785, 3221)	53	4		57	57				$13,338,804	$2,077,798
Office Buildings (101)	16	17	11	44	42	2			$8,604,692	$3,670,733
Operations Buildings (261, 297, 551, 561, 591,601, 611, 614, 621, 641, 642, 693, 694, 6271, 6719, 7009)	31	11	9	51	50		1		$22,244,596	$5,694,354
Storage Buildings (400, 401, 410, 4010, 4020, 4171, 450, 4500, 4221)	88	36	11	135	119	6	6	4	$22,484,571	$886,085
Residential Buildings (300, 691)	61	1	1	63	62			1	$1,869,697	$553,437
Other Building Types (234, 294, 295, 298, 644, 801, 2449, 2909)	21	3		24	18	6			$528,597	$406,438
Utility Infrastructure (508, 525, 531, 595, 5171, 5569, 5789, 5906, 6919, 7261, 8129, 8131, 8171, 8329, 8549, 8561, 8629, 8719, 8929, 8939, 8949, 8979)	12	4	8	24	23	1			$22,280,034	$4,263,864
Roads and Walkways (1129, 1169, 1729, 1739, 1749, 1769, 1789)	8	4		12	12				$4,593,709	$208,907
Culverts, Dams, Fences (2429, 2629, 2819, 2619)	12			12	12				$210,423	$97,182
Total	322	89	43	454	427	15	7	5	$115,866,264	$19,868,457

Of the 454 structures, 427 are operating at or near 100% utilization. Of those, over 25% are inadequate or substandard. Office buildings (FIMS-101) remain a particular concern; 64% are either inadequate (17) or substandard (11), but they remain near full utilization with $8.6M in deferred maintenance. Laboratory and experimental spaces are at maximum utilization, despite 38% being below adequate condition, and $19.7M of deferred maintenance. The accelerator complex is likewise at maximum utilization but in better condition, with 93% of the facilities rating adequate, though they carry a $13M deferred maintenance balance.

Fermilab's campus strategy is aligned with addressing these inadequate and substandard conditions by migrating functions to the central campus and into facilities that are modern and capable. The IERC is nearing the transition to operations and providing a world class facility, the UIP has achieved CD-1 providing a pathway to resolve end-of-life infrastructure issues, and a project to address the needs of Wilson Hall that are ready for validation. Also in construction, on schedule and under budget, is a sanitary sewer project addressing urgent repairs of the most compromised elements. As less than adequate facilities are vacated, their maintenance footprint can be reduced until those assets can be repurposed or demolished. Additional projects are planned through the 2030s, as determined through the infrastructure prioritization process, to address the most pressing site needs. Currently, the greatest limitation to reducing unutilized and unsatisfactory space is funding for small projects, including demolition. Given the opportunity, shutdown space could be reduced as a function of funding levels.

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

	Operating		Standby		Shutdown	
	Total	GSF	Total	GSF	Total	GSF
Building/Trailer	389	3,481,373	5	5,772	10	28,913
OSF	62	-	2	-	0	-

In FY 2021, Fermilab transitioned to a CFM system. CFM immediately began to demonstrate its value, identifying previously unknown or under-reported building needs and initiating repairs and improvements to address them. In addition, the facility condition assessment will soon begin the third and final evaluation segment. Establishing baseline data for every facility at the laboratory will enable in-depth infrastructure metrics to greatly enhance maintenance and strategic planning.

Campus Strategy

Fermilab's campus strategy will enable four objectives:

- Close infrastructure gaps associated with emerging science frontiers and existing projects including LBNF, DUNE, PIP-II, and the quantum science program
- Identify facility capability gaps and modernization and demolition needs using detailed information from the Strategic Facility Assessment and the ongoing condition assessments of facilities
- Improve the sustainment and resiliency of existing assets
- Recapitalize or dispose of overaged, obsolete, and severely deteriorated infrastructure

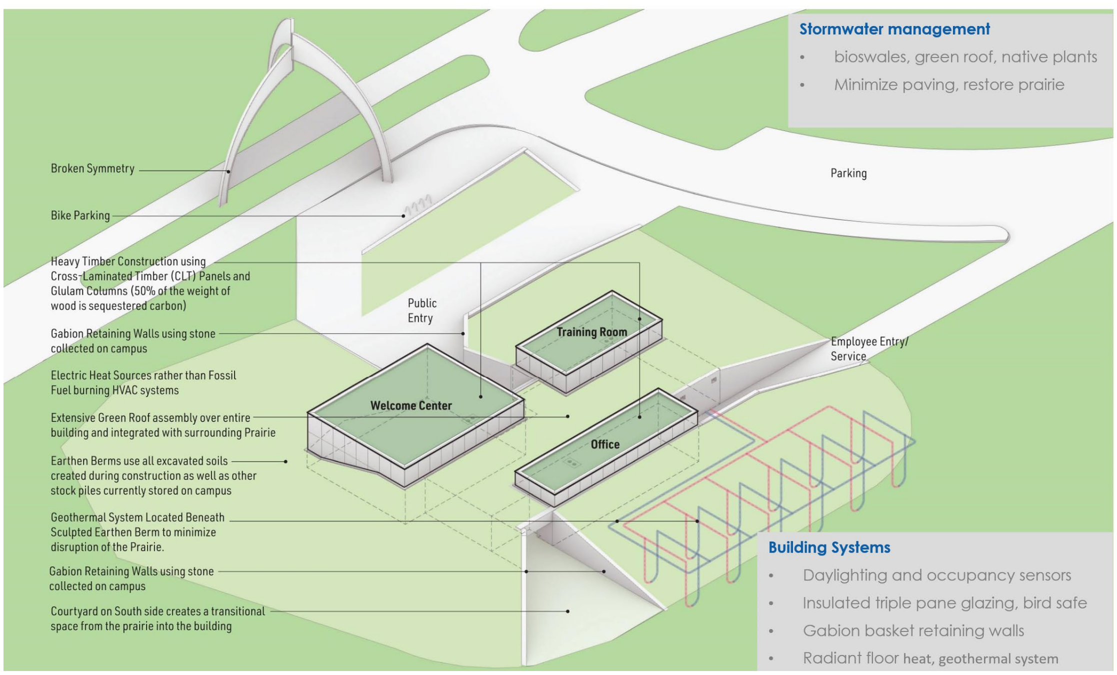
Fermilab's infrastructure planning and investment strategy addresses these objectives and ensures Fermilab will continue to provide modern, world-class facilities for scientific research. Fermilab's 10-year science and technology plan is the basis of the campus strategy which provides an integrated approach to achieve a campus fully supportive of current operations and future mission requirements. The strategy incorporates facility and utility strategic assessments and a program to centralize facilities management.

Planning infrastructure improvements is a major part of the laboratory's Campus and Facility Planning Board (CFPB) responsibility to support future/major initiatives identified in Section 4. The cornerstone of the campus strategy is the annual process to identify, coordinate, prioritize, and communicate infrastructure needs. The outputs of the FY 2021 CFPB process and the view of emerging science and supporting infrastructure projects are each described in greater detail below. The prioritized list consists of both larger DOE Order 413 projects (i.e., greater than $20M) and smaller minor construction projects (i.e., less than $20M). This list is prioritized based on impact to the scientific mission, infrastructure reliability and safety/environmental factors. The laboratory continues to develop and advance these projects in anticipation for program funding. For the minor construction projects, the laboratory has worked with the DOE/HEP program office to develop a funding profile of $15M per year as a planning tool to execute minor construction projects necessary for safety compliance and mission critical projects; however, in FY 2021 and in FY 2022 this assumption has not been valid. Continued funding shortfalls threaten the laboratory's infrastructure strategy and increases operational risk for safety and compliance issues.

Site Sustainability Plan Summary

In FY 2021, Fermilab made great strides toward establishing its first net-zero building to be constructed using carbon neutral techniques. The Fermilab Welcome and Access Center, slated to start construction in FY 2022, will feature bioswales, green roofs, native plantings, restored prairie, minimized paving, earthen berms, triple pane bird safe glazing, gabion basket retaining walls, radiant floor heating, and geothermal systems. The Welcome and Access Center also greatly enhances the laboratory's site security by moving the pre-badge activities of the badging and ID office, subcontractor orientation training and a welcome space outside the secure perimeter established by the guardhouse to enter. Security is further enhanced with barriers, gates and cameras covering Fermilab's main entrance.

Welcome and Access Center (FY22 priority #13 subproject)



Net Zero Energy Ready

Carbon Neutral

Extensive Green Roof System Manages Stormwater, Reduces Heat Island Effect, and Improves Air Quality

Green Roof & Earthen Berms Insulate Building

Engineered Timber Structure Sequesters Carbon (50% of mass)

Geothermal Heat Pump Radiant Floor Heating and HVAC Systems

Minimized Paving for Stormwater Management

Fill Materials for Earthen Berms and Gabion Retaining Walls Incorporate Materials on Campus

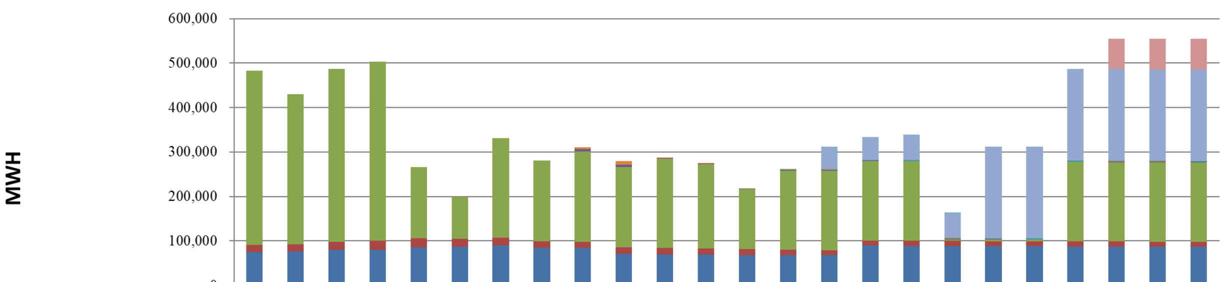
Eight of 58 eligible buildings currently comply with High Performance Sustainable Building Guiding Principle requirements, and Fermilab looks forward to adding two facilities to that list in FY 2022. An additional ten new facilities and two sustainable renovation projects are projected for completion over the next five years to support LBNF, DUNE, and PIP-II projects. When completed, these 12 facilities will add an additional 277,238 GSF (29% of building count, 21% of total building footprint area) of compliant sustainable buildings to the Fermilab site.

The water efficiency and resilience of Fermilab's site will get a boost when UIP is kicked off. UIP will be executed in three phases: 1) construction of a new chilled water plant and renovation of the existing central utilities building, 2) replacement and modernization of the Kautz Road Electric Substation, and 3) repair or replacement of significant segments of linear utility systems across the site including potable water, chilled water, industrial cooling water, storm sewers, and electrical distribution infrastructure.

While not a water efficiency measure, Fermilab made significant progress toward reducing inflow and infiltration (I&I) into the site sanitary sewer system in FY 2021. The project is being planned to repair, replace or reline 19,000 linear feet of pipe and services, repair or replace 117 manholes, and plug and abandon 1,400 linear feet of pipe. The reduction of I&I into the system will alleviate system overwhelm during storm events.

Significant changes to Fermilab’s projected energy consumption are anticipated over the coming decade as the new PIP-II accelerator is brought into service and the LBNF/DUNE complex is tied into the existing accelerator complex beginning in 2029. The connection of LBNF will require a shutdown that is currently scheduled to begin in 2027. The addition of the PIP-II accelerator and beam requirements for LBNF are expected to increase Fermilab’s overall energy consumption by 30% over historic peak levels.

Electricity Use and HEMFs – Actual and Projected FY08-FY31



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

	FY20	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30	FY31
LBNF										68,328	68,328	68,328
PIP-II			51,430	51,430	56,993	56,993	205,913	205,913	205,913	205,913	205,913	205,913
SBN Near & Far Detectors	700	631	701	701	701	701	701	701	701	701	701	701
Mu2e (MC-2)	471	488	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752	1,752
Muon G-2 (MC-1)	1,057	1,144	876	876	876	876	876	876	876	876	876	876
Existing Particle Accelerators HEMSF	133,600	178,662	178,662	178,662	178,662	3,462	3,462	3,462	178,662	178,662	178,662	178,662
Existing High Performance Computing HEMSF	13,131	11,564	11,564	11,564	11,564	11,564	11,564	11,564	11,564	11,564	11,564	11,564
Site Base	68,533	68,151	67,772	89,384	89,013	88,646	88,282	87,922	87,565	87,212	86,863	86,517

To prepare for and offset the anticipated future increase in energy consumption, Fermilab launched an Energy Systems Working Group (ESWG) of its Campus and Facility Planning Board. The ESWG will foster new ideas and coordinate efforts around clean and renewable energy, energy storage, and energy resilience applications. By feeding into the Campus and Facility Planning Board, new and emerging projects have a defined pathway for prioritization and funding. The laboratory will continue to use renewable energy certificates (RECs) as the primary mechanism to offset greenhouse gas emissions associated with electrical consumption.

Finally, in partnership with the Fermi Site Office, a Fermilab Resilience and Efficiency Project (FREP) was proposed as part of an application to the Department of Energy’s Assisting Federal Facilities with Energy Conservation Technologies (AFFECT) funding program. The application details a project to execute an Energy Savings Performance Contract (ESPC), which would fund a four-pronged energy efficiency and renewable energy strategy including an aggressive suite of energy conservation measures, a 2 MW solar photovoltaic array, an energy storage facility, and micro/nanogrid infrastructure to improve the resilience of critical facilities onsite. Fermilab was awarded the AFFECT grant and is actively engaged in the ESPC portion of the project.

LAWRENCE BERKELEY NATIONAL LABORATORY

Lab-at-a-Glance

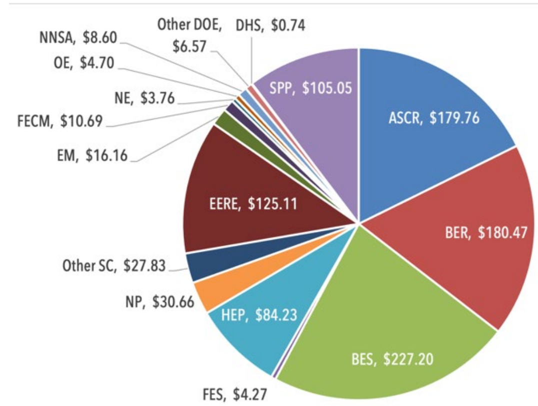
Location: Berkeley, California
Type: Multi-program Laboratory
Contractor: University of California
Site Office: Bay Area Site Office
Website: www.lbl.gov

- **FY 2021 Lab Operating Costs:** $1015.81 million
- **FY 2021 DOE/NNSA Costs:** $8.60 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $105.05 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 10.3%
- **FY 2021 DHS Costs:** $0.74 million
- **FY21 added $0.571M for LCLS-II and $0.997M for LCLS-II-HE**

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:
- 3,693 Full Time Equivalent Employees (FTEs)
- 1,781 Scientists and Engineers
- 242 Joint Faculty
- 503 Postdoctoral Researchers
- 297 Graduate Student
- 119 Undergraduate Students
- 13,990 Facility Users
- 1,736 Visiting Scientists and Engineers

FY 2021 Costs by Funding Source ($M)



Mission and Overview

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

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

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

We have continuing partnerships with other national laboratories on a wide range of projects from subatomic physics to quantum information, biomanufacturing, climate science, water-energy, ecosystem science, and innovative energy technologies.

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

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

Core Capabilities

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

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

Large Scale User Facilities/Advanced Instrumentation

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

The Advanced Light Source (ALS) is the world-leading facility for high-brightness soft X-ray science, with additional excellent performance ranging from the infrared through hard X-ray spectral regions.

Scientists use the data they collect to understand, predict, and ultimately control matter and energy at length scales ranging from the atomic to the macroscopic. This research underpins many of DOE's Core Capability areas, including those involving chemical, material, and biological systems. In FY21 the ALS had 1,159 users (247 of whom were onsite). ALS-based results appear in nearly 1,000 refereed journal articles annually, ~20% of which are in high-impact journals. Annual budget: ~$68 million (BES).

The Molecular Foundry provides communities of users worldwide – 750 in FY20 (643 of whom were onsite) – with access to expert staff and leading-edge instrumentation to enable the understanding and control of matter at the nanoscale in a multidisciplinary, collaborative, and safe environment. Established 15 years ago, the Foundry's stellar reputation attracts expert scientists from around the globe. It 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. Annual budget: ~$31 million (BES).

The ***DOE Joint Genome Institute (JGI)*** is a national user facility carrying out projects of central relevance to DOE missions in bioenergy, global carbon cycling and biogeochemistry. JGI is the world's largest producer of plant and microbial genomes, with programs focused on large-scale generation of DNA sequences; development of innovative DNA analysis algorithms; and functional genomics, a strategic focus that includes a growing DNA design and synthesis program and metabolomics capabilities. In FY21, JGI served 2,180 primary users and over 14,000 active secondary users; FY21 budget: ~$82 million (BER). JGI's strategic plan lays out the I5 Strategic Framework, encapsulating guiding principles for JGI's activities (identification, interrogation, investigation, integration, and interaction) to guide its transition to an Integrative and Collaborative Genome Science User Facility that will integrate sequence and functional capabilities for systems-level biology. At the end of the 2-year period, 85% of JGI's 2-year milestones are complete.

The National Energy Research Scientific Computing Center (NERSC) supports more than 7,500 users from universities, national laboratories, and industry – the largest and most diverse research community of any DOE user facility. NERSC is the mission High Performance Computing center for the DOE Office of Science, providing resources for SC's six scientific program offices. NERSC deploys large-scale, state-of-the-art supercomputing and data storage systems, networking, and expert consulting and support services. Over the last decade NERSC's workload has expanded so that a growing number of scientists can use NERSC to analyze data from DOE SC's experimental and observational facilities, including light sources, sequencers, telescopes, and microscopes. This increased workload requires new capabilities, including more robust support for AI, data analytics, data management, transfer and sharing and the ability to support complex workflows that originate outside of NERSC. As such, NERSC developed and deployed key enabling technologies, including containers that run on HPC platforms, interactive notebooks for data analysis, and scaling ML and deep learning frameworks to take advantage of HPC scale resources. The need to integrate data with new AI models is not unique to experimental science; it is increasingly being required by NERSC's traditional simulation and modeling workloads as well. This thrust, to enable new modes of scientific discovery through the integration of simulations, data analysis, and AI is a core principle in the NERSC-10 Mission Need (signed in the fall of 2021) for NERSC's next generation system to be deployed in the 2025 timeframe. The Perlmutter (NERSC-9) system, represents a significant step forward in supporting SC user workflows and provides a boost in computing performance and capability to the user community with more than 6000 NVIDIA GPUs, an all flash file system, and TB/s gateway to ESnet's network. The system will also continue the transition to exascale-era architectures by introducing GPU resources to the broad SC user community. The NERSC Exascale Science Application Program (NESAP), pairs application developers with NERSC performance engineers and vendor experts to prepare teams and optimize applications for the Perlmutter system. Thus far

NESAP has enabled six key SC applications to achieve significant performance improvements. One example is a 25X speedup on the Dark Energy Spectroscopic Instrument (DESI) code that has enabled the project to make use of GPUs. In 2021, NERSC systems provided more than eight billion computational hours to researchers. NERSC's FY21 funding: $111 million (ASCR).

The Energy Sciences Network (ESnet) is SC's high-performance network user facility, delivering highly reliable data transport capabilities optimized for the requirements of large-scale science. ESnet serves as a vital "circulatory system" for the entire DOE national laboratory system, dozens of other DOE sites, and ~200 research and commercial networks around the world—enabling tens of thousands of scientists at DOE laboratories and academic institutions across the country to transfer vast data streams, access remote research resources in real-time, and collaborate on important scientific challenges. In essence, ESnet is a force multiplier that enhances scientific productivity and expands opportunity for discovery. In the past year, the network transported over an exabyte of data. During FY20, ESnet completed a successful CD 2/3 for ESnet6, a strategic facility project to upgrade its network to meet the increasing data needs of science. In addition, ESnet deployed a new router platform across its backbone transitioning services across 40 sites as part of its project. Greater optical capacity, with 400 Gbps wavelengths, was also added across the new optical substrate built in 2020 bringing the aggregate network capacity to > 20Tbps. Further, ESnet continues to develop and deploy software automation tools, and high-touch packet inspection services as part of the project. The project continues to transition the routers placed at the various labs to the new platform in 2022, working through supply chain issues and restrictive maintenance schedules. ESnet's FY21 funding was ~$90M (ASCR).

Basic Research in Energy

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Berkeley Lab has deep expertise in theory and computational simulations in conjunction with novel synthesis approaches that rely on machine learning and AI concepts, which are critical to the discovery and design of new materials. Researchers develop models for understanding, predicting, and controlling complex materials with targeted properties. The Center for Computational Study of Excited-State Phenomena in Energy Materials develops new general software, theories, and methods to understand

and predict excited-state phenomena in energy-related materials from first principles with exascale performance. Open access to analysis tools and computed information on known and predicted materials provided by the Materials Project helps the Lab to conduct computational work in high-throughput modalities.

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

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

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

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

Earth Systems Science and Engineering. This Core Capability is associated with Berkeley Lab's geosciences group, the largest and most comprehensive in the DOE complex. We have deep expertise in developing knowledge, data, monitoring tools, and predictive models to investigate complex subsurface processes and their impacts on energy, water, environmental and infrastructure systems. We use diverse laboratory and field methods to probe chemical, physical, thermal, mechanical, and biological processes under relevant subsurface conditions and on length scales from nanoscale pores to reservoirs. Using Berkeley Lab's key facilities, we move knowledge from the atomistic level of cryo-EM at the Molecular Foundry through in situ X-ray tomography at the ALS and the Rock Dynamics Laboratory to field-scale monitoring of dynamic subsurface processes using acoustic, earth strain, and electromagnetic methods including satellite data and distributed fiber optic methods. A particular expertise lies in our ability to work across spatial, temporal, and development scales to move from insight to impact in what we term Science to Hubs. This is particularly apparent in our geothermal energy and geologic carbon storage portfolios but also in more recent research directions focused on negative emissions, water resource management, and critical mineral supply. Experimental field research efforts at LBNL and across the complex benefit from the Geosciences Measurement Facility (GMF), which provides exceptional expertise and tools to design, build, test, and deploy new equipment and instrumentation, and sampling tools required for geoscience investigations, including large field scale deployments.

BES support enables researchers to discover the molecular-scale mechanisms of fluid-rock processes and to translate molecular- and nano-scale insights into larger-scale models and capabilities. Our flagship geosciences program is unique in the U.S. and unifies the disciplines and the expertise needed for mechanistic understanding of how rock-fluid systems evolve in response to stress and reactive fluids and solutes, knowledge that is required for assessing functionality and system responses of subsurface geologic resources. We develop and integrate powerful experimental methods with exceptional expertise in molecular-to-continuum scale theory and modeling. World class instrumentation is used to quantify geologic fluids, solutes and minerals under elevated temperature and pressure, including *in situ* X-ray imaging and spectroscopy and facilities. The group designs and constructs novel instruments capable of measuring the geochemical and mechanical evolution of out-of-equilibrium interfaces or rocks. The group is a world leader in the use of cryogenic transmission electron microscopy of clay minerals to provide insights into the pathways for clay swelling and ion exchange. We also advance and integrate stable isotope measurements, including clumped isotope methods, to identify and interpret chemical signatures of rock-fluid interactions. Advanced experiments on geologic samples help to understand chemical-mechanical dynamics on timescales of picoseconds to millions of years. Emerging computational capabilities include the first coupled geochemical and geomechanical model for chemically mediated deformation and the integration of ML and molecular simulation for efficient prediction of complex fluid and interface properties. ECRP awardee Laura Lammers is developing predictive, first-principles models for mineral formation under relevant geochemical conditions through interfacial experimental science and molecular modeling. An approximately 10-year development effort on micro-continuum reactive transport models for clay-rich media resulted in the release of a 3D high-performance computing version of the 2017 R&D 100 winner CrunchFlow, here referred to as CrunchClay. This software is the only one available in the world that can address electrostatic effects on transport in clay media in multiple dimensions.

Translation of fundamental knowledge to increasingly accurate subsurface simulations is a cross-cutting goal and one that ultimately requires HPC. Supported by ASCR, Berkeley Lab leads the only two subsurface exascale application projects in the complex. The first project, Subsurface Exascale, focuses on scale-adaptive approaches to simulate, from the micro- to the reservoir scale, the coupled hydrological, geochemical, thermal, and geomechanical processes that are critical to many subsurface energy applications, including geologic CO_2 sequestration, geothermal energy production, subsurface energy storage, and nuclear waste isolation. The project is providing the ability to resolve dynamic subsurface features like fractures at very high resolution using a combination of the latest computer architectures and new software designed specifically for heterogeneous architectures. The centerpiece here is the Chombo-Crunch code, which is approaching exascale performance on both CPU and GPU platforms. The second project, EQSIM (EarthQuake SIMulation), is preparing to exploit emerging DOE exascale computers for a transformational advancement in the ability to simulate earthquake processes at regional scale. Over the past three years, EQSIM has made major computational and algorithmic advancements and regional scale simulations (e.g., the entire San Francisco Bay Area) can now be performed routinely at unprecedented frequencies of engineering interest – up to 10 Hz – with computer run times on the order of 6-7 hours. This new capability is being used to improve the understanding of the complex spatially varying distribution of regional earthquake risk with ultimate broad applicability to urban, transportation and energy infrastructure systems. This advanced computational technology has already begun the transition to practice in the regional-scale risk assessment of distributed energy systems with support from the Risk Management and Modeling Tools Program of CESER.

The Lab's applied subsurface portfolio is primarily supported by the Geothermal Technologies Office (GTO) in EERE, by Fossil Energy and Carbon Management (FECM), and by NE's Office of Spent Fuel and Waste Disposition, with other support coming from OE, EM, CESER and NNSA, and from 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 (e.g., for geothermal energy extraction, CO_2 sequestration, subsurface energy storage) can be manipulated for beneficial utilization while minimizing environmental risks. It is critically important to extend geoscience theory and approaches to the field scale, where research can be done under in situ conditions, across compartments and scales, and in the presence of natural forcings. To this end, the Lab has developed and is conducting significant research at several field-based subsurface energy test facilities. For example, our geothermal research 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 Enhanced Geothermal Systems (EGS) Collab project, where novel fracture stimulation and heat mining production methods are tested in situ in testbeds developed from deep tunnels at the SURF facility in South Dakota. We are also conducting two research projects focused on field-scale characterization at GTO's Frontier Observatory for Research in Geothermal Energy (FORGE) in Utah: one led by the Lab involves joint electromagnetic, seismic and InSAR imaging of fractures, and the other led by Rice University uses fiber-optic methods to monitor the evolution of the EGS reservoir following stimulation.

Berkeley Lab has a significant and broad GTO-funded portfolio beyond research on enhanced geothermal systems, including discovery of conventional hydrothermal resources, direct use of geothermal energy for heating and cooling, thermal energy storage, and exploration of synergistic benefits such as the extraction of critical materials from geothermal brines. For example, working with LLNL and Rice University, LBNL is leading a project using dark fiber within the Imperial Valley to investigate if distributed acoustic sensing (DAS) and distributed thermal sensing (DTS) can identify the presence of hidden geothermal resources and better characterize faults and fracture networks. We have just kicked off a new project with partners from UC Riverside and Geologica Geothermal Group to better characterize the lithium resource associated with the Salton Sea geothermal field and assess potential environmental impacts associated with lithium recovery from geothermal brines. We are also involved in three research projects funded by GTO as part of the international Geothermica consortium: 1) SPINE, developing a new tool and protocols to conduct stress profiling in crystalline rock for improved EGS reservoir creation; 2) DEEP, developing improved seismic monitoring technologies, modeling capabilities and process understanding to reduce the risk of induced seismicity associated with EGS; and 3) DEEPEN, developing a play fairway analysis methodology for geothermal plays associated with magmatic geothermal systems.

GTO also funds the Community Geothermal Project, which integrates low-temperature geothermal energy and subsurface energy storage techniques directly with the needs of communities. The project works with internal and external teams to couple building energy management simulations with subsurface models to optimize how the subsurface can be used for energy storage as well as heating and cooling of the built environment. It also explores new ways to combine other renewable energy resources like solar with long-duration energy storage in the subsurface to create the hybrid energy systems of the future. Researchers are exploring additional energy storage technologies, including porous media-compressed air energy storage (PM-CAES) and subsurface hydrogen storage — activities that are well aligned with the goals set in DOE's Energy Storage Grand Challenge Roadmap. Considering the future energy revolution will depend on access to critical materials and minerals, Berkeley Lab has initiated several activities and projects to ensure ready supplies of these elements. This includes a focus on lithium with the Lithium Resource Research and Innovation Center (LiRRIC): five lithium resource characterization and recovery projects have already been launched with key partners as described earlier. Through partnerships, LiRRIC is also addressing issues of energy justice through comparison of priorities between planning entities and local stakeholder communities.

The Lab's Carbon Storage program focuses on enabling geologic carbon sequestration at scale to support an effective transition from a hydrocarbon-based to a clean energy future. Key aspects of our mostly FECM-funded program include evaluating carbon sequestration risks through DOE's National Risk Assessment Partnership (NRAP) program, developing advanced monitoring and accounting solutions, and testing them at various demonstration sites, such as the Decatur project in Illinois, the Aquistore and CaMI FRS sites in Canada, and the Otway site in Australia. In another field demonstration site in Switzerland, our researchers have pioneered and demonstrated an experimental method that allows controlled fault activation tests deep underground, providing a window into the complex processes leading to induced seismicity. The Lab is a key partner in the Brine Extraction Storage Test in Florida, developing synergistic approaches to couple CCS pressure management with brine desalination methods. We also assist the Gulf of Mexico Partnership for Offshore Carbon Storage (GoMCarb) project by carrying out novel offshore modeling (CO_2 blowout into water column) and monitoring (seafloor dark fiber) of CO_2 leakage for risk assessment and assurance monitoring. Our future goal is to continue to refine and 'harden' these measurement technologies such that they can be applied at full scale carbon storage sites to provide a low-cost monitoring solution. This is an example of our 'Science-to-Hubs' technology pathway mentioned above.

The Lab has also been providing leadership in FECM's multi-institutional SMART Initiative (Science-informed Machine Learning for Accelerating Real Time Decisions in Subsurface Applications). Here, we apply ML techniques to monitor data and reservoir simulation that will contribute to real time visualization of CO_2 saturation at depth, rapid forecasting, and the development of a virtual learning environment applicable to design and management of subsurface geologic carbon sequestration sites. Beyond research on geologic carbon sequestration in deep reservoirs, we continue developing and refining a Lab-wide Carbon Negative initiative, including terrestrial and geological solutions based on enhanced mineralization of rock resources for carbon removal.

With funding from FECM and several industry partners, our Hydrocarbon Research portfolio includes efforts to identify and mitigate leakage of methane from oil and gas infrastructure and optimize methods for more efficient and environmentally sustainable hydrocarbon recovery. Berkeley Lab continues to advance the understanding of gas hydrates including the energy and environmental impacts of hydrate production through research projects to develop tools for assessment of production methods from hydrate resources or to evaluate production techniques for an ongoing field test in Alaska; and through scientific outreach such as providing technical assistance to India's Ministry of Oil and Natural Gas. We are a partner in field-based research at the Austin Chalk/Eagle Ford Field Laboratory (ACEFFL) in Texas, using continuous geophysical monitoring to assess reservoir processes associated with production.

Finally, through support from NE's Office of Spent Fuel and Waste Disposition, we are developing advanced approaches to enable safe long-term geologic disposal of nuclear waste and concomitant environmental protection. We study complex coupled subsurface processes — thermal, hydrological, mechanical, and chemical (THMC) — triggered by perturbations from the repository construction, engineered barrier emplacement, and waste disposal. Numerical modeling methods for evaluating and predicting these coupled processes are being developed and tested against experiments conducted at multiple laboratory and field scales, from micro-scale imaging of clay swelling and clay rock damage in laboratory settings to large in situ experiments conducted in Underground Research Laboratories (URLs).

The latter is part of an international collaboration program with various waste management organizations, coordinated by Berkeley Lab on behalf of DOE NE. THMC studies are critical for the evaluation of the potential long-term impacts on repository site safety. For example, temperature rise from radioactive decay may trigger an increase in pore pressure, mechanical deformations, and chemical reactions, possibly causing rock damage and mineralogical changes, which could strongly affect radionuclide transport. The THMC model is now being integrated into a system assessment framework via surrogate models derived with ML methods. New 3D HPC capabilities in the CrunchClay simulator enable accurate simulation of 10-year long experiments on rock-bentonite-concrete interfaces conducted in the clay-rich rock in the Mont Terri lab.

Complementary to the DOE-supported research at Berkeley Lab are several significant recently awarded projects with the California Energy Commission. One project is focused on the use of fiber optic monitoring of wind turbines thereby creating a link between our sensor development work and energy infrastructure deployment. A second is demonstrating at the Geysers geothermal field in California how seismic and electromagnetic data can map geothermal reservoirs and create enhanced structural imaging to better target production wells. A third is developing networked observational systems to quantify methane fluxes from energy infrastructure using aircraft, towers, and intensive ground-based sensors. These awards are in addition to those related to mineral recovery from geothermal brines mentioned earlier.

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

We are also working on exciting new characterization and monitoring methods to better constrain risk-relevant properties of natural and engineered systems, quite often using LDRD support. For example, a past LDRD project developed the ultra-dense monitoring methods for subsurface parameters and ground motions using dark fiber DAS technology, which is now deployed in the Imperial Valley to find hidden geothermal systems. A new LDRD uses "Earth Tides" (subsurface strain and fluid movement induced by tidal gravitational changes) to probe the permeability of the subsurface in uncharacterized areas. Another new LDRD is developing the next generation of low impact mineral extraction methods through electrochemical manipulation of the subsurface. We have also developed and tested advanced optical sensor and wireless communication systems that allow, for the first time, rapid determination of potential damage in critical building structures immediately after a natural hazard event. These sensors have been installed in B59 and are currently being designed for installation in BioEPIC. The application space of these technologies and tools is quite broad and can impact a wide range of infrastructure systems including energy facilities, industrial complexes, pipelines, levees, bridges, and buildings.

Biological and Environmental Sciences

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

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

The Joint BioEnergy Institute (JBEI) is one of the four DOE BRCs whose mission is to advance science, engineering, and technology to support the maximum possible conversion of carbon from lignocellulosic biomass to liquid transportation fuels and bioproducts. JBEI has successfully altered biomass composition in model plants and bioenergy crops, demonstrating that ionic liquids can deliver near-complete dissolution of plant biomass to facilitate its conversion to sugars and lignin-derived intermediates needed to produce energy-rich biofuels and advanced bioproducts. In a project funded by the California Energy Commission, JBEI scientists worked with Aemetis, the leading biofuel company in CA, to scale-up a conversion process pioneered at JBEI. This project successfully developed, optimized, and scaled an innovative “one-pot” ionic liquid pretreatment technology developed to convert waste woody biomass to fermentable sugars at 83% yields. This technology was scaled-up to the pre-commercial scale, and then the hydrolysate was converted into cellulosic ethanol by *Saccharomyces cerevisiae* with an overall fermentation efficiency exceeding 90% and achieved overall carbon conversion efficiency from biomass to fuel of nearly 80%. This process required no solid-liquid separations. Scale-up from prior lab scale (~2 liters) to a working volume of 680 liters in a 1,600 liter industrial-level fermenter was an important validation of commercial feasibility and scalability of the entire process.

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

The Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) provides capabilities for scale-up of biofuels pretreatment, saccharification, and fermentation methods. In collaborations with national labs and with industry, this facility develops new and optimizes existing processes for biofuels and bio-based chemicals and materials processes. In FY21, the ABPDU helped three companies scale-up production of new technologies that could aid in ending the pandemic. For CASPR bio, ABPDU optimized the fermentation process, scaled-up to 10 liters, and purified their CRISPR enzymes which were tested in rapid COVID detection tool kits. ABPDU also scaled-up technologies from Swiftscale on COVID antibodies and Digestiva on enzymes for protein digestibility to 300L. These projects were each executed within two just months. The facility has been instrumental in developing and optimizing new processes for bio-based chemicals and materials. Our partners have brought eight products to market as a result of ABPDU's process improvements and optimizations. 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 the 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 BETO. Led by Berkeley Lab, the ABF leverages capabilities across the complex; its partners include ANL, LANL, NREL, ORNL, PNNL, and SNL. The ABF integrates computer-assisted biological design, advanced metabolomics and proteomics techniques, ML, techno-economic and sustainability analysis, and process integration to optimize biological process design and develop methods for predictable scaling. The consortium engages with stakeholders through its industry engagement team and its advisory board of experts from companies in the bio-based products and biological computing fields. In FY21, the ABF continued 14 projects and completed 7 projects that resulted from directed funding opportunities (DFO) in FY17 and FY21 and two EERE FOAs from FY18 and FY19, enabling industry and university partners to access ABF expertise. 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 consortium has initiated an FY22 DFO to solicit additional industry and academic partner projects and has built strong relationships with LanzaTech, Lygos, Teselagen, and Agilent. In FY22, the NSF is supporting a DFO that aims to increase ABF interactions with university partners and to incorporate new biomanufacturing technologies into the platform.

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, we sustain leading capabilities in systems biology, genomics, secure biodesign, structural biology, and imaging at all length scales. 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 and infrastructure at the ALS, DOE JGI, the Molecular Foundry, NERSC, NMDC, and JBEI. The Lab has the capability to characterize complex microbial community structure and function; manage highly complex biological data; visualize biological structure; and produce large-scale gene annotation.

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

JGI produces a variety of environmental omics data that requires everything from a single node to a supercomputer to process and analyze. The single-node workload is supported through personal computers, or LBNL IT resources, whilst the large-scale computing needs are well met by resources at NERSC. To address growing scientific productivity to support analysts and researchers running complex workflows, as well as organizational resilience, JGI has developed and is deploying software and hardware infrastructure that distributes work across LBNL IT, NERSC, and at EMSL. In FY22, JGI will fully deploy this distributed computing system, maintain a central data repository at NERSC, and offsite backup data repositories at ORNL and EMSL. JGI has also engaged in a significant effort to make all data and analysis products Findable, Accessible, Interoperable, and Reusable (FAIR). Finally, informed by a rigorous user-centered design approach, JGI will deploy a new interface to its data that will make it more discoverable by humans and machines.

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). It 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 500 analysis tools spanning QA/QC of sequencing reads, genome and metagenome assembly and annotation, basic comparative genomics, RNA-seq analysis, and metabolic modeling of organisms and their communities.

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

As both JGI and KBase exist to serve a broad scientific community, our focus is on expanding user engagement and partnership with other User Facilities. KBase has established four user working groups (UWGs) on metabolism, microbiome, functional genomics, and data science to collaboratively integrate datatypes, data, tools, and analyses from DOE-sponsored groups operating in each topic area. These resources are available via the KBase platform, and regularly leverage shared infrastructure run by KBase, JGI, and other user facilities (e.g., NERSC, EMSL). Additionally, these UWGs act as cross-program users (KBase, JGI, EMSL, NMDC, etc.) that enable DOE programs to generate interoperable user-driven designs, science, and data standards. Together, JGI and KBase have continued to host joint outreach activities and booths and hold workshops. JGI users who submit proposals to their Community Science Program are encouraged to utilize KBase tools for their data analyses.

In partnership with JGI and NERSC, KBase is developing a scalable open platform for foundational genomics based on homology, taxonomy, and environmental sources of genomes and metagenomes. A JGI-KBase-NERSC call was launched in late FY18 under the Facilities Integrating Collaborations for User Science (FICUS) umbrella. This award is continually evaluated and revised as data and analysis linkages continue to improve. 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 to take advantage of new relationship types using results from the JGI co-development work and new tools being generated by the KBase team. Planned KE approaches require large-scale meta-analyses of diverse data types including ML-based inferences of microbial associations, protein structures and interactions, and biogeographic distributions. 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 is its deep and enduring ties with industry to drive the use-inspired research that will propel the bioeconomy forward, including the companies Aemetis, Novozymes, SAPPI, and Total.

The NMDC also provides critical support through leveraging existing resources, unique capabilities, and expertise across our four National Laboratory partners to deliver a set of unique microbiome data science capabilities aligned with the FAIR Data Principles. Led by Berkeley Lab, the NMDC Phase I 27-month Pilot (July 2019 – Sept. 2021) established a collaborative framework for coordinated integration of multi-omics data generated at JGI and PNNL's EMSL. The NMDC develops core capabilities in metadata standards for sample and environmental descriptors; standardized bioinformatic workflows; prototype interface for data search and access; and a robust strategic engagement plan for research teams, scientific societies, funding agencies, and publishers. Further, the Pilot builds upon integral efforts underway at the JGI and KBase (described above) and HPC systems, in particular NERSC, to provide an unparalleled integration of multi-omics data for DOE mission-relevant environmental microbiome research. Following the first annual review in August 2020, the DOE extended the NMDC Pilot for an additional 12 months to September 2022 with support to broaden collaborative infrastructure with ESS-DIVE and NSF's NEON.

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

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

Fabricated ecosystems hold the potential to bridge the gap between highly constrained lab experiments and field-scale experiments that are challenging to control, allowing researchers to dissect microbial community dynamics and effects in relevant environments. EcoFABs, small chambers with control of liquid flows and spatially defined imagining capabilities, have been employed in two BER-funded projects, m-CAFEs and TEAMS (Trial Ecosystems Advancement for Microbiome Science). Under development at Berkeley Lab, EcoPODs are meter-scale enclosed environments that allow direct and intensive monitoring and manipulation of replicated plant-soil-microbe-atmosphere interactions over the complete plant life cycle. EcoPODs are being employed to study the fate and transport of engineered microorganisms in the m-CAFEs project and will enable the “twinning” of field conditions in the BER-funded Twin Ecosystems project. This project is piloting laboratory and field ‘twin’ ecosystems that use sensors and autonomous controls leveraging unique resources in fabricated ecosystems at Berkeley Lab, PNNL’s field ecology expertise and resources, EMSL’s sensor and omics expertise, JGI’s lab automation and omics expertise, and CAMERA’s mathematical and computational expertise.

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

At the ALS, BER-funded programs 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 understanding of biomolecules at atomic resolution and in solution. The National Center for X-ray Tomography uses soft X-ray microscopy to visualize 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 2021, BER gave an ECRP award to Ben Cole for his work on understanding molecular responses to stress in energy crop plants and how those responses influence interactions with soil microbiomes. Ben employs cutting-edge sequencing and molecular profiling techniques to examine the genes and gene-regulating processes underlying how individual cells in two prominent bioenergy crops – sorghum and switchgrass – respond to drought and nutrient limitation. This work will also investigate how beneficial microbes and fungi interact with the plants under stress conditions.

Three BER ECRP awards to EESA scientists benefit greatly from Biosciences collaborations and DOE user facilities. One project, led by Neslihan Tas, involves understanding the impacts of increasing global temperatures on microbial activity in Arctic permafrost. She has identified novel permafrost microorganisms, examined of their responses to changes in soil moisture and temperature, and showed how permafrost microorganisms acclimate and take advantage of permafrost thaw. The project makes good use of collaborations with Trent Northen and Hoi-Ying Holman as well as JGI resources. A second project, led by Nicholas Bouskill, examines the mechanisms underpinning the microbial ecosystem's response to drought in tropical forest soils, and the feedback to the carbon cycle. Multi-scale field and laboratory approaches are being used to ascertain the role climate history plays in regulating the microbial response to hydrological disturbance. The project makes use of JGI and ALS to non-destructively characterize a cell’s biochemical phenotype under stress. The third project, led by Kolby Jardine, characterizes the metabolism of cell wall ester modifications and volatile intermediates and their roles in plant physiology in the emerging biofuel tree species, California poplar. Understanding and manipulating the metabolism of cell wall modifications could provide a basis for engineering plant resistance to environmental extremes as well as contribute to the sustainable production of biofuels and bioproducts. The project benefits from JBEI and EMSL collaborations to address 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 hydrologic and geochemical fluxes of both biologically critical elements, such as carbon, nitrogen, and phosphorus, and energy-related waste products, such as radionuclides and heavy metals. Such interactions also exert primary controls on processes impacting water and energy security, water availability for energy, industry, and urban use, as well as agriculture production.

With support from BER, Berkeley Lab is developing a predictive understanding of watershed responses to extreme hydroclimatic behavior and impacts to biogeochemical function—from microbial to watershed scales. The Watershed Function SFA is developing new constructs and approaches to predict how vulnerable mountainous watersheds respond to increasingly frequent perturbations, such as droughts, floods and early snowmelt, and the associated impacts to downgradient water quality and quantity. Important advances over the last year include: improved prediction of hydroclimate impacts on downgradient water discharge; tested 4D digital watershed and functional zone approaches for characterizing complex watersheds in a scalable and transferable manner (e.g. inter-watershed transferability); demonstrated the first satellite monitoring of groundwater depletion at management scales; advanced ML for predicting watershed organization and functions; documented the heretofore unrecognized role of bedrock weathering in nitrous oxide, a potent greenhouse gas; predicted the influence of wildfire and snowmelt dynamics on groundwater recharge in mountainous systems; and advanced the first watershed-based documentation of the impact of wildfire on water quality. As soil-plant-microbe-interactions play a key role in water and biogeochemical cycling, the Watershed SFA is an anchor tenant of BioEPIC. BioEPIC platform technologies, such as the EcoSENSE SMARTSoils testbed, are adding critical value by addressing key questions posed by the Watershed SFA and its related research enterprises in sensing-data-model integration, with a near-term focus on improving estimates of evapotranspiration and nitrogen cycling.

As noted earlier, with the co-location of overlapping BER investments at the East River experimental watershed in Colorado, the Watershed SFA community has continued to advance a predictive understanding of multi-scale mountainous watershed processes spanning the bedrock-to-atmosphere continuum. Field deployment of DOE ARM's Second Mobile Facility (AFM2) and instrumentation associated with a companion atmospheric research campaign led by NOAA began in late summer 2022, with real-time data generating in late September. These data streams are quantifying where, when, and how precipitation falls within a large portion of the Upper Gunnison River basin and aims to link hydrologic processes spanning the atmosphere-to-bedrock continuum to concomitant measurements being made by the Watershed SFA. Such linked measurements are being used to constrain predictive models in ways that have little precedent in North America, with important implications for assessing key hydroclimatological drivers impacting the future of water in the Western US.

To improve prediction of future watershed function, a range of HPC, AI and data approaches are being developed, including adaptive mesh refinement methods to enable models that can telescope into a watershed to capture fine-scale processes. Advanced simulation capabilities are being developed for watersheds through the multi-institutional Interoperable Design of Extreme-Scale Application Software (IDEAS-Watersheds) and ExaSheds projects, both funded by BER. This effort yielded the first HPC watershed flow and biogeochemical reaction capability that was used to predict concentration-discharge relations in the Copper Creek catchment within the East River watershed. Deep-time models have been used to quantify the nitrogen cycle with unprecedented rigor. ExaSheds has made advances this year in hybrid physics and machine-learning approaches, as previously described, with development of a first-of-its-kind reduced dimensional modeling approach for computing biogeochemical fluxes at the river basin scale. A BER ECRP is investigating the impacts of hydrometeorological disturbances, such as floods, droughts, and heat waves, on river water quality at continental scales. The study utilizes data-driven methods including a novel data integration tool, BASIN-3D, and ML techniques for classification and prediction to understand water quality response and resilience to disturbance in different watersheds.

With BER support, expertise and capabilities associated with monitoring and predicting hydrobiogeochemical watershed dynamics have been extended to address challenges associated with agriculture, environmental remediation, the onset of harmful algae blooms, and water quality impacts from wildfire. With EM support, we are developing a new AI-based paradigm for long-term monitoring of DOE's legacy contaminated sites, and specifically at the Savannah River Site. The Lab was also chosen by DOE's Office of Legacy Management (DOE-LM) in response to a report issued by the U.S. Government Accountability Office (GAO) examining the resilience to future climate disturbance of critical DOE-LM infrastructure. BER-developed capabilities are being used and extended through the California water agency and CalFIRE support to address surface and groundwater quality in regions impacted by the recent significant California wildfires. They are providing the first watershed-based strategy for investigating wildfire impacts on water quality. We are engaging in various wildfire-focused city, state, and Western U.S. science panels. LDRD investments have extended BER-developed insights about coupled biological-environmental-climate systems to advance ML and systems approaches for predicting the onset of algae blooms; and to advance approaches to estimate subsurface biogeochemical interactions using volatile organics sensed from above the ground.

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

Berkeley Lab conducts internationally recognized research on advancing the understanding and prediction of ecosystem responses and feedbacks to climate. We lead the TES Belowground Biogeochemistry SFA, which contributes to developing a new paradigm for soil organic matter dynamics through basic research on soil carbon turnover, storage, and loss. This SFA is producing new understanding and improved predictions of belowground biogeochemistry in the soil-plant-microbial system and the role of soils in global change. Soil warming experiments are ongoing at Blodgett Forest, CA, and efforts are underway to develop a more extensive SFA experimental site at Point Reyes, CA. The Lab-led NGEE-Tropics advances cutting-edge predictive representation of tropical forest carbon balance and climate system feedbacks in DOE's E3SM climate model using a modeling-experimental (ModEx) approach that combines model development and extensive field research. NGEE-Tropics is global in scale, with tropical forests accounting for the largest terrestrial carbon, water, and energy fluxes, comprising Earth system feedbacks that are widely recognized as essential for accurate climate projections. NGEE-Tropics leads the development of a process-rich tropical forest ecosystem model—the Functionally Assembled Terrestrial Ecosystem Simulator (FATES)—which enables the representation of physiology, growth, competition, and mortality of individual plants at scales tractable for global simulations. FATES introduces a mechanistic and trait-based approach to vegetation dynamics and climate impacts on ecosystems within the DOE E3SM climate model. The Lab is applying FATES to understand potential drought response and tree mortality in California as part of a BER ECRP, and to model wildfire and vegetation distribution in the western U.S. as part of a UC-funded collaboration. FATES development is expanding as E3SM's global dynamic vegetation model to address critical terrestrial-climate system carbon, water, and energy feedbacks. As a key partner in the NGEE-Arctic project, the Lab contributes its expertise in environmental geophysics, soil biogeochemistry, microbial ecology, and mechanistic modeling of ecosystem-climate feedbacks. For example, the team developed a distributed temperature profiling system and coupled such measurements with electrical-resistance tomography and remote sensing data to quantify the controls on permafrost thaw with unparalleled resolution; measured CO_2, CH_4, and energy fluxes and evaluated how spatial heterogeneity in plant and soil properties drives CO_2 fluxes measured at flux tower sites; revealed the impact of rain and heat advection on accelerating permafrost thaw; projected that 21st century changing high-latitude seasonality will significantly increase the spring net carbon uptake; and forecasted that fire and 21st century climate will double deciduous plant productivity in high-latitude regions.

Six BER ECRP projects showcase the Lab's efforts to scale from microbial mechanisms to ecosystem processes to landscapes. Two ECRP awardees are focused on global change impacts on soil microbiomes and their consequences for global biogeochemical cycles and atmospheric feedbacks. One project tackles the microbial metabolic response to permafrost thaw, using microbial communities as integrators of site conditions to predict forward trajectories of biogeochemistry following permafrost thaw. The other is focused on drought in tropical systems and its impact on carbon processing and stabilization by the soil microbiome and implications for drought resilience and forest productivity. As described above in the Biological Systems 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 NGEE-Tropics project research and connects climate-relevant plant volatile emissions to biochemical roadblocks of biomass deconstruction. A fourth project explores the implications of western U.S. climate extremes and recent severe droughts on western forests using FATES, using these droughts to predict forests' response to increasing disturbances, as well as to predict similar forest responses to the northward shift in the mid-latitude storm tracks, and the associated shifts in rainfall patterns, predicted and now observed under global anthropogenic climate change. A complementary ECRP on terrestrial ecosystem vulnerability to wildfire in coastal zones is led by a joint faculty member. The sixth project, described above, is an investigation of the impacts of streamflow disturbances on water quality using a data-driven framework. This study is designed around extensive application of ML to understand water quality changes in the river corridors and watershed attributes that confer resilience to extreme events.

Berkeley Lab also leads the AmeriFlux Management Project (AMP), which serves the AmeriFlux network of 560 sites and the broader scientific community by producing high quality data products of ecosystem-atmosphere fluxes of carbon, water and energy that enable scientific and modeling advances. Approved for Phase 3 (FY21-FY25), the renewal proposal scales AMP activities to serve a bigger network and accommodate network growth; scales AmeriFlux to more of the Americas' geography and people; and scales the impact of fluxes for science and stakeholders. AMP has worked to keep the AmeriFlux community connected in the past year, organizing virtual events that reached a larger and more diverse audience: AMP produced 17 community webinars, an annual meeting attended by >250 people from 30 countries, and a joint ARM/ASR/ESS workshop on land-atmosphere interactions with >350 attendees. The 2021 theme, "The Year of Water Fluxes," was meant to increase the quality and visibility of water-cycle measurements across the network and expand coordination through the US-GEWEX consortium. AmeriFlux data continue to see widespread usage: the site data in FLUXNET2015 and BASE products were downloaded more than 40,000 times by more than 6,000 unique users in the past five years. AMP increased by 20% the number of sites for which data were available. AmeriFlux contributes directly to BER ESS's Coastal Systems program, with over 200 flux-measurement sites located within 50 miles of a coastline.

We are advancing AI to explore many challenges associated with carbon cycling and healthy soil. "Rice'n Grits," an ongoing SMARTFARM project funded by ARPA-E, is using ML to quantify the carbon intensity and budget in farming. In addition, Berkeley Lab leads the data integration and scaling project (CARBON STANDARD) in the SMARTFARM program, wherein all SMARTFARM field teams will provide data for ML-based data synthesis and scaling. Berkeley Lab also leads a project in the ARPA-E ROOTS program: the TERI (Tomographic Electrical Rhizosphere Imager) technology developed via the project recently won first prize in the international RootScanner challenge organized by Bayer Crop Science. We are part of a multi-lab organizing team partnering with BER's Earth and Environmental Systems Sciences Division to advance a new initiative on AI for Earth system predictability (AI4ESP). This initiative explores how AI can be harnessed—together with multi-scale mechanistic models, diverse observations, and technologies such as edge computing and exascale capabilities—to engineer paradigm-changing advancements in Earth system predictability with a particular emphasis on hydrological extremes.

Berkeley Lab is one of the primary science centers studying hydroclimate and land-atmosphere interactions, and currently leads several major BER projects in the Atmospheric System Research (ASR) and Atmospheric Radiation Measurement (ARM) programs. The Lab-led Surface Atmosphere Integrated Field Laboratory (SAIL) Campaign successfully deployed DOE's Second ARM Mobile Facility (AMF2) to Colorado's East River Watershed in September 2021 to measure the atmospheric processes and land-atmosphere interactions that govern hydroclimate in the Upper Colorado River. SAIL's data collection is funded by ARM; the Lab is supported by ASR to perform scientific research activities associated with SAIL. With strong partnerships across its partner institutions, SAIL is also tightly integrated with the Watershed Function SFA to achieve the world's most comprehensive mountainous atmosphere-through-bedrock observatory. Furthermore, SAIL has precipitated additional campaigns, including

NOAA's Study of Precipitation, the Lower Atmosphere and Surface for Hydrometeorology (SPLASH) and NSF's Sublimation of Snow (SOS) Campaigns, as well as international collaborations with Deutsche Forschungsgemeinschaft (Germany). These collaborations are co-located with SAIL; they are making additional measurements to achieve mountainous hydroclimate benchmark data at unprecedented scope and scale.

With five other National Labs, we have developed and operate the ARM Carbon Project and ARM Aerosol Observing System Infrastructure to conduct measurement of trace gasses, to contribute to cross-program research on land-atmosphere interactions and multi-agency validation of satellite-based column CO2 estimates. The Lab's ASR project on Convection and Land-Atmosphere Coupling in the Water Cycle is advancing climate prediction by improving representation of land-atmosphere coupling. We are pioneering the use of digital stereo photogrammetry to observe clouds, which play a critical role in weather and Earth's radiation balance. The Lab deployed six new cameras ringing the SGP ARM site in Oklahoma that provide a 4D gridded view of shallow clouds. Every 20 seconds, these generate a 50 m grid of cloudiness and cloud geometry, called Clouds Optically Gridded by Stereo (COGS). These new capabilities are providing unprecedented data on cloud sizes, lifetimes, and life cycles—critical information for developing cloud schemes for next-gen weather models.

Berkeley Lab is a major contributor to DOE's flagship Earth system modeling project, continually advancing the Energy Exascale Earth System Model (E3SM). The Lab's contributions include improved biogeochemistry representation between the soil, plant, and abiotic processes responsible for constraining the global carbon budget. Within ELM, the Lab has also developed an extensible and scalable three-dimensional hydrology and thermal module, a multi-phase reactive transport solver, and is leading the development of the FATES dynamic vegetation model. 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. These developments will allow for future projections of U.S.-relevant carbon pathway scenarios using state-of-the-science treatments of physical, chemical, and biogeochemical processes. Lab researchers serve as members of the E3SM leadership team for the land model group and NERSC exascale applications. Ongoing work in E3SM v2 includes a new AI fire model, land-use land-cover change capabilities in FATES which will interact with E3SM's IAM component (i.e., GCAM), and evaluation and analysis with plant hydraulic dynamics and plant nutrient competition in FATES. Outside of terrestrial processes, the Lab is developing high-resolution ice sheet modeling using an Adaptive Mesh Refinement to accurately model the physical processes of ice sheet retreat 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 2022, the Lab quantified anthropogenic, atmospheric, and oceanic drivers of hydroclimate extremes in the continental U.S. via an extensive analysis of climate simulations produced for the Coupled Model Intercomparison Project version 6 (CMIP6). Several recent deliverables illustrate this success, including publication of the latest versions of the Toolkit for Extreme Climate Analysis (TECA) and the software tool climextRemes, both of which allow sophisticated analysis of extreme events in massive datasets.

Co-led by LBNL, the RUBISCO SFA studies the interacting roles of biogeochemical and water cycles and their feedbacks in the Earth system. Our diverse team studies a wide range of Earth system science problems across multiple spatial and temporal scales, including permafrost carbon dynamics, carbon–climate feedbacks, land-use change, methane emissions from wetlands, wildfire effects on the terrestrial carbon cycle and atmospheric composition, and the application of machine learning methods. We are also active in CMIP6 model analyses, including using our ILAMB benchmarking package.

BER is the primary sponsor of the research in the Lab's climate change and atmospheric science core capabilities. Other sponsors include DOE ARPA-E and SBIR, SERDP, NASA, UC, 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. The Lab has substantial expertise and research activity to meet the challenges of exascale computing, including performance analysis and algorithms, programming languages, systems and tools and alternative computer architectures for increasing future computing capability. Also significant is our work on high performance parallel I/O, ML, scientific workflows, data management, user experience, and data-intensive visualization and analysis targeted at exascale computing. Not all computer science challenges are associated with exascale computing. Our development of scalable solutions for scientific data, including management, curation, archiving quality-assurance, distribution, and analysis, troubleshooting and performance-analysis tools for complex, distributed applications will substantially impact the broad computational challenges faced by those who seek to understand data produced by experiments and observations coming from environmental sensors, genomics, light sources, and cosmological observations, etc.

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

- *Resource Disaggregation:* The cost and complexity of existing interconnects prevent designing datacenter racks tailored to emerging applications such as ML. Resource disaggregation is a system-level approach to runtime customization of heterogeneous system elements, in which compute, memory or storage modules are flexibly combined through one-model-fits-all embedded photonic connectivity and better utilize distant resources.
- Heterogeneous Int*egration:* This approach looks at co-integrating diverse "blocks" of chip designs from vendors like Arm and government innovations to create designs tailored for HPC. Currently this is supported by Project 38, an interagency collaboration between DoD and DOE, focusing on a set of vendor-agnostic architectural explorations.
- *Custom Acceleration for Science:* A complementary approach is to select a high-value application target and design a custom accelerator around that application's requirements. Over the past two years, we have co-designed a custom accelerator design targeting Materials Science Codes (Density Functional Theory); these codes account for a large fraction of DOE's HPC workload. This has led to a more rigorous mathematical approach to translating procedural algorithms into a form suitable for dataflow acceleration with custom circuits and has also demonstrated 22x speedups on CGRAs like GraphCore and SambaNova compared to NVIDIA's latest GPUs.

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

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

The Lab is a pioneer in scalable workflow solutions for scientific data, including meta-data generation, management, curation, quality-assurance, distribution, usability, and analysis. The growth in scientific data volumes has resulted in a need to scale up processing and analysis pipelines using HPC systems. These workflows need interactive, reproducible analytics at scale. Our efforts bring together core technologies based on the Jupyter Platform to create interactive, reproducible analytics at scale on HPC systems. Berkeley Lab leads the data processing and curation aspects of the BER-sponsored AmeriFlux Management Project and NGEE-Tropics, described in the Climate Change Science and Atmospheric Science core capability, which focus on distributing high quality, standardized datasets to a variety of end users. We also developed and run the Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository, whose mission is to preserve, expand access to, and improve usability of critical data generated through DOE-sponsored research of terrestrial and subsurface ecosystems. We lead the work on the Neurodata Without Borders: Neurophysiology (NWB:N) data standard for neurophysiology, providing neuroscientists with a common standard to share, archive, use, and build analysis tools for neurophysiology data. We lead the Software Engineering Team for the FE-funded Institute for the Design of Advanced Energy Systems (IDAES), Carbon Capture Simulation Industry Initiative (CCSI2), National Water Alliance Initiative (NAWI), and PARETO Produced Water projects that are developing next-gen modeling and optimization platform to aid in the design of novel energy and water systems, where our 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. Science Capsules are enabling automated capture of scientific workflow executions. Our work in HDF5 is expanding its impact on data across the science areas that benefit from the improved organization, performance, and search our HDF5 work enables. Our user experience work has crosscut the sciences, helping to better understand the critical needs in each area and translate those requirements into needs-focused research and development.

Berkeley Lab is a leader in developing software to enhance, troubleshoot and debug performance of complex, distributed scientific applications. Lab-developed open-source software has had tremendous impact worldwide. The PERFormance Service Oriented Network monitoring ARchitecture (perfSONAR) application, is now deployed at over 2,000 sites worldwide in national laboratories, commercial and research networks, universities, and corporations. Our researchers are piloting 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 and data management software like RUCIO. This approach has been adopted by the ExaFEL ECP project and deployed worldwide through the AutoGOLE project. In addition, we are exploring the application of ML techniques on network traffic prediction to optimize traffic engineering and routing of large scientific flows over uncongested paths, and revolutionizing measurement and monitoring of elephant data flows. We will find these performance issues by developing a nano-second precision packet telemetry system leveraging FPGAs, programmable data planes, and an innovative software processing infrastructure as part of the 'high-touch' component of the ESnet6 project. The same FPGA platform is being leveraged for edge-computing with prototype deployment at an ALS beamline, NCEM, and an innovative edge computing/load balancing project with JLAB. Now complete, the first phase of FABRIC (whatisfabric.net), an NSF mid-scale project, will 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. The team is turning next the design phase.

We are pursuing a comprehensive strategy for edge computing and *in situ* data processing at data sources – a crucial technology to address the increasing data volumes from new experimental facilities. Our goal is to design and deploy specialized computing workflows that include new/efficient algorithms, codes, programming systems, specialized hardware, and networking to enable real-time computing for streaming data in-situ with the experiment.

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

The Lab has unsurpassed expertise in algorithms for modeling and simulating compressible, incompressible, and low-Mach-number flows in many applications, from combustion processes to ice-sheet formation and retreat to atmospheric and cosmological flows. Adaptive Mesh Refinement techniques pioneered at the Lab are globally recognized as a key enabling technology, and our Exascale

AMR Co-Design Center continues to improve AMReX, a software framework leveraging a variety of hybrid CPU/GPU systems that supports ECP and SciDAC scientific simulation codes for combustion, astrophysics, cosmology, accelerator technology, and multi-phase flow.

For example, we are collaborating with researchers at Princeton University, University of Michigan, UC Berkeley, and the University of Maryland to develop a method to model axion dark matter cosmology at high resolution. The multiple scales necessary for modeling axion cosmological strings have previously made it difficult to provide a precise prediction of the dark matter particle mass. However, using the AMReX framework to increase resolution of the axion string cores, has led to a significantly more precise prediction of the axion particle mass, suggesting new experimental designs for detecting dark matter particles.

Lab mathematicians have also developed a 3D phase field modeling framework for simulations of low-energy consuming ferroelectric material-based field effect transistors. Ferroelectric materials are being explored for beyond-CMOS microelectronics by one of the DOE microelectronics co-design teams. Existing codes for ferroelectric field effect transistors (FeFET) utilize 2D formulation and simplified models for semiconductor charge transport. The new 3D code, based on the AMReX library, serves to bridge the gap between material discovery and device design by performing predictive simulation of multi-physics processes at device level. It utilizes material parameters obtained from experiments or ab-initio calculations and predicts device characteristics to be used by circuit and system designers. It will also perform the converse function, i.e., motivate material discovery by providing device level metrics.

Berkeley Lab has also made significant strides in developing methodology for simulating the dynamics of physical systems at microscopic and mesoscopic scales. In collaboration with San Jose State University, we developed a hybrid Lagrangian-Eulerian approach for simulating complex fluids at the mesoscale. Dubbed Discrete Ion Stochastic Continuum Overdamped Solvent (DISCOS), this method captures important molecular scale features of a flow using fluctuating hydrodynamics and immersed boundaries – at much lower cost than the traditional molecular dynamics method. This has been previously applied to model bulk electrolytes at the nanoscale and is now being used to simulate confined flows and fluids containing complex molecules such as polymers. Fluctuating hydrodynamics simulation techniques are also being used for studying the effect of thermal fluctuations in microscale flows of multiphase mixtures using a thermodynamically consistent approach for an arbitrary number of phases and components based on Flory Huggins theory. These techniques lay the foundation for studying spinodal decomposition processes relevant to the manufacture of organic photovoltaics and separation membranes, liquid nanothreads, and nanodroplets.

The Center for Applied Mathematics for Energy Research Applications (CAMERA), an integrated, cross-disciplinary center, is jointly funded by ASCR and BES. Its aim is to develop the fundamental new mathematics required to support DOE user facilities. In recent years, CAMERA scientists have developed a series of breakthrough mathematics that are being used at multiple DOE facilities and around the world:

- CAMERA invented the first mathematical and algorithmic formulation for extracting rotational diffusion coefficients from x-ray photon correlation spectroscopy data (XPCS). The new methods reconstruct these coefficients with an error less than 1% and are now being carried into 3D; these methods are poised to take advantage of coming synchrotron upgrades at several DOE facilities.
- We have continued to customize and exploit CAMERA's Multi-Tiered Iterative Projection (M-TIP) approach, with new applications to coherent surface scattering imaging (CSSI), joint with Argonne's Advanced Photon Source. This allows 3D imaging of thin materials.

- With NSLS-II, we have developed a new approach for alignment of tomographic data, which handles jitter and non-uniformities in measured data. This approach works with relatively sparse data and relies on a customization of M-TIP.
- CAMERA has developed the gpCAM mathematical environment, algorithms, and software suite to drive autonomous experimentation, relying on various forms of Gaussian Processes as well as incorporating known physical knowledge. These methods are in use across multiple DOE facilities and in Europe and have led to numerous advances and cost-savings, including Brookhaven's six-fold decrease in the number of experiments required to obtain the same information; a 50-fold decrease in data collected at LBNL's Berkeley Synchrotron Infrared Structural Biology (BSISB) beamline; and a reduction of experiments from one month to one night at the Institute-Laue-Langevin in Grenoble, France.

CAMERA scientists are engaging with new BER-funded projects, including developing the image analysis and recognition algorithms as well as the autonomous driven experiment algorithms for the EcoTwins project which builds, measures, and analyzes plant structures grown in a controlled environment and mirroring experiments in the field. This is a collaboration between CAMERA, Molecular Physics and Integrated Biophysics (MBIB) and the JGI at LBNL, and PNNL's EMSL.

In numerical linear algebra, Berkeley Lab is the only SC lab that has expertise in large-scale eigenvalue calculations and direct solutions in sparse matrix inversion. Direct and pre-conditioned iterative solutions of high-frequency wave equations are critical components for many ECP and SciDAC applications, including MFEM at LLNL, accelerator modeling at SLAC, and EM simulation codes at Sandia. Their fast solutions require leveraging the recently developed numerical linear algebra tool, Butterfly, to exploit the low rank structures of the linear systems similarly to what is done in the classical FFT algorithm. The resulting hybrid algorithms have enabled us to push the capability of STRUMPACK for high frequency wave equations from 300^3 to 500^3. They also developed butterfly-enhanced integral equation alternatives to STRUMPACK that require 5x lower mesh density and added high-order basis functions to enable improved accelerator cavity modeling. The Lab also developed the first sparse direct solver for multi-GPUs using a multi-precision approach, resulting in 30-40% faster performance than the original double precision code by reducing the memory footprint and lowering communication volume. This takes advantage of the recent addition by hardware vendors of faster units for low-precision arithmetic that were originally for the ML community.

As part of an early career project, a high-order quadrature algorithm, used for solving partial differential equations, e.g., to solve complex multi-phase multi-physics problems, has been developed that can automatically handles various kinds of complex geometry, including multi-component domains, tunnels, junctions, self-intersections, and cusps.

To meet the needs of DOE SciDAC partnerships, DOE Computational Materials Software center, DOE Computational Chemical Science center, and EFRC projects in quantum chemistry and nuclear physics, Berkeley Lab developed better Kohn-Sham density functional theory based nonlinear eigensolvers, configuration interaction based sparse linear eigensolvers, linear response eigensolvers and tensor eigensolvers. Some of these have now been ported from many-core CPUs (NERSC Cori KNL) to multi-GPUs (NERSC Perlmutter). These eigensolvers are integrated with application software tools such as Quantum Espresso, SIESTA, NWChemEX, BerkeleyGW, MFDn, and Omega3P.

These capabilities and their applications are sponsored primarily by ASCR, with support from other DOE program offices and SPP. They support DOE missions in fusion energy science, biological and environmental research, high-energy physics, nuclear physics, accelerator technologies, 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 energy and environment DOE mission areas.

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, environmental management, and all Core Capability areas described in this Plan. The Lab has effectively integrated these research areas in conjunction with HPC resources to obtain significant results in 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. In addition to providing senior leadership and leveraging our Applied Math and Advanced Computer Science, Visualization and Data core capabilities in the two SciDAC Institutes, FASTMath, and RAPIDS, we are involved in 14 of the 30 SciDAC-4science partnership projects. We provide advanced computer science methods and robust applied math techniques and algorithms for enabling and accelerating scientific discoveries. Under SciDAC-5, we are participating in all five partnership projects funded by BES. These benefit from the results of FASTMath and RAPIDS. Furthermore, the Lab plays key roles in 12 Application Development subprojects in the ECP, supporting computational science development for exascale systems across many disciplines. RAPIDS' roofline methodology has been extended to analyze deep learning workloads and emerging accelerator technologies and has been integrated into the production vendor tools of Intel Advisor and NVIDIA Nsight Compute. RAPIDS has enabled a two-order of magnitude improvement of data sharing (compared with disk I/O) by transferring variables directly on two BOUT++ simulations computing ELM and transport. A collaboration between RAPIDS and NERSC explored important scientific ML workloads in cosmology and climate analytics and increased overall performance by up to 10x. A FASTMath and RAPIDS collaboration led to the first multi-node/multi-GPU sparse triangular solver, which shows 6x speedup over that in NVIDIA's cuSPARSE using 16 GPUs. The Lab's SciDAC researchers' paper in the *SIAM Journal on Matrix Analysis and Applications* described a factor of two-five improvement of an implementation of an approximation algorithm for a Traveling Salesman Problem arising in the optimization sparsity structure for GPU implementation of certain sparse matrix computation. The Lab's researchers developed a reinforcement learning-based eigensolver for selected configuration interaction for molecular systems. They also developed GPU-accelerated implementations of eigensolvers for nuclear structure calculations and many-body localization studies. Others have contributed to an effort to better understand uncertainties in projections of future ice sheet contributions to sea level rise and are co-authors of a high-profile *Nature* paper reporting the results of that effort. Working with SciDAC collaborators, Lab researchers in ProSPect have helped develop a new way to model the calving processes that occurs in Antarctic ice shelves, along with a novel model for subglacial hydrology which uses adaptive mesh refinement to resolve subglacial channelization under an ice sheet.

The Quantum Information, Science, and Technology Group (QuIST) is a multidisciplinary team developing quantum computing hardware based on superconducting electronic circuits. QuIST concentrates on all aspects of design, co-design, fabrication, characterization, operation fidelity optimization, and deployment of superconducting quantum computing processors. This group is implementing quantum protocols and algorithms that advance and push the frontiers of QIS. Further, they are interfacing with the wider QIS community through the Advanced Quantum Testbed User program, which has been running a wide range of experiments in collaboration with users and recently completed its second call for proposals.

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

The Computational Biosciences Group brings together experts from our core capabilities of Computational Science, Applied Mathematics, Machine Learning, Data Management and Analytics, with strategic partners in the Biosciences Area to understand the dynamics and multi-scale nature of many biological problems. Recent work has focused on molecular inverse design through ML to recommend molecules which meet a desired specification, along with the pathways to synthesize them. We have built several general-purpose statistical-machine learning tools to reveal interpretable latent structure and applied them to complex biomedical data sets as part of an AI-codesign project. This project also evaluates diverse ML-hardware accelerators towards sustainable AI. We have developed tools to enable FAIR data ecosystems for diverse biological communities in environment, bioenergy, and health.

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.

While 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. Others 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 the accurate description of complex systems.

Cyber and Information Sciences. Berkeley Lab conducts research into a broad array of cyber and information sciences (secpriv.lbl.gov) including security for scientific and high-performance computing environments, high-throughput networks, "open science" computing workflows, and the power grid. Examples include the development of RISC-V based hardware trusted execution environments (TEEs) appropriate for HPC to isolate data and computing from cyberattacks and leveraging differential privacy to enable privacy-preserving analysis and ML model training without exposing raw data. Ongoing, current, and future work in trustworthy hardware/software co-design for "edge to HPC," scientific computing, from architecture to OS and runtime, is being performed to ensure both the integrity and the confidentiality of scientific computing in the face of accidental or malicious threats, without significant cost to either usability or performance. Gem5-based hardware architectural simulations are being constructed to enable security and performance design space exploration, and formal verification is being applied to prove correctness of protocols, APIs and key elements, and interfaces.

Novel research techniques are also leveraging the "physical" aspects of cyber-physical systems, such as the power grid, to detect cyber-attacks against equipment controlling this grid. Because these systems must act within the laws of physics, these properties can be exploited to detect malfeasance or failing sensors. In two current power grid cybersecurity projects, we are leveraging AI to automate the use of defensive control logic to maintain power grid stability in the face of solar inverters or grid-attached storage, with the development of the PyCIGAR software being integrated into the NRECA Open

Modeling Framework (OMF). With LDRD funding, AI is also being examined for its vulnerabilities by developing means to detect and mitigate attacks on complex, automated, AI-driven cyber-physical systems, including power grid control elements and synthetic biology “self-driving labs.”

The Lab serves in prominent leadership roles in cyber sciences, including with IEEE Security & Privacy; the NSA Science of Security Distinguished Expert committee; the DARPA Information Science and Technology (ISAT) Study Group, where it is leading a “cyber moonshot” study on accelerating security of systems with emerging technologies; and the DOE Securing Energy Infrastructure (SEI) Executive Task Force Technical Project Team (TPT) on Developing a National Cyber-Informed Engineering (CIE) Strategy.

In addition to our cybersecurity research, ESnet provides an integrated set of cyber security protections designed to efficiently protect scientific 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, promotes cybersecurity research at scale. The Lab leads the world in developing technologies to optimize science data transfers across local and wide-area networks. ESnet’s “Science DMZ” model champions an architecture to transfer data securely across the national and international research and education community. This model continues to be developed since many data sets have special privacy and security concerns. In particular, the “Medical Science DMZ” was designed to help address the concerns of HIPAA/HITECH while supporting the high-performance needs of big data science.

Formerly known as Bro, the Zeek network security analysis framework started at Berkeley Lab in 1995 to monitor network traffic in open scientific environments. It is now deployed at National Labs, major universities, supercomputer centers and, particularly through the Corelight commercial spinoff, *Fortune 100* companies. Starting in 2010, Zeek went through a major overhaul to support next generation networks at 100Gbs, with one of the first production 100Gbps deployments at the Lab in 2015. Currently, ESnet is exploring novel techniques to apply Zeek on a WAN environment where geographically dispersed, asymmetric traffic breaks the assumptions of most network security monitors. New technologies in ESnet6 will potentially provide the building blocks to solve this security challenge and more at scale. ESnet maintains leadership both formally on the Zeek management team, and with the many technical contributions back to the project.

Berkeley Lab also co-leads Trusted CI, the NSF Cybersecurity Center of Excellence (https://trustedci.org), where it has had leadership roles in recent years in directing the development of groundbreaking reports on profiling cybersecurity risks to open science, evaluating trustworthy data,, identifying issues in data confidentiality and privacy in scientific computing, and the state of software assurance in research computing, and the security of *operational technology* (or *cyber-physical systems*), such as sensor and control elements, used by major scientific research facilities. It has also participated in one-on-one engagements with developers of software used in research computing.

ASCR, the CEDS R&D and CEDS Threat Mitigation programs in the CESER office (including GMI/GMLC), and NSF are the primary supporters of this Core Capability, as well as recent DOE SETO, DHS S&T, CSR and LDRD support, and with additional previous support from EERE/BTO, OE, OCIO, NNSA, NSF, and NSA/LTS. Significant benefits accrue for all SC offices and other elements of DOE, as well as strategic partners such as the DoD, the IC, and NIH. This capability supports SC’s mission with disciplines, technologies and practices designed to protect, analyze, and disseminate information from electronic sources, including computer systems from edge devices to HPC, computer networks, sensor networks, and network-connected scientific instruments and user facilities.

High Energy and Nuclear Physics

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

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

On the Energy Frontier, Berkeley Lab is playing leading roles in the ATLAS pixel and silicon strip tracking upgrades for HL-LHC (including major contributions to the tracking reconstruction software), has the leadership role in the core offline software while contributing more generally to computing and software systems, plus substantial contributions to Higgs, SM, and BSM physics analyses. The Lab plays a leading role in the international R&D program to develop the pixel readout ASIC for both ATLAS and CMS HL-LHC upgrades and developed the silicon strip stave concept that has been adopted by the ATLAS collaboration. The Lab leads the Global Mechanics upgrade for the new tracker in the U.S. ATLAS HL-LHC Upgrade project.

We also play leading roles in the ATLAS software framework, and more recent efforts have focused on the applications of ML and quantum computing techniques, as well as more efficiently harnessing NERSC's HPC capabilities. Over the years, the Lab scientists has led all aspects of ATLAS, including as Physics Coordinator (twice), Deputy Spokesperson, Upgrade Coordinator, Computing Coordinator, Simulation Convener (twice), Upgrade Physics Working Group Convener, SM Working Group Convener, SUSY Working Group Convener and Higgs Working Group Convener. We are 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 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 2012-17. We are leading the LUX-ZEPLIN (LZ) experiment. LUX completed data taking in 2016 and produced results that are still among the most sensitive limits in the search for dark matter. After LZ received CD-4 in September 2020, installation and commissioning of the detector were completed at the end of 2021. The experiment began routine physics operations in December 2021. Berkeley Lab played many leading roles in the LZ construction project, including the Project Director and Project Manager, and is leading the Operations phase. We continue a leadership role during the Operations phase of the experiment. Our scientists served as spokesperson, physics coordinator, calibration coordinator, as well as leading many analysis working groups. Supported by a DOE ECRP Award, we are pursuing R&D on an LZ upgrade that would involve freezing the xenon to trap radioactive impurities and dissolving lighter species in the liquid xenon to enhance low-mass sensitivity. We are also pursuing advanced low-mass dark matter detection techniques supported by a new QuantISed consortium grant to develop new quantum-enabled sensors and readout and the TESSERACT concept to deploy TES readout on multiple targets supported by DMNI R&D funding. In addition, LBNL designs and oversees fabrication of skipper CCDs for the SENSEI and DAMIC dark matter experiments.

The Lab led the successful design and construction of the Dark Energy Spectroscopic Instrument (DESI), a Stage IV BAO experiment to create the largest 3-D map of the universe, with close to 40 million galaxies. DESI successfully passed CD-4 in May 2020 and started its main survey in mid-2021 after re-commissioning and survey validation. The Lab has developed a detailed DESI operations plan and will continue to manage it during the five-year survey. Lab staff's roles in DESI including Project Director, Project Manager, Project Scientist, co-Spokesperson 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. 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. Our CMB-S4 project roles include lead lab, Project Director, Project Manager, Project Engineer, co-Spokesperson, Technical Baseline Development and L2 leadership roles in detectors, small aperture telescopes and data management.

On the Intensity Frontier, the Lepton Flavor group is involved in two flagship experiments at Fermilab. On Mu2e, Berkeley Lab leads the Software and Computing group which leads the simulation and reconstruction software efforts and has completed two Mock Data challenges. We redesigned the Mu2e simulation production chain, improving the efficiency by an order of magnitude, and added simulations of cosmic ray calibrations. LBNL built and operated the first working prototype of the straw tube tracker and is supporting readout electronics testing. We lead the development of the firmware and readout system of the full tracker. We developed and currently maintain the track reconstruction software and lead the development and testing of the tracker's calibration and alignment software. We developed a conversion electron analysis based on ML regression that improved the sensitivity by 15%. We are also involved in the Snowmass effort to explore follow-on experiments to Mu2e, for which we developed simulation tools for studying the physics reach of new experiment setups and detector designs to detect lepton flavor violation.

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. Berkeley Lab has demonstrated the scalability of our novel low-power, cryogenic pixelated readout (LArPix) for the DUNE ND, producing and testing more than 200,000 channels and instrumenting two successful ton-scale prototype detectors. The group has also developed a highly parallelized pixel detector simulation designed for the new NERSC 9 (Perlmutter) GPU-based supercomputer and used this to benchmark the prototype pixel detector performance and guide further ND design. We are the technical lead of the DUNE Near LArTPC effort and the center of engineering development for the Near Detector complex. The Lepton Flavor group also has had leading roles in the analysis of Daya Bay, a ground-breaking reactor neutrino experiment which was conceived of and led by Berkeley Lab. Daya Bay made the first observation of the third neutrino mixing angle and has the most precise measurements to date, resulting in many awards and prizes. Daya Bay data has concluded operation and the group is completing final analyses of reactor neutrino oscillation using the complete data set. Berkeley Lab is also now facilitating a joint neutrino oscillation analysis of the T2K and NoVA experiments using the NERSC supercomputing facility.

Computation is a central aspect of our program. We have taken a leading role in software, simulation, and computing for ATLAS, Daya Bay, Mu2e, BOSS, DESI and CMB experiments, and leveraged resources at NERSC and the Lab's Computing Research Division for HEP. We've also incorporated ML as a tool in several of our simulation and analysis efforts. The Center for Computational Excellence has provided additional resources to take advantage of the NERSC HPC for HEP, and we have obtained other resources from ASCR. We are poised to take advantage of the latest HPC advances 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. We have a growing and active cross-cutting ML group that brings together scientists across the frontiers and even extends beyond HEP.

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.

We are proud to host, lead, and support the Particle Data Group, an essential resource for the field. PDG is an international collaboration that annually produces the most comprehensive and trusted compendium of measurements and averages in particle physics and cosmology, as well as curated reviews on many topics and techniques.

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

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

In the study of neutrinos, Berkeley Lab's critical role in the discovery of neutrino oscillations at the Sudbury Neutrino Observatory has been widely recognized. KamLAND and IceCube resulted in the first observations of geo-neutrinos and ultra-high-energy cosmic neutrinos, respectively. Experiments also search for the rare nuclear process known as neutrino-less double-beta decay, which will demonstrate if the neutrino is its own antiparticle. This effort may provide information on the absolute neutrino mass scale and determine if lepton number is conserved. We 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 and has accumulated over 1 ton-year of exposure, the most for bolometric detectors. We are developing new detector technologies to enhance the physics sensitivities by two orders of magnitude in next-gen experiments: the Large Enriched Germanium Experiment for Neutrinoless Double-Beta Decay (LEGEND), and the CUORE with Particle Identification (CUPID) experiments. We have leading analysis roles in the recent sub-eV neutrino-mass limit of the direct measurement by the KArlsruhe TRItium Neutrino (KATRIN) experiment.

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 carry out experiments at ANL's CARIBU facility. This tradition continues with the next-generation Gamma-Ray Energy Tracking Array (GRETA) which received CD-2/3 in 2020.

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

The Lab's strong nuclear theory group is building the science cases for the next generation of advanced nuclear physics facilities to be built in the U.S. Notable is work that elucidates the nature of gluonic matter and the structure of the nucleon, which is of great relevance to the next generation EIC. 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 via the Lab's ECP award. Daniel Kasen received a recent E.O. Lawrence Award in recognition of his pioneering contributions in multi-messenger astrophysics and for his leadership in the application of HPC.

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 led in defining physics goals and detector components for the future EIC.

To develop detectors for the EIC, we have initiated and formed a consortium (seeded by the UC Multi-campus Research Programs and Initiatives (MRPI) program), with 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.

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 has led to regular use of NERSC HPC machines for reconstruction and simulation studies for STAR, and large-scale simulation efforts for ALICE. We are developing infrastructure to allow user analysis of large data sets from these experiments.

The Lab's Applied Nuclear Physics program is growing, with applications ranging from international safeguards, radiological monitoring, biomedical applications, and detectors for astrophysics. This work takes advantage of the Lab's capabilities in innovative instrumentation, including the world-renowned Semiconductor Detector Laboratory (SDL), and attracts many cross-divisional collaborations at the Lab. In late 2019, Berkeley Lab scientists in this program won one of the coveted R&D 100 Awards for their portable radiation imaging, spectroscopy, and mapping (PRISM) device. In late 2021, scientists in this program won an R&D 100 Award for Neutron and Gamma Ray Source Localization and Mapping Platform 2.0.

The U.S. Nuclear Data Program evaluates and organizes nuclear data for national interests. This 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 developing new gamma-ray databases, including language processors, for nuclear reaction modeling.

The 88-Inch 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 Nuclear Data and Isotopes Program targeted measurements represent the second thrust for the 88. This facility also contributes to 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 has now finished taking data, utilizing multiple components produced by the Lab. We've upgraded the design components and installed them in the successor LEGEND-200 experiment at Gran Sasso. CUORE is also taking production data here, and we have a strong lead role. CUPID-Mo was a prototype setup for CUPID and completed its data-taking in mid-2020. KATRIN is taking production data and will establish the best upper limit of the neutrino mass in a model-independent measurement. 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. We completed construction of two Monolithic Active Pixel Sensor layers for the ALICE inner tracker upgrade. This novel silicon pixel technology will be utilized for the sPHENIX experiment at RHIC and will be further developed for the EIC detector. The Semiconductor Detector Lab provides world-class instrumentation for development of advanced germanium and CdZnTe detectors.

The Office of Nuclear Physics recently funded a collaborative proposal led by the Lab's Nuclear Science Division and Workforce Development & Education Department, and several minority-serving institutions (San Jose State University, UC Merced, and UC Riverside) to develop and administer a traineeship program to diversify the workforce in Nuclear Science and STEM.

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 and Fusion Science

Berkeley Lab has core expertise in the physics of beams (particle and light) and accelerators, plasma, fusion, and laser-plasma interactions; synchrotron radiation sources and free-electron lasers (FELs); high performance magnetic systems; laser-plasma accelerators (LPAs); linacs, rings and colliders; accelerator and laser controls and instrumentation; accelerator front-end systems, high brightness electron and ion sources. Supported by HEP, FES, and BES, with further sponsorship from ARDAP, ASCR, NE, NNSA, DHS, DoD, ARPA-E, other federal agencies, and industrial partners, this core capability of Accelerator Science and Technology and Fusion Science 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. It is a center of excellence and community leadership in advanced modeling of accelerator, beam, and plasma physics. AI/ML is advancing these accelerator science and technology research areas. We are also working to improve QIS and on algorithms that could leverage future quantum computers for accelerator science. In this appendix additional detail is provided on the program.

Strong participation in campus, community and agency activities to develop unified visions for our fields and aligns activities towards leading roles. A staff member served on the recent FES Long Range Plan. In the ongoing Snowmass process for HEP, staff are serving in several leadership roles and a local working group coordinates accelerator and physics input to design the next generation of experiments. The ATAP director serves as one of the co-conveners for advanced accelerators at Snowmass. A BELLA member serves on a joint task force, and a staff member is an Early Career representative. Two BCMT scientists serve co-convener roles for Snowmass. The BELLA and BCMT programs were also deeply involved in the European LDG planning exercise this year. AMP has three staff serving respectively as co-convener, liaison, and early career. BACI has staff serving in the muon collider forum and early career. AMP is also leading the development of the roadmap for the Prediction Grand Challenge of the HEP GARD Accelerator and Beam Physics thrust, as well as the Consortium for Advanced Modeling of Particle Accelerators, a collaboration between LBNL, SLAC, FNAL and UCLA. This will position the Laboratory to lead accelerator capabilities that will enable that science.

We engage strongly with campus, including via a recent appointment of Carl Schroeder as Adjunct Prof. in Nuclear Engineering. We hosted the remote Advanced Accelerator Concepts Seminar Series in 2020-21 to provide a forum for the advanced accelerator community.

The program is strongly engaged with the workforce and IDEA development efforts described in Section 7 and the Appendix, including through active teaching at the U.S. Particle Accelerator School, mentorship for the SAGE program (Science Accelerating Girls Engagement in STEM), leadership of Laboratory and American Physical Society employee resource groups, incorporation of content in planning activities, and an active committee and set of practices.

Accelerator and Laser Science. The Lab's strong interlinked capabilities support accelerator projects and long-term technology development required to enable next gen capabilities.

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 for HEP under the multi-institutional U.S. Magnet Development Program (MDP) and a key member of the High-Luminosity-LHC-Accelerator-Upgrade-project (HL-LHC AUP), which is contributing half of the new high-field interaction-region magnets for the LHC upgrade. The project was recently awarded CD-3, enabling full production to proceed. In 2018 the

BCMT delivered the fully tested magnet system for the FRIB 28GHz ECR Source, and the device was recently commissioned at FRIB, meeting a key final CD-4 milestone. The Lab leads the large-bore high field dipole for a future HTS Cable Test Facility funded by HEP and FES (other FES projects are detailed below).

Berkeley Lab is the world leader in ultrahigh-gradient laser-driven plasma acceleration technology. Its BELLA Petawatt laser is used for research in support of the SC-HEP mission, including developing 10 GeV beams from a sub-meter-scale accelerator (current record: 8 GeV). Such an accelerator is envisioned as a module of a future electron-positron collider concept with potential for energies to many TeV. An HEP funded project to add a second beamline (an independent laser arm) on the BELLA Petawatt is nearing completion. The second beamline project will provide the capability of staging two multi-GeV laser plasma accelerator modules which is a key next step to establish potential collider applications of plasma accelerators. BELLA Center is now operating two new 100 TW class laser systems for LPA applications. One system, funded by the Moore Foundation and an early career grant from BES, is used for LPA-driven FEL studies. The other system, funded by NNSA, studies LPA use for nuclear security applications. Both, along with the petawatt system, are used for studies of high brightness beam injection as a third major component for a future collider. These experiments inform theory and simulations in an integrated program to develop the accelerators and project potential for future colliders. Intense ion pulses from laser plasma acceleration have been used for radiation biology studies in the FLASH regime. Expansion of the BELLA program also includes the iP2 project and FES applications as detailed below.

The Berkeley Accelerator Controls and Instrumentation (BACI) Program brings together decades of deep expertise in electron and ion acceleration, innovative RF structure design and engineering, advanced field programmable gate array (FPGA)-based precision digital RF controls, and femtosecond synchronization including novel high average power fiber-laser technology, and qubit control. It is a world leading center in advanced FPGA-based precision digital controls for accelerators. In collaboration with several DOE national labs, BACI plays a leading role in technology development in LLRF controls for upgrades of Argonne Wakefield Accelerator (AWA) at ANL, SNS at ORNL, and PIP-II accelerator complex at Fermilab and at the LCLS-II and its high energy upgrade project at SLAC (LCLS-II-HE). BACI's research programs target the most pressing problems and potential limitations impacting the scientific capabilities of accelerator-based facilities and collaborate closely with fellow national laboratories and institutions. BACI staff also apply its FPGA expertise to the precision control of fiber lasers and superconducting qubits and are exploring adaptation of these techniques to other qubits, including trapped ions.

A cross program ATAP initiative is developing a new class of lasers combining high peak power (required to drive plasma accelerators) and high average power (required to enable operation at application repetition rates as well as active correction for precision and performance). A proof of principle system is being developed at the kHz, 0.2 Joule level with support from DOE ECRP and the Moore Foundation. This program, related research under the Accelerator Stewardship Program and ARDAP, and collaborations establish the basis for such lasers. The kBELLA initiative would be a new 1 kHz multi-J-class laser for high-repetition-rate LPA science and applications. The kBELLA initiative would be a new 1 kHz multi-J-class laser for high-repetition-rate LPA science and applications. It will be a key step towards the needs of future colliders at the 10 Joule and tens of kHz level. Together with the accelerator research in the BELLA program, this laser work establishes the basis for a future collider.

Integrating magnet and BACI contributions, 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 contributed to linac systems, RF controls, and accelerator physics. We are also a partner in construction of the LCLS-II HE upgrade now underway, leading the delivery of the undulator sources, including design and procurement of new magnetic modules as well as the procurement of additional magnet structures to complement the existing FEL lines and to achieve FEL saturation at the higher beam energy.

Leveraging the development of the LCLS-II injector is the High-Resolution Electron Scattering (HiRES) beamline at BACI, 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 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 of the LCLS-II injector, we developed the beam dynamics, RF, and engineering design for the next generation normal-conducting CW RF gun – APEX2. This has potential application for the LCLS-II high energy upgrade (LCLS-II HE) and as an electron source for electron cooling in the EIC.

The Lab is a world leader in developing simulation tools and techniques that model advanced accelerators, plasmas, and high-intensity laser-matter interaction physics. Our Accelerator Modeling Program (AMP) is a center of excellence and community leadership in particle accelerator modeling. AMP activities cover a broad range of accelerator technology (e.g., linacs, rings, sources, plasma-based), and beam and plasma 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 pioneered many advances in algorithms that make the codes more accurate and faster. AMP scientists are also leading the U.S. DOE ECP application project on "Exascale Modeling of Advanced Particle Accelerators," where a team 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.

ATAP's ALS Accelerator Physics Program is matrixed with the ALS division. Besides being responsible for ALS operation, it also develops new concepts and technological improvements to enhance the performance of ring based light sources, with a particular attention to the ALS. Through a series of key upgrades, the 25-year-old ALS continues to operate as the world's brightest soft X-ray source. The group skill set and areas of expertise include theoretical (both analytical and numerical) capabilities, software development, electron and photon beam diagnostics and experimental capabilities. This has allowed the group, over almost 30 years of ALS operation, to conceive and develop upgrades to maintain the facility as the world leading soft x-ray 3rd generation synchrotron light source. A notable example is the development and implementation of a machine learning application that allowed us to dramatically improve the beam size stability of the ALS in operation. 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.

Plasma and Fusion Energy Science. The Laboratory's capabilities in magnet, laser, diagnostic, accelerator, and ion beam science as well as exascale plasma simulations enable strong contributions to magnetic fusion via high field magnets and diagnostics, and to high energy density science. This also prepares for contributions to any emerging efforts in inertial fusion.

Core capabilities in superconducting magnet technology are being applied to improve future fusion reactors, and several public-private collaborations have been initiated between LBNL and US Industry via SBIR, ARPA-E, and INFUSE programs. Starting in FY17, the Laboratory has received funding from FES for a new program to investigate HTS technology for Fusion applications, focusing on technology aspects common to FES and HEP applications. Most recently, funding has been provided for FY21 and FY22 to continue research into HTS fusion magnet technology, where we currently focus on REBCO tape and cable performance characterization as well as the development of diagnostics that are essential for the application of HTS materials to fusion magnets, and new modeling capabilities tailored to HTS materials. The research has been further advanced through judicious collaboration with industry in areas including advanced modeling, diagnostics developments, and cable testing. We lead the large-bore high field dipole for a future HTS Cable Test Facility jointly funded by FES and HEP. This is based on LBNL leadership of the HEP funded US Magnet Development Program. In addition, SBIR proposals and sponsored projects have been funded whose goals are aligned with the FES-funded technology development, in particular those related to REBCO-based cable concepts.

The laser systems within the BELLA Center, which include the BELLA PW laser, the new iP2 beamline, and two independent 100 TW systems, are available to the user community through the LaserNetUS program funded by FES. We host users and collaborate where desired to conduct experiments in discovery plasma science and high energy density science. The BELLA iP2 project focuses the present BELLA laser for ion acceleration and high energy density physics. This FES-funded high-intensity beamline project is nearing completion and will enable the BELLA PW laser to produce very small focal spots (and corresponding very high intensities) for a variety of experiments in high energy density physics (e.g., ion acceleration). Thanks to the high repetition rate at BELLA, many experiments will be performed within hours that would take weeks at other facilities. These high repetition rate lasers are a vital part of the emerging core capability in Fusion Energy Sciences for relativistic plasma science and the development of advanced X-ray and gamma diagnostics beams for HEDP experiments. Intense ion pulses from laser plasma acceleration at BELLA have been used for qubit synthesis and are relevant to inertial fusion. The particle and photon sources developed under these programs also offer unique opportunities in precision diagnostics for high energy density and fusion plasmas. Unique, intense lasers and particle beams are used for qubit synthesis very far from equilibrium, enabling formation of novel color center qubits with tailored properties for QIS applications (Fusion for Quantum).

The Laboratory's programs in highly efficient, high-power lasers and particle beams offer future potential capabilities relevant to advanced driver technologies. As detailed above, we are developing techniques to enable orders of magnitude advances in laser efficiency and repetition rate. The Lab has significant expertise in developing ion beams and sources. A series of projects funded by ARPA-E are led by Fusion Science and Ion Beam Technology (FS-IBT) staff which leverage and reinforce this capability, including the imaging of carbon in soil with neutrons, and the development of multi-beam RF linacs made using low-cost MEMS techniques. It is developing novel accelerator architectures based on micro-electromechanical systems (MEMS) for fusion plasma heating, materials testing, and manufacturing applications. Advanced plasma-based coating techniques support low temperature plasma technology applications, including for QIS (and, at the Laboratory, also the needs of projects such as ALS-U, LCLS-II).

AMP's WarpX code and team are also inaugural members of SimNet, a new network of high-performance laser-plasma interaction simulation codes and teams in support of LaserNetUS. These codes are also used at LLNL, in collaboration with AMP, for the modeling of laser-plasma interaction and fusion physics.

These capabilities enable strong support of both magnetic and inertial approaches to fusion.

Artificial Intelligence and Machine Learning. Accelerator, laser, QIS, fusion and plasma science and technology systems are complex and require both precision active control and intelligent parameter space exploration beyond the limits of conventional techniques to meet the goals of upcoming projects and initiatives. The Accelerator Technology & Applied Physics (ATAP) Division develops and applies the latest techniques in AI/ML to further enhance progress and enable next generation system performance.

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

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

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

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

BACI has developed an advanced AI-based design tool for RF cavity designs, supported by LDRD. The tool has been successfully applied to the RF designs of APEX2 and ALS-U RF cavities. BACI program has applied its high precision timing and RF control technology, taking advantage of BACI's well-developed control systems for particle accelerators, to develop ML-based advanced feedback systems for fiber laser systems and quantum computer bit control in solving the scalability problem in the control electronics.

In collaboration with the UC Berkeley Quantum Nanoelectronics Laboratory (QNL) under the support from HEP and ASCR, we have prototyped a qubit control system (QubiC) and demonstrated single and two qubits gate operation on superconducting qubits. Associated software has been developed to streamline the qubit chip characterization, gate optimization, and execute circuits provided by users. The prototype system allows for further study of the parameter space of an overall control system that interacts with the qubits. In addition, we will further develop more compact modules and interconnection among them to build up a system needed for more complex quantum computers.

Applied Science and Energy Technology

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

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

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

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

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

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

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

This Core Capability is sponsored by BES, EERE, DHS, ARPA-E, and SPP programs, including DoD and industry. It is underpinned by DOE-supported basic chemistry, materials, and computational research, and contributes to DOE missions in energy, the environment, and national security. This work benefits DOE technology programs such as water desalination, solar-energy conversion, electrical-energy storage and transmission, solid-state lighting, energy efficiency, and the study of materials in extreme energy environments.

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

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

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

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

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

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

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

Within the national lab network, Berkeley Lab leads management of transmission reliability programs (CERTS); collaborates with DOE, independent power authorities, and states (with the Demand Response

Research Center); and collaborates with other national labs on energy storage for ancillary services and renewable integration.

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

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

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

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

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 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.

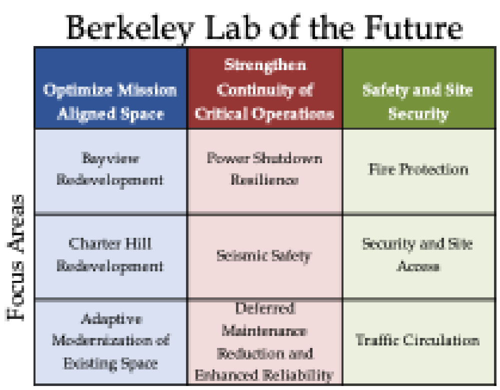
Science and Technology Strategy and Major Initiatives

To sustain our ability to provide critical research to the nation requires both a strategic vision of the most promising research directions and prudent stewardship, both 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 strategic vision and stewardship, thus maximizing the opportunities for scientific breakthroughs in the future.

Infrastructure

Overview of Site Facilities and Infrastructure

To sustain our ability to provide critical research to the nation requires both a strategic vision of the most promising research directions and prudent stewardship, both 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 strategic vision and stewardship, thus maximizing the opportunities for scientific breakthroughs in the future.



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

The main campus building space consists of ~1.74 million gross square feet (gsf) of operating DOE-owned buildings (1.71M gsf) and trailers/storage containers (.027M gsf). For the DOE owned properties, the main campus net square footage decreased by 71k gsf from FY20 due to removal of six assets and administrative corrections. Two UC-owned facilities (B30 Chu Hall and B59 Shyh Wang Hall) at 202,788 gsf are used for DOE purposes under the UC occupancy agreements. There are 24,317 sq ft of UC-owned space within the Advanced Light Source building. The Guest House (B23) is UC-owned; it is not managed in the Facilities Information Management System (FIMS).

As of 9/30/21, the Lab leased nine off-site facilities totaling 268,519 gsf, including a 55,000 rentable sq ft warehouse to support ongoing operational storage needs. The Lab has no-fee use of 48,211 sq ft of UC space at UC Berkeley. For FY22, we are working with the SC Consolidated Service Center to extend the two lease properties – ESnet's office suite (1.8k RSF) in Champaign, IL, and JBEI (65k RSF) in Emeryville, CA, which will expire in mid-2023. We plan to lease a new 3k RSF GSA office space for five ESnet staff members who reside in Bloomington, IN.

Building and Trailer Ownership Summary		
Ownership	Size (GSF)	Property Count
DOE Owned	1,736,651	168
Contractor Leased/License	268,519	9
Contractor Owned	202,788	2

Grand Total	2,207,957	179

Overall Condition Summary

Below is the overall condition summary by mission dependency as reported in FIMS at the close of FY21. All the mission critical assets with inadequate condition rating are due to either poor or very poor seismic rating. Refer to the section on 'Improve Seismic Safety and Reduce Landslide Risks' for more details regarding how the Lab's plan to address these assets.

Overall Condition – Mission Critical Assets				
Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$392.5M	31.9%	408,881	21
Substandard	$476.3M	29.5%	472,014	14
Inadequate	$363.0M	38.7%	693,653	28
Grand Total	$1,231.8M	100%	1574,548	63

Overall Condition – Mission Dependent, Not Critical Assets				
Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$48.0M	54.7%	71,017	24
Substandard	$14.0M	16.0%	12,121	17
Inadequate	$25.8M	29.4%	67,152	7
Grand Total	$87.8M	100%	150,290	48

Overall Condition – Not Mission Dependent Assets				
Condition	RPV	% of RPV	GSF	Asset Count
Adequate	$3.5M	27.9%	7,542	56
Substandard	$0.0M	$0.0M	$0.0M	0
Inadequate	$9.1M	72.1%	4,271	1
Grand Total	$12.6M	100%	11,813	57

Operating Status Summary - DOE-Owned Real Property Assets						
Status	Building		Trailer		OSF	
	GSF	Asset Count	GSF	Asset Count	GSF	Asset Count

Operating	1,705,560	89	26,820	78	N/A	67
Shutdown	16,172	3	1,281	2	N/A	2
Standby	4,271	1	0	0	N/A	4
Grand Total	1,726,003	93	28,101	80	N/A	73

Below is the overall asset condition summary of our utility systems by their Mission Dependency as percentage of their replacement value (RPV). 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., tele-communications, optical fiber). These systems and their respective components vary greatly in age and condition, reflecting generations of alterations and improvements over Berkeley Lab's long history. The Lab's Institutional General Plant Project (IGPP) is invaluable to our strategic goal to modernize core infrastructure elements, and over the past several years our investment has grown substantially. In FY19 and FY20, the Lab invested about $9M and $16M towards IGPP, respectively, which grew to over $23M in FY21 costs. The Lab is currently working through a backlog of approved IGPP projects and plans to maintain annual IGPP investments on the order of $25-$35M. The average IGPP index over the planning period is 1.2%.

Overall Condition – Site Utility Systems as $ of RPV				
Condition	Mission Critical (% of RPV)	Mission Dependent, Not Critical (% of RPV)	Not Mission Dependent (% of RPV)	Total (% of RPV)
Adequate	$170.0M (53.5%)	$31.8M (26.6%)	$.2M (5.6%)	$202.0M (45.9%)
Substandard	$83.3M (20.3%)	$87.9M (73.4%)	$0 (0%)	$171.2M (38.9%)
Inadequate	$64.4M (26.2%)	$0 (0%)	$2.7M (94.4%)	$67.1M (15.2%)
Total	$317.7M	$119.7M	$2.8M	$440.2M (100%)

FIMS Status Summary

Below is the FIMS status summary of all DOE-owned buildings, trailers, and structures at the close of FY21. Overall, 95.1% of all assets were in operating status. Less than 4.9% were in either standby (2.0%) or shutdown (2.9%) status. Of the seven assets in shutdown status, two (46D trailer and 79B structure) were demolished in FY22. Three (B54, B54A, and 54-EL-2 structure) are pending D&D.

FIMS Status Summary - DOE-Owned Real Property Assets							
Status	Building		Trailer		OSF		Total Assets
	GSF	Asset Count	GSF	Asset Count	GSF	Asset Count	
Operating	1,705,560	89	26,820	78	N/A	67	234 (95.1%)
Shutdown	16,172	3	1,281	2	N/A	2	7 (2.8%)
Standby	4,271	1	N/A	N/A	N/A	4	5 (2.0%)

Total	1,726,003	93	28,101	80	N/A	73	246 (100%)

Asset Utilization Summary

The table below provides the asset utilization summary of DOE-owned buildings and trailers. All operating buildings and trailers are fully utilized at 99.94%. Less than .06% of assets are underutilized and there are no unutilized assets. All six unutilized assets are either in standby or shutdown status. The Lab's disposition and demolition program continues to make progress removing assets that no longer support the DOE mission. Seven assets, including six buildings and trailers (28,930 gsf) and one structure were demolished and removed from the site in FY21.

Building and Trailer Utilization Summary				
Status	Utilized (GSF)	Underutilized (GSF)	Unutilized (GSF)	Total (GSF)
Operating	1,731,420	960	N/A	1,732,380
Standby	0	0	4,271	4,271
Shutdown	0	0	17,453	17,453
Total	1,731,420	960	21,724	1,754,10

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

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

Objective 1: Optimize mission aligned space

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

After analyzing Future of Work implications and new modes of work, fully leveraging telework allows the Lab to reclaim office space for conversion to research, lab, and support space. This also enables a fresh approach to space policies and allocations to be based on research and operational need rather than employee class. Another opportunity is to repurpose outdated conference space into modern research space. We consistently work to identify creative ways to leverage the Future of Work and support modernizing space for research needs.

Bayview Redevelopment

Our multi-year strategy includes facilities construction to support full integration of biosciences and related programs adjacent to the IGB in the Bayview cluster. Now under construction, the Biological and Environmental Program Integration Center (BioEPIC) will house exciting new research capabilities that will advance interdisciplinary priorities, such as fabricated ecosystems, new sensors, new simulation capabilities, new levels of lab to field connectivity, and cryo-EM for biological and environmental science. Construction activities for BioEPIC are planned to occur through Q2 of FY25, with program moves into the building shortly thereafter.

Redevelopment activities will continue at the northern section of the Bayview cluster throughout the planning horizon. A planned EM-funded Bayview Cleanup Phase 2 will address the demolition of B56 and B64, including cleanup of any local site contamination. The Lab is developing plans for relocating the remaining occupants of B56 and B64 to accommodate the future cleanup project. The demolition of B56 and B64 will free up the acreage necessary to construct the third biosciences-focused facility, the Biosciences Genome Engineering and Manufacturing (BioGEM) facility. An FY20 preliminary study helped scope and size this proposed building, set to house the Joint BioEnergy Institute (JBEI), the Advanced Biofuels and Bioproducts Process Development Unit (ABPDU), and the Agile BioFoundry (ABF). BioGEM could enable those programs to move from their leased location in Emeryville to the Lab's main site. Additional D&D efforts farther north, to remove B55, B55A, B60, and B63, will eventually follow, creating new acreage for additional facilities at Bayview.

Charter Hill Redevelopment

Berkeley Lab's multi-year strategy includes constructing a materials and chemical sciences and technology building cluster at Charter Hill, adjacent to the ALS user facility. Charter Hill is being developed on the Lab's former "Old Town" area, which is being cleared of buildings and foundation members under the current Old Town Demolition Project. This Project's final phases address the removal and cleanup of B4 and B14 slabs, nearby utilities, B7, and B7C. Currently, substantial completion is planned for early FY23. Early interim uses of the newly available acreage in the Charter Hill cluster are already in place, including a new tensile structure and additional parking and laydown areas in support of projects and operations. A second tensile structure will be installed and commissioned in FY23. The Linear Assets Modernization Project (LAMP) will extend utility infrastructure into the Charter Hill area.

As part of the long-term vision, the Lab's Energy Storage Center will be centralized at Charter Hill. We are evaluating the optimal use of the current footprint, given the expanding needs of energy storage research at the Lab and the significant benefits of leveraging similar equipment and research already in the Charter Hill area. The Energy Storage Center will harness, guide, and galvanize the expertise, capabilities, and innovation in energy research across Berkeley Lab, from discovery to deployment. At Charter Hill, the current research teams in Chu Hall (B30) initiated a building-wide agreement to share space and equipment with compatible but distinct research programs designed to efficiently utilize space and allow for other economies of scale. We will extend this model to nearby buildings as the Energy Storage Center and other Charter Hill related collaborative research concepts develop.

Envisioned to enable collaboration and accelerated discovery, Charter Hill's future lab spaces would leverage advances in ML, AI, and automation; other next-gen science concepts; and proximity to the ALS beamlines, to pursue the understanding and control of materials phenomena and chemical transformations across size and time scales. The first anticipated facility would be the Advanced Materials Discovery Building (AMDB), a 3-4 story, ~68,500 gsf lab/office facility with approximately 150 occupants. This would house personnel and programs from B70, which has a poor seismic rating and is planned for demolition. The second would be the Interdisciplinary Chemical Sciences Building (ICSB), a

~68,500 gsf lab/office facility with approximately 150 occupants. The “Chemical Observatory,” is a key component of the envisioned capabilities for the site. It will be an innovative research facility designed to integrate multiple probes, such as those derived from the ALS’s soft X-ray beamlines, into more traditional lab spaces. Site preparation would include grading, installation of modern utilities, and realignment of Segre Road. A Modular Utility Plant (MUP) would be constructed in stages nearby to efficiently distribute utilities between the buildings. One or more ALS beamlines may be extended into the Charter Hill cluster.

Redevelopment Needs Outside Bayview and Charter Hill

Electron Microscopy (EM). Specialized space for new types of EM will enable Berkeley Lab to remain an international powerhouse. Infrastructure that incorporates a number of synergistic plans across the site would result in a renewed state-of-the art, world-leading electron imaging capability for a diverse set of scientific challenges in areas such as materials synthesis, catalysis, earth and environmental science, soft matter characterization, quantum materials, energy storage and structural and cellular biology. Instruments to be developed requiring state-of-the-art space include novel in situ, time-resolved and cryo and variable temperature EM instruments, and an analytical transmission electron microscopy (TEM) with high energy resolution. A future conventional construction project would build an addition onto B62 – approximately 7,000 gsf of specialized laboratory space to house EMs, supporting infrastructure and systems. Further, the construction of a new addition to house EMs would allow for a full overhaul and modernization of the B72 complex, which has housed the National Center for Electron Microscopy for decades and needs modernization.

Accelerator Science and Engineering Building. Accelerator science and engineering are closely integrated at Berkeley Lab, which is essential for the efficient operation of our accelerator facilities, for world-leading R&D in advanced accelerators and superconducting magnets, for engineering of advanced scientific instruments for key stakeholders in HEP, BES, FES and NP, and for development of new applications of accelerator technology. However, accelerator and engineering staff are currently distributed across the laboratory. Many activities are housed in legacy buildings that do not encourage collaborative work, and do not meet current seismic standards. A new Accelerator Science and Engineering Building will bring together scientists and engineers working on activities critical to the mission of DOE across the Office of Science. High bay space for large structure assemblies remains in short supply when compared to the needs of numerous programs across the Lab. The inclusion of an Accelerator Science and Engineering Building in the out-years of the strategic planning horizon represents one significant step in addressing this critical space need at the Lab.

Laser-Plasma Acceleration Infrastructure Modernization at B71. Utility infrastructure is needed to support the installation of a future high average power laser system, kBELLA, to enable high repetition rate applications of laser plasma accelerators. This would include new radiation shielded target areas, a lab clean space for the laser and control room, and associated mechanical, electrical, and HVAC infrastructure. Possible sites include a new shielded cave within the existing high bay, and a new underground tunnel facility. A design study and estimates for the in-building site have been prepared. The tunnel option is also being explored on the hillside directly north of the B71 facility as an alternate site.

Adaptive Modernization of Existing Space

Given the high utilization rate of existing facilities and the elevated cost of new construction across the region, the Lab is renewing efforts to improve existing space and infrastructure to better align with evolving research needs.

The Lab will fully leverage telework and Future of Work concepts to return substandard space to the institution and convert it into modernized laboratory and technical space aligned to the Office of Science Mission. Leveraging telework will create more opportunities to reduce or eliminate occupancy in substandard space so that renewal activities can occur with less operational impacts. These efforts are aligned with the ongoing task of identifying potentially underutilized spaces for modification and redeployment for current and future program needs.

Three examples of proactive improvements and revitalization include renovating high bay space in B62, modernizing lab space in B66, and converting a conference room with an exceptionally high ceiling to assembly space in B2. Examples of reconfiguring space to accommodate a more robust Future of Work implementation are converting office and substandard conference room space to lab space in B90 and optimizing office and cubicle layouts in B59 and B91 to accommodate more researchers in our newer facilities. These future endeavors are in the early planning stages and will be prioritized in FY22 and incorporated into the Lab's multiyear infrastructure investment strategy.

Objective 2: Strengthen continuity of critical operations

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

Power Shutdown Resilience

A major 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 encountering debris or vegetation when gusty winds and dry conditions are forecasted or are present. Prior to 2019, the Lab had never been impacted in such a manner. However, in 2019, the Lab was forced to shut down operations for five business days across two separate events. Direct costs related to these events were approximately $1.7M per business day – $8.5M total. In addition to the productivity losses caused by the shutdowns, significant strain was placed on the Lab's aging infrastructure through repeated equipment de- and re-energizations. The likelihood of additional PSPS events over the next decade and beyond increases the urgency to reduce DM and increase the degree to which back-up generation power is available for use.

The Lab receives power from PG&E at the Grizzly Substation via overhead 115kV transmission lines. Power is distributed at 12.47kV from the Grizzly Substation to seven switch stations throughout the site. Each switch station, in turn, serves multiple buildings. In response to the 2019 PSPS events, feasibility studies considered various options to quickly add power generation capacity in preparation for the 2020 fire season. This analysis concluded that temporary backup generation at the 12kV switch stations provided the optimal near-term solution. Besides helping to mitigate the impacts of PSPS events, this approach also minimizes the impact of maintenance activities and construction related shutdowns. In partnership with PG&E, pilot projects were executed to provide temporary power generation at Switch A6 during the 2020 and 2021 fire seasons, providing backup power to critical business systems. Although PG&E has taken actions to reduce the likelihood of a PSPS event at the Lab, the risk remains. The Lab is installing 2MW of open transition temporary power at Switch A6 to mitigate this risk during the 2022 fire season and has initiated the conceptual design for 4 MW of permanent close transition backup generation at the location. There are also several other investments being made through GPP, IGPP, and

LAMP, described in further detail throughout this subsection, that will modernize distributed utilities and increase reliability.

While the Lab is making significant investments, they unfortunately fall short of a sitewide solution that ensures mission critical Lab operations can be fully maintained during planned (PSPS) and unplanned power outages (e.g., caused by earthquakes or local wildfires). A future state of power resilience will include utilizing onsite power generation capabilities, demand side management, and advanced site wide supervisory control and data acquisition control systems. This future state transitions the electrical distribution system into a flexible microgrid of interconnected loads and distributed energy resources that can operate in both a grid-connected or island mode. In 2021 an independent study assessed the Lab's energy resilience and identified capability gaps in maintaining critical operations during a power outage. This 2021 energy security assessment has helped steer the Lab's energy resilience objectives.

The Lab's near-term strategies include increasing asset reliability and power metering to support development of load shedding and demand-side management strategies, closed transition backup at 12kV switch stations, replacing aging equipment, upgrades to building automation system controllers and optimization of existing generator capacity. Longer term strategies include implementing a microgrid strategy, incorporating alternative energy technologies such as solar PV, energy storage, fuel cells, hydrogen electrolyzers, EV charging, and implementing new backup power strategies serving critical loads for new buildings (vs. traditional backup diesel generator approaches). Longer-term resilience strategies are being coordinated across the Facilities Division, Sustainable Berkeley Lab, and the Lab's Energy Technologies Area to foster "living lab" opportunities to advance resilience and sustainability while creating opportunities to develop and test emerging technologies.

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

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

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

The SLI-funded LAMP will significantly improve the Lab's utility resilience. The project will construct common utility corridors centered on Grizzly Substation and serving the East, Northwest, and Southwest areas of the Lab. These corridors will be connected into redundant system loops, where logical and affordable, to modernize system operations and increase utility service reliability. The multi-year LAMP project prioritizes essential system improvements, based on mission impacts and future programmatic needs into earliest work packages.

The first phase of this project will expand the Grizzly Substation and increase the Lab's power capacity to 70MW to cover planned load increases, including building electrification, datacenter expansions and full-power operations at NERSC. The expansion will enable modern, state of the art sitewide electrical SCADA capabilities, as well as safer, segregated high voltage duct banks for improved reliability and reduced maintenance outages that impact research. A common utilities corridor will be created along Lawrence Road to provide improvements for segregated high voltage duct banks, sanitary sewer, natural gas, communications and data, compressed air, controls, and hydraugers. The second phase of the project will focus on two additional common utilities corridors, first in the East Canyon service area, and second along McMillan Road.

Our multiyear capital investment strategy identifies several projects to further respond to the risks posed by PSPS events, other potential unplanned outages, and planned outages necessary for construction and/or maintenance. The Sitewide Generator Upgrades Phase 1 was begun in FY22; it will provide standby power to the Bayview MUP and BioEPIC. It will provide a permanent switch station to allow for temporary generator installations for future fire seasons, as well as a dedicated, full capacity back-up for the Lab's Fire House and Fire Station. The Lab has also proposed an SLI-funded Emergency Generator Upgrade project to modernize the generator, automatic transfer switch, generator docking station, and load bank serving the Lab's permitted Hazardous Waste Handling Facility (B85). In future years, installation of permanent back-up power capabilities at switch stations A5 and A6 will be top funding priorities, as well as renewal needs for aging generators already in place at several other Lab facilities.

Improve Seismic Safety and Reduce Landslide Risks

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

After more than a decade of mitigation efforts, the Lab's number of buildings expected to perform poorly in a seismic event dropped from 34 to 19. However, national standards for seismic evaluations were revised in 2013 and 2017 and implemented into the California Building Code in 2019. Berkeley Lab has refreshed evaluations of many buildings based on the new standards, and as expected, more facilities were rated less favorably than before, up from 19 to 45. However, all currently occupied facilities met the California Building Code in effect at the time of construction, thus fulfilling DOE seismic requirements.

Recognizing the hazards presented by nearby faults, the Lab utilizes a comprehensive risk-ranked prioritization process to manage and mitigate seismic risks and will continue to partner with DOE on implementing appropriate corrective measures (e.g., retrofit, demolition, etc.). The Seismic Safety and Modernization (SSM) Project will improve the safety of Lab employees and visitors by addressing existing critical Operations facilities (e.g., B48, B54) that are currently in an inadequate seismic condition. The B6 (ALS) addition, B83, and B90 are near the top of the Lab's revised prioritized mitigation schedule, due to the mission critical nature of each facility, the number of people in each building, and their seismic performance ratings. The Bayview redevelopment plan discussed previously includes demolishing several seismically poor buildings. Building 79 was demolished in Q1 of FY22 to make the site ready for future upgrades to the Grizzly Substation. As indirect funding allows, other small seismically deficient buildings and trailers will be demolished. 53B was demolished in FY21 and 46D was demolished in FY22 using indirect funding. As part of the overall strategy, we are reducing staff levels in some buildings and vacating others during the multi-year seismic risk reduction efforts.

Chemical Lifecycle Management

In 2020, we embarked on a substantial initiative to understand the state of chemical management, to identify programmatic and performance problems, and to provide recommendations for improvement as expected by Lab leadership, UCNL, and the Site Office.

The "Chemical Lifecycle Management Corrective Action Plan" (CLM CAP) addresses these recommendations. Significant time and effort are needed from both research and operations divisions over the next few years to improve all aspects of the chemical lifecycle, including work planning, receiving/onboarding, procurement, inventory management, and disposal.

Execution of the CLM CAP began in early January 2021. Substantial progress has been made on near- and long-term objectives. Notable accomplishments in 2021 include completion of an evaluation of concept study for central chemical receiving, launching a new training course for time-sensitive chemicals, and improving the chemical inventory transition process for departing researchers. Work will continue through 2022 on key initiatives, which include:

- Radio Frequency-Identification (RFID) technology to facilitate chemical inventory reconciliation and improved tracking of high-risk chemicals, such as those that are time-sensitive.
- Performing a conceptual design study for central chemical receiving, which will take several years to fully implement. Temporary and permanent solutions are being evaluated.

- Configuring, customizing, testing, and implementing a new chemical management system procured in 2021. Implementation is on schedule to start in mid-2022.

Importantly, while EHS leads the CLM CAP management, research divisions are closely partnered with all aspects of successful execution through participation in work groups, feedback from institutional committees and subcommittees, and additional outreach efforts.

As the CLM CAP progresses, chemical management performance will continue to improve until a high level of performance is achieved. These efforts will decrease the Lab's risk profile in both safety and security, address previous performance issues and findings, and ensure compliance with all applicable DOE orders and regulations. Once implemented, R2A2s – critical to the sustained success of CLM – will be communicated and enforced.

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

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

The Lab prioritizes DM reduction efforts via building and utility system owners' annual review of each facility's condition assessment. Subject matter experts validate scope, status, and cost estimate of each deficiency and assign a risk score based on probability and consequence of failure. The Lab's annual review process includes identifying and categorizing deficiencies as DM, repair needs, and modernization. The Lab then uses an industry-standard pairwise methodology to develop an overall ranking strategy. For FY21, the Lab adopted and incorporated the Guidance for Categorizing DM, RN, and Modernization, developed by the SC DM working group to improve reporting accuracy and consistency. Each year, we reprioritize, categorize as DM, and address repair needs. Once DM deficiencies are addressed, they are then closed out and retired from the facility condition assessment database. Currently, DM represents approximately 47% of the entire repair needs balance. The Lab focuses its investments on high-risk facilities and infrastructure deficiencies with the most significant mission and operational impact.

We are working through the IGPP funded Sitewide Mechanical Plant Maintenance Upgrades Phase 1 and the Sitewide Electrical Safety and Maintenance Upgrades Phase 1 projects. The former has already replaced and added redundancy to the B62 boiler plant. It will begin construction in FY22 to provide increased cooling capabilities at B2 and B43, as well as renew and upgrade B43's compressed air plant. The latter project will begin construction to replace and upgrade electrical gear at B70A in FY22, with additional construction work planned at B50A to begin in early FY23. With a warming climate and aging building-specific mechanical and electrical infrastructure across its site, the Lab will continue to propose mechanical and electrical improvements across the planning horizon to modernize enduring building systems responsible for supporting mission delivery. For example, B71 mechanical requires a modernized chiller plant that will provide cooling redundancy to address single points of failure and replace other antiquated HVAC and electrical systems to improve overall facility systems' reliability and meet the demands of research programs. B71's existing systems cannot adequately control and maintain temperatures for experiments that are sensitive to minor fluctuations and air currents. This utility infrastructure will be increasingly important as multi-program activities and user operations increase, and the costs of downtime or nonperformance escalate. Similar challenges include B90, B62, B66, and the B50 complex.

Maintenance and repair (M&R) funding is projected at 2.69% as an average across the entire planning period. The Lab is nearing completion of the SLI-funded Storm Drain Repair/ Replacements GPP, which has retired the highest priority DM related to its sitewide storm drain system. Over the past several years, the Lab has replaced several boilers that were out of compliance with local air quality standards, and this year will complete the replacement of the final boiler plant with this issue at B88. The Lab is also replacing gas switches in the Strawberry Canyon cluster that leaked SF6 gas and are at the end of their useful life. Another important mechanical repair is the B50B exhaust flue system, which is leaking. The Lab will begin an ongoing program of overhauling boilers and chillers that are at highest risk of failure to accelerate DM reduction related to aging building-specific mechanical equipment. Other mechanical equipment replacements in FY22 and FY23 include an inoperable humidifier at B86, liquid nitrogen distribution stations serving numerous programs at B70, replacement of fume hoods providing service to the Lab's permitted Waste Handling Facility (B85), and replacements of multiple isolation valves, a pump, a tank, and a steam trap related to the steam system providing comfort heating for the B50 complex. The Lab will also invest in numerous perimeter fencing repairs identified through a recent condition assessment. The Lab is completing the sitewide elevator assessment study which will allow us to prioritize and address deficiencies. Finally, we have engaged the NNSA's Roof Asset Management Program to assess our roof systems to prioritize roof repairs and replacements into the future.

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

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

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

This objective includes implementation of fire protection upgrades, security related infrastructure improvements, and modernization of traffic circulation.

With the inception of the new Security and Emergency Services (SES) Division in 2020 and increased direct and indirect funding streams provided by DOE, we have reinvigorated our commitment to sitewide security improvements to bring systems to modern-day standards. In FY21, SES completed upgrades to Berkeley Lab's access control and access management systems. This included modernizing lab-wide video surveillance to the latest industry standards including the use of digital cameras, analytics, and an integrated access control. These improvements allow the Lab to integrate video surveillance, access control, and intrusion detection systems with the ability to upgrade software versions and system components to meet present and future requirements.

Berkeley Lab is making significant hardware upgrades as well in response to Design Basis Threat (DBT) requirements. Currently, the Lab is undergoing a $1.3M upgrade to build out new Property Protection Areas (PPA) for the protection of certain assets that meet DBT protection requirements. This includes expanding onsite camera coverage from 130 views to 250 views and adding 121 access control readers. Berkeley Lab has also updated our physical security systems requirements for all new construction and remodel projects. Based on known projects, these changes are driving the increases of up to 49 new camera installs and 150 access control readers associated with new construction over the next decade.

Perimeter Protection Another cornerstone of physical security protections is the perimeter protection formed by fencing and by site vehicle and pedestrian access gates. Fencing integrity is a challenge due to the varied geography of the main site. With the proximity to the UC Berkeley campus and hiking trails, trespassing events are somewhat frequent. Improvements will likely be necessary in the next 5-10 years (or sooner) barring new DOE requirements.

Vehicle Gates: At the main site, the Lab's three vehicle and pedestrian entry points are an area of concern and require improvement. Both the Strawberry Gate Guard House (B33A) and the Grizzly Gate Guard House (33C) were constructed in 1965 and were not designed or positioned to meet today's security standards. In FY20, in response to an increasing baseline security posture, the Lab implemented new security requirements, including 100% badge-in at site vehicle and pedestrian gates, and 100% ID checks for non-LBNL personnel. Geographic challenges, dated configuration and technology, and new security procedures have made these entry points marginally adequate. Further increases to the Lab's security posture in these locations will be extremely challenging, if not impossible, without significant reconfiguration. The Lab is leveraging the planned UC Berkeley-managed Centennial Bridge Replacement Project starting in 2022 to improve the configurations of the Strawberry Canyon and Grizzly entry points. Such projects would improve vehicular safety and the Lab's security posture.

FireSAFE The average age of fire protection systems at the Lab is 27 years. Frequent equipment failures have led to costly building evacuations and operational interruptions. The Fire and Safety Alarm Future Enhancements Project will replace and upgrade our existing fire and safety alarm systems have exceeded their end-of-life. The new fire alarm systems will have mass notification capabilities that would replace the Lab's dated public address system. The plan is sequenced over a funding-dependent, multi-year period based on building risks, operational priorities, and the condition of existing systems. The highest priority phase of this project is for B6 since this fire detection and alarm system is a critical component to the life safety systems at the ALS.

Maximize Transportation and Parking Improvement Opportunities

The past two years have fundamentally redefined how people across the world work and commute. The Lab is no exception, with much of our community continuing to telework. Recognizing that we can work differently, telework is central to the Lab's strategy to reduce commute impacts to local communities and the environment, as well as parking demand onsite. We are transitioning from maximum telework to a mix of onsite, hybrid, full-time telework, and remote workers. Initial indications are that as the Lab settles into these new work modes, the Lab's daily, onsite population will be approximately 60% of the pre-pandemic daily average. This will play an important part of the Lab's future transportation strategy. The Lab has pursued several improvements in our shuttle system over the last couple years including improved technology, vehicle reliability and communications media, with a goal to drive future ridership through more reliable service supported by more robust information. Further efforts to reduce demand for single occupancy vehicles on-site include partnering with the LBNL Bike Coalition, pursuing avenues to leverage recent micro-mobility permits issued by the City of Berkeley, and reestablishing a rideshare partnership to facilitate carpooling.

Site Sustainability Plan Summary

Sustainable Berkeley Lab (SBL) pursues three broad initiatives to reach sustainability targets driven by requirements of the federal government, California or federal law, and University of California policy. The initiatives, listed below, are described in greater detail at the Sustainable Berkeley Lab website, 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

The Lab's strong performance in energy savings is driven by ongoing efforts to improve building operations, optimize the NERSC cooling plant, and consistently follow sustainability standards in new construction. Efficiency efforts are significantly enabled through strong capabilities in applying data analytics for operations within a software platform called Skyspark. The Lab's energy and water management system is certified to ISO 50001 and recognized by the DOE as 50001 Ready. As well, the Lab is adapting efficiency retrofit project planning to meet the requirements of the Energy Act of 2020. Key efficiency performance metrics include:

- **Maintained Energy Savings**: As of spring 2022, Berkeley Lab is maintaining energy savings of 13.3 million kWh, water savings of over 19 million gallons, and utility cost savings of $1.1M annually. Maintained efficiency savings are updated monthly at sbl.lbl.gov/data.
- **Energy Use Intensity Reductions**: As of the start of FY22, Lab-wide weather-corrected energy use intensity (excluding major process loads) has decreased 29% since FY15. Energy use intensity for all loads is down 27% since FY15. Efficiency metrics are updated every six months at sbl.lbl.gov/data.

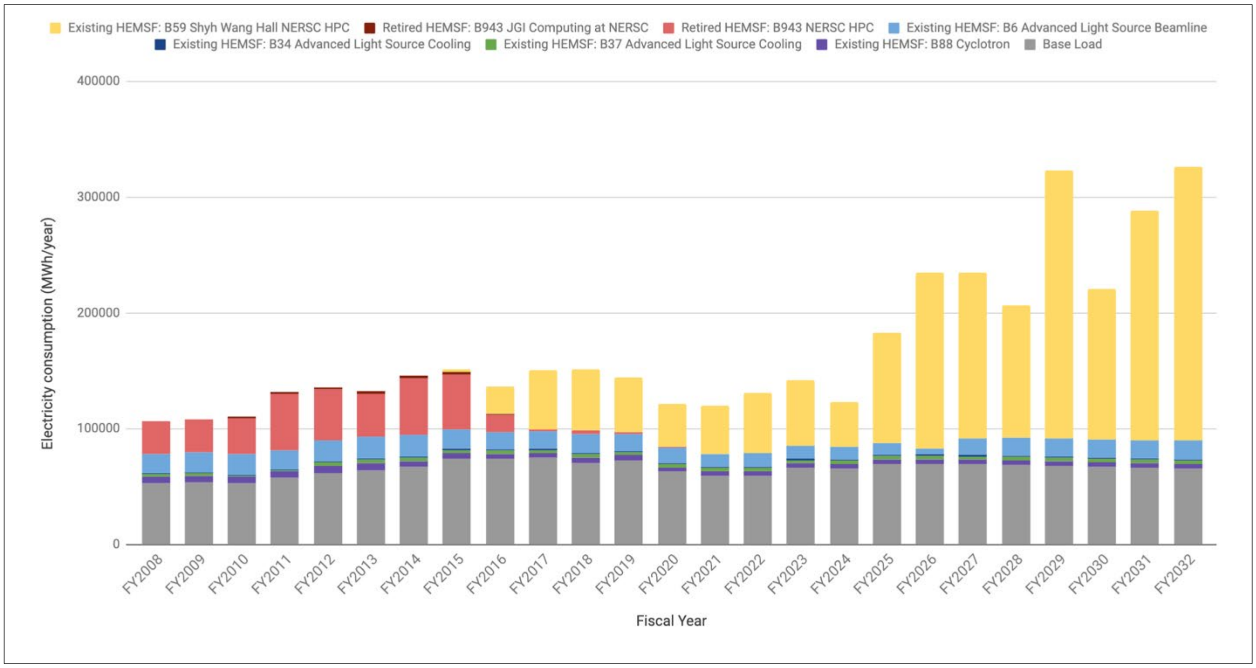
Per Executive Order 14057, the Lab is initiating net-zero planning, building on its strong foundation in energy efficiency performance. The Lab is also prioritizing planning to meet key requirements of the Order, such as fleet electrification and 100% carbon free electricity.

Our Net-Zero Lab Visioning Team has representatives from across the Lab. It will work over the coming year to inform net-zero planning. With consultant support, we have developed a scalable strategy for renewable energy procurement to meet carbon-free electricity and greenhouse gas reduction requirements of E.O. 14057. We are working with the Site Office for related approvals. We are exploring technical aspects related to electrification, moving away from natural gas, to inform the development of retrofit projects. The Lab is assessing EV fleet charging infrastructure requirements and will incorporate those needs to its planning. SBL is continuing resilience planning exercises that are being led by the Facilities Division and are discussed above in the section under Objective 2. Our planning seeks to maximize the role of solar and storage within a flexible microgrid as a complement to traditional deployment of diesel generation. The Lab is also working to prepare its Vulnerability Assessment and Resilience Plan as required by the end of FY22.

Actual and projected energy consumption for Lab, with separate identification of High Energy Mission Specific Facilities, is included in the figure and data table below. As to future changes in consumption:

The projection reflects an anticipated 9-month shutdown at the ALS beginning in Sept. 2025 followed by a 9-month commissioning period for the ALS-U project; for NERSC, the projection assumes additional load from NERSC-10 in FY25 and FY26, a retirement of NERSC-9 (Perlmutter) in FY28, plus increases in FY29 and FY31, which are more speculative.

Figure 1. Electricity Consumption Actuals and Projections



	FY08	FY09	FY10	FY11	FY12	FY13	FY14	FY15	FY16	FY17	FY18	FY19	FY20
Existing HEMSF: B59 Shyh Wang Hall NERSC HPC	0	0	0	0	0	0	0	1,832	23,546	50,571	53,188	47,184	37,323
Retired HEMSF: B943 JGI Computing at NERSC	0	0	1,491	1,491	2,058	2,477	2,409	2,294	1,020	0	0	0	0
Retired HEMSF: B943 NERSC HPC	28,627	27,875	30,514	48,951	43,903	36,727	48,449	47,785	14,511	2,026	3,383	1,734	603
Existing HEMSF: B6 Advanced Light Source Beamline	16,593	17,524	18,014	16,405	18,202	18,623	18,883	16,520	15,264	14,747	15,962	14,380	13,006
Existing HEMSF: B34 Advanced Light Source Cooling	879	982	750	952	915	1,000	1,044	1,096	1,040	1,329	1,072	954	1,055
Existing HEMSF: B37 Advanced Light Source Cooling	2,224	2,317	846	842	3,104	2,869	2,999	2,827	2,909	2,401	2,856	2,748	3,108
Existing HEMSF: B88 Cyclotron	5,423	5,316	5,498	5,870	6,032	6,917	4,512	4,689	4,001	4,316	4,624	4,140	2,803
Base Load	52,868	53,814	53,306	57,466	61,765	63,739	67,296	74,041	74,066	74,896	70,665	72,913	63,556
Total LBNL Electricity Consumption	106,614	107,828	110,419	131,977	135,979	132,352	145,592	151,084	136,357	150,286	151,750	144,054	121,454

	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30	FY31	FY32
Existing HEMSF: B59 Shyh Wang Hall NERSC HPC	42,001	51,467	57,131	38,157	95,126	152,014	143,688	113,918	231,568	129,943	198,077	236,684
Retired HEMSF: B943 JGI Computing at NERSC	0	0	0	0	0	0	0	0	0	0	0	0
Retired HEMSF: B943 NERSC HPC	0	0	0	0	0	0	0	0	0	0	0	0
Existing HEMSF: B6 Advanced Light Source Beamline	10,848	12,061	10,980	10,980	9,860	5,080	14,270	15,850	15,850	15,850	15,850	15,850
Existing HEMSF: B34 Advanced Light Source Cooling	986	951	982	982	982	982	982	982	982	982	982	982
Existing HEMSF: B37 Advanced Light Source Cooling	3,080	3,109	3,011	3,011	3,011	3,011	3,011	3,011	3,011	3,011	3,011	3,011
Existing HEMSF: B88 Cyclotron	4,087	3,859	3,986	3,986	3,986	3,986	3,986	3,986	3,986	3,986	3,986	3,986
Base Load	59,072	59,132	66,011	65,699	69,640	69,872	69,193	68,520	67,855	67,195	66,543	65,897
Total LBNL Electricity Consumption	120,074	130,579	142,101	122,815	182,605	234,945	235,130	206,267	323,252	220,967	288,449	326,409

OAK RIDGE NATIONAL LABORATORY

Lab-at-a-Glance

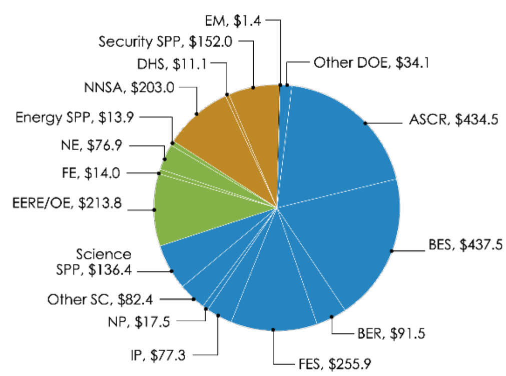
Location: Oak Ridge, TN
Type: Multi-program Laboratory
Contractor: UT-Battelle, LLC
Site Office: ORNL Site Office
Website: www.ornl.gov

- **FY 2021 Lab Operating Costs:** $1,771 million
- **FY 2021 DOE/NNSA Costs:** $1,458 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $302 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 17.7%
- **FY 2021 DHS Costs:** $11 million

Physical Assets:
- 4,421 acres and 265 buildings
- 4.5 million GSF in buildings
- Replacement Plant Value: $8.4 B
- 1.16M GSF in 58 Excess Facilities
- 0.87M GSF in Leased Facilities

Human Capital:
- 5,867 Full Time Equivalent Employees (FTEs)
- 110 Joint Faculty
- 324 Postdoctoral Researchers
- 250 Graduate Students
- 196 Undergraduate Students
- 1,564 Facility Users
- 671 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Mission and Overview

Oak Ridge National Laboratory (ORNL) has a rich history of scientific discovery and application of world-leading resources to the most pressing national problems. ORNL complements signature strengths in materials, neutrons, nuclear energy, isotopes, and computing with deep capabilities in chemistry, biological and environmental sciences, advanced manufacturing, energy technologies, and security science. ORNL advances and integrates this extraordinary range of expertise for scientific and technical breakthroughs that accelerate deployment of solutions for clean, resilient, and secure energy systems and global security. Convergent science and translational research are engrained in the laboratory's ethos and strategy, yielding solutions with national scale and impact.

ORNL's user facilities and major projects provide a cornerstone for ORNL's science and technology (S&T) and a unique set of resources to allow researchers worldwide to contribute to the Department of Energy (DOE) mission. ORNL operates four DOE Office of Science (SC) user facilities—the Spallation Neutron Source (SNS), High Flux Isotope Reactor (HFIR), Center for Nanophase Materials Sciences (CNMS), and Oak Ridge Leadership Computing Facility (OLCF)—and leads the Manufacturing Demonstration Facility

(MDF) and other applied energy facilities critical for clean energy. Extensive project management expertise enables new, large-scale capabilities, including the SNS Second Target Station (STS); the Exascale Computing Project (ECP); US ITER; and Frontier, America's first exascale system.

ORNL collaborations with laboratories, universities, industry, and communities lead to new insights, impacts, and economic development. As the only SC laboratory in the Southeast—within a Southern Appalachian laborshed categorized as distressed, at-risk, or transitional—ORNL is deeply invested in enhancing new partnerships and galvanizing a vibrant regional innovation ecosystem.

The extraordinary synergies among ORNL's 23 core capabilities; a creative, dedicated and mission-ready workforce of more than 5,800 employees; a unique ecosystem of facilities; diverse partnerships; and a disciplined strategic plan enable ORNL to find solutions essential to advancing DOE's clean energy, environment, and security missions.

Core Capabilities

The 23 core capabilities assigned to Oak Ridge National Laboratory (ORNL) by the US Department of Energy (DOE) provide a broad science and technology base that catalyzes fundamental scientific advances and technology breakthroughs to support DOE's mission of addressing the nation's energy, environmental, and nuclear challenges. These capabilities, each of which has world-class or world-leading components, reflect a combination of exceptional people, equipment, and facilities. Synergies among these core capabilities accelerate the delivery of scientific discovery and technology solutions and allow ORNL to respond to changing priorities and the critical needs of the nation.

Accelerator Science and Technology

ORNL has world-leading expertise in the basic physics of high-intensity hadron beams and the technology to support the production, acceleration, accumulation, and utilization of such beams. The Spallation Neutron Source (SNS) accelerator complex, operating at 1.4 MW power on target, is the world's most powerful pulsed proton accelerator and the world's highest-power superconducting linear accelerator (linac) for hadrons. The SNS enables ORNL to lead the investigation of the dynamics of high-intensity hadron beams and the development of high-power proton targets. The Proton Power Upgrade (PPU) project, which will provide up to 40% more power to the SNS First Target Station (FTS) and will enable novel neutron scattering experiments with thermal neutrons at high-energy resolution, is on track for completion in fiscal year (FY) 2025.

Other ORNL leadership areas include expertise in negative hydrogen ion (H^-) sources and low-energy beam chopping and manipulation; superconducting radio-frequency (SRF) technology; high-power target systems; high-power and low-level radio-frequency (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.

ORNL's strengths in computational science are used to develop beam dynamics modeling (including six-dimensional models) and data management tools to design next-generation spallation neutron sources, high-intensity linacs, storage rings, and associated radiation shielding. Expertise has been developed in artificial intelligence (AI) and machine learning (ML) with the goal of using large sets of accelerator data to predict and mitigate accelerator and target systems failures. The combination of state-of-the-art beam dynamics modeling tools and access to robust experimental data on collective, halo-formation, and instability effects in high-intensity hadron linacs and accumulator rings is unique to ORNL. These strengths underpin efforts to systematically increase the power level at which SNS operates reliably.

The comprehensive SRF and Cryogenic Test Facility supports a robust research program that has led to the development and successful deployment of a novel in situ plasma-cleaning technology that has increased the peak gradients of selected superconducting high-beta accelerator cavities by up to 25%. This project was extended into the medium-beta cavities, where a plasma ignition technique was successfully deployed to two medium-beta cryomodules. Additionally, ORNL is transferring this technology to other important accelerator projects in the DOE portfolio. ORNL is also developing capabilities for laser-assisted charge exchange of energetic H^- ions to facilitate high-power beam injection into advanced rings, pursuing novel approaches to power conversion technology for klystron modulators, and developing advanced beam instrumentation systems. Continued advances in high-level real-time applications, in combination with improvements in warm accelerator structure vacuum systems, have led to a significant reduction in the time required to complete facility turn-on after planned outages.

The Beam Test Facility (BTF) is a functional duplicate of the first 5 m of the SNS accelerator, the portion of the accelerator structure with the most complex beam dynamics and the most challenging reliability issues. The BTF supports continuous development and testing of critical hardware toward higher reliability, in particular new RF quadrupoles (RFQs), novel beam measurement instrumentation, and ion sources. It also serves as a high-availability, easy-access research station for understanding the beam dynamics in the low-energy portion of the accelerator, aimed toward improving control of the beam in the production accelerator. The research program at the BTF is an essential resource to enhance accelerator science opportunities that attract, engage, and retain staff with the expertise to drive innovation in several areas of accelerator science and technology relevant to the ORNL mission.

ORNL staff members also collaborate with similar international accelerator facilities as reviewers and advisors. DOE's Office of Science (SC) is the primary source of funding.

Recent advances to this core capability include the following:

- New capabilities at SNS include an RFQ, which will be delivered in FY 2022 and will greatly improve performance and maintenance of the SNS front end and the installation of a new upgraded servo-manipulator system with much higher camera resolutions and functionality. The cryogenic moderator system was demonstrated to have the capacity to operate at 1.9 MW, which will be critical to support SNS operations after the PPU is completed.
- At the BTF, the speed and dynamic range of phase space measurements have been increased at all dimensional orders. The dynamic range for emittance measurement now is at the 10^7 level, and for four-dimensional phase space, it is increased an order of magnitude to 10^4. The speed of measuring high-dimensional measurements such as five-dimensional phase space is increased an order of magnitude. The technique paves the way for better understanding mechanisms that generate beam halo, beam loss, and residual radiation in the linac.
- ML infrastructure and methods that aid in equipment prognostics, errant beam detection, and target modeling were developed to improve the reliability of the accelerator. First results in the past year indicate the potential for ML to aid in early detection of errant beams, early detection of hardware degradation in the High Voltage Converter Modulator, and modeling of the jet flow liquid mercury target. Work in this area will continue toward developing demonstration systems that operate on live equipment or data and ML for modeling of the jet-flow mercury targets with gas injection.

Advanced Computer Science, Visualization, and Data

ORNL staff are deeply engaged in research and development (R&D) to enable the deployment of scalable computing infrastructure to support the DOE mission, with an emphasis on the programs, facilities, and operations at ORNL. The laboratory participates in numerous Scientific Discovery through Advanced Computing (SciDAC) application teams and leads several components of RAPIDS (a SciDAC Institute for Resource and Application Productivity through Computation, Information, and Data Science). ORNL staff are prominent in the Software Technology focus area of the Exascale Computing Project (ECP). They are expanding ORNL capabilities in high-performance computing (HPC), including leading projects to develop an open-source algorithm and a software stack that will automate the process of designing, executing, and analyzing the results of quantum algorithms, thus enabling new discovery across scientific domains.

Three interconnected areas of emphasis distinguish the ORNL computer science research program: exploring and evaluating emerging accelerated computing technologies; developing the tools and methods needed for the analysis and management of data from the computational, experimental, and observational facilities across DOE; and developing the tools and methods needed to federate facilities in support of the DOE mission. Accelerated computing technologies will be deployed throughout the resources used to federate facilities, from the edge to our large HPC systems. Exascale applications are becoming more complex in their data flows (e.g., multiscale and multiphysics simulations that need to exchange data between separate codes, simulations that invoke data analysis and visualization services to extract information and render it, simulation output that needs to be stored to the file system for later analysis). The ORNL-developed Adaptable Input/Output System (ADIOS) provides a simple way to tackle data management challenges posed by large-scale science applications running on high-performance computers. Much of the opportunity for acceleration will be related to in situ data management and analysis. Support for data management and analysis spanning multiple facilities is also a key foundation for federating facilities.

In addition to these research foci, the ORNL computer science program stewards two service-oriented capabilities: the engineering of research software and the engineering, curation, and visual analysis of data sets. These software and data engineering capabilities focus on ensuring quality in the software and data-related artifacts being developed across the laboratory. The overarching purpose of the computer science program is to ensure that the programs, facilities, and operations at ORNL and throughout DOE utilize the best technologies available. While the computer science program is focused on long-term impact, the service-oriented capabilities provide a critical linkage between the research program and the programs that rely on the results of the research program.

ORNL is committed to developing the tools and technologies needed to advance accelerated node computing, from extreme-scale systems deployed by the Oak Ridge Leadership Computing Facility (OLCF) to those deployed by the Experimental Computing Laboratory (ExCL). The HPC resources of the OLCF, including the 200-petaflop IBM AC922 Summit and highly anticipated Frontier (OLCF-5), which promises a peak performance over 1,500 petaflops, will be available to users to advance knowledge in areas such as designing fusion power plants, designing new materials, engineering proteins to treat diseases, efficiently releasing energy from biomass, and understanding the impact of climate change. Frontier will achieve around 50- to 100-times performance improvement in real science applications or, alternatively, around 5- to 10-times application performance improvement over Summit. Systems available through ExCL explore a wide range of accelerated processing technologies, from quantum and neuromorphic processors to near-memory computing systems such as an Emu Chick and systems with field-programmable gate arrays. ORNL is building capabilities in predictive performance and future-generation high-end computing architectures. Additionally, ORNL is leading one of the SC Advanced Scientific Computing Research (ASCR) program Quantum Testbed Pathfinder teams.

ORNL is equally committed to developing tools and approaches that support the evolution of applications needed to effectively utilize the computing capability enabled by computational accelerators. ORNL staff are deeply engaged in the standards activities related to directive-based programming systems, including OpenMP and OpenACC, to ensure that these standards address the needs of DOE applications. QCOR, a novel open-source software stack specific for quantum computing, enables single-source quantum computing. The high level of abstraction in the developed language is intended to accelerate the adoption of quantum computing by researchers familiar with classical HPC. ORNL staff are also developing tools aimed at supporting the transformation of scientific software. For these and other applications, ORNL researchers bring significant expertise in system software, component technologies, run-time optimization, architecture-aware algorithms, and resilient computations.

In recent years, the DOE community has begun to recognize the need for advanced computer science, visualization, and data capabilities to provide a deeper understanding of data generated at DOE user facilities, such as light sources, neutron sources, and nanoscience centers. For example, bringing OLCF resources to bear at SNS can provide a deeper understanding of materials samples. To this end, ORNL has established research programs in workflow systems (including ADIOS, BEAM, and ICE), system science (including networking), and data and information visualization (including EVAL, Eden, and Origami). The Compute and Data Environment for Science (CADES) provides focus for deploying these research capabilities. Launched internally to provide a fully integrated infrastructure offering compute and data services for researchers, CADES is now being applied to the needs of users at SNS, the High Flux Isotope Reactor (HFIR), and the Center for Nanophase Materials Sciences (CNMS). With this platform, researchers can process, manage, and analyze large amounts of data using scalable storage, data analysis, and visualization tools.

ORNL also enables scientific discovery and accelerates the deployment of technologies in energy and national security by developing, managing, and accessing scientific data repositories (e.g., the Atmospheric Radiation Measurement [ARM] Data Archive, the Distributed Active Archive Center, the Earth System Grid Federation, the National Extreme Events Data and Research Center, and A Large Ion Collider Experiment [ALICE] USA Tier 2 Center). Through software and architectural advances such as quantum and neuromorphic computing for next-generation architectures, ORNL accelerates the deployment and utilization of petascale- and exascale-capable systems that will contribute to solving critical national challenges in science, energy assurance, national security, advanced manufacturing, and health care. ORNL also applies its capabilities in advanced computer science, visualization, and data in geographic information system R&D.

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 University of Tennessee–ORNL Bredesen Center for Interdisciplinary Research and Graduate Education. This capability is supported by SC, the Office of Electricity (OE), the US Department of Homeland Security (DHS), and Strategic Partnership Projects (SPP) sponsors, including the US Department of Defense (DoD) and the US Department of Health and Human Services (HHS).

Recent advances to this core capability include the following:

- Developed the first filtering method that directly estimates parameters without solving the estimated model state.
- Led important advances in the development of Discontinuous Galerkin methods for multiscale kinetic equations with diffusive limits.

- Designed new structure-preserving, multiscale methods for kinetic plasma simulations that are more efficient than direct methods in near-equilibrium regimes but still competitive in non-equilibrium settings.
- Developed efficient data-driven approximations to replace expensive entropy-based closures in kinetic simulations.
- Developed a new high-performance implementation (SNAPSHOT) of the Floyd-Warshall algorithm to assist in utilizing ORNL's Summit supercomputer to respond to COVID-19 challenges.
- Used the DCA++ application, a popular code for predicting the performance of quantum materials, to verify two performance-enhancing strategies for ORNL's Frontier supercomputer.
- Developed a stochastic approximate gradient ascent method to reduce posterior uncertainty in Bayesian experimental design involving implicit models.
- Developed novel compressed sensing approaches for simultaneous reconstruction of multiple signals that are endowed with similar sparsity patterns.
- Designed, implemented, and evaluated an HPC runtime system that uses the design pattern concept to orchestrate resilience capabilities for efficient protection against faults, errors, and failures.

Applied Materials Science and Engineering

ORNL closely couples basic and applied research to develop next-generation structural materials for applications in fission and fusion energy, transportation, buildings and other structural applications, high-efficiency steam generation, the hydrogen economy, supercritical carbon dioxide power cycles, and concentrated solar power. Teams of internationally renowned researchers in fundamental condensed matter science and materials science and engineering programs (supported by the DOE Office of Basic Energy Sciences [BES]) enable the development of new functional materials for energy and national security applications. ORNL's integration of basic and applied sciences combines characterization and computational tools with experimental synthesis, accelerating the progression from foundational science advances to technology innovation and providing an opportunity to deliver forward-looking materials science solutions that can readily be translated to high-impact applications.

Research associated with this core capability is the source of the majority of ORNL's patents, including novel processing techniques for advanced manufacturing of metals, alloys, and polymer composites. For example, ORNL recently advanced synthesis, production, and evaluation capabilities for radioisotope power systems to enable planned future space missions for the National Aeronautics and Space Administration (NASA) and other federal entities.

ORNL is also home to the Fusion Energy Sciences (FES) materials program, with an emphasis on developing and understanding structural materials relevant for fusion environments. Foundational research in plasma-materials interaction is key to preparation for fusion component studies. ORNL has expanded capabilities in materials theory, modeling, and simulation to enable structural and fuel cycle materials for fusion energy and taming plasma-materials interactions.

Specialized world-leading capabilities in applied materials science and engineering include materials joining, surface engineering and processing, corrosion studies under harsh but well-controlled conditions, mechanical testing in a variety of environments, and physical property determination. Specific materials expertise exists in the development and advanced manufacturing of alloys, ceramics, nanomaterials, carbon fiber and composites, nanostructured carbons, polymers, thermoelectrics, and energy storage systems. ORNL recently developed an ultrapure lithium metal deposition capability for all-solid-state batteries and fabrication, processing, and test capabilities for laboratory-scale solid-state batteries.

ORNL's applied materials science and engineering program takes advantage of state-of-the-art capabilities for materials development and testing, such as the SC user facilities CNMS, SNS, HFIR, and OLCF; the Carbon Fiber Technology Facility (CFTF) and the Manufacturing Demonstration Facility (MDF), supported by the DOE Office of Energy Efficiency and Renewable Energy (EERE); and other nonreactor nuclear and radiological facilities, such as the Low Activation Materials Development and Analysis (LAMDA) Laboratory and the Irradiated Materials Examination and Testing hot cell facility. ORNL leverages these capabilities for national security interests within secure manufacturing facilities, including export-controlled facilities (e.g., CFTF) and classified manufacturing (classified MDF).

Moreover, ORNL continues to increase and optimize automation for materials characterization and to apply advances in digital tools, computation, AI, and ML to its capabilities. ORNL is advancing capabilities that integrate advanced functional imaging, data science and informatics, and image-informed modeling for advanced characterization and performance prediction of materials for harsh environments. ORNL research also maximizes the lifespan of existing energy infrastructure; for example, ORNL recently developed improved repair welding technology and advanced capabilities to evaluate service-irradiated steels that enable the life extension of the current fleet of nuclear reactors.

advanced heat-resistant structural materials, and procedures for testing them. For example, ORNL recently developed the capability to conduct creep tests at up to 1300°C in an inert (Ar) environment for testing refractory metal alloys and other environmentally sensitive materials at high temperatures. Overall, the core capability of the 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, the Office of Nuclear Energy (NE), the National Nuclear Security Administration (NNSA), DHS, the Advanced Research Projects Agency–Energy (ARPA-E), DoD, and other SPP customers.

Recent advances to this core capability include the following:

- Enhanced ORNL's capabilities to develop and evaluate materials for plasma-facing component solutions and robust structures to operate in the extreme fusion and nuclear environment.
- Expanded capabilities that enhance our expertise in solid-state batteries through investments in lithium-metal deposition capabilities that enable controlled engineering of ultrapure lithium thin films.
- Furthered capabilities that enable the reuse and recycling of materials for energy storage through the development of an automated battery disassembly line that makes battery disassembly safer and 10 times faster.
- Advancing capabilities that integrate advanced functional imaging, data science and informatics, and image-informed modeling for advanced characterization and performance prediction of materials for harsh environments.
- Developed the capability to conduct creep tests at up to 1300°C in an inert environment for testing refractory metal alloys and other environmentally sensitive materials at high temperatures to enable the development of advanced heat resistant structural materials.

Applied Mathematics

ORNL's applied mathematics program spans four highly visible and externally recognized areas of research: (1) multiscale modeling and simulation; (2) mathematical tools for the analysis of scientific data, including AI and ML; (3) discrete mathematics, including graph theoretic methods and matrix factorizations; and (4) systems analysis and decision making, including statistics and the analysis of complex networks. Strategic foci include (1) scalable, architecture-aware, and resilient mathematical and computational capabilities for modeling and simulation; (2) robust algorithms for ML and data analysis, including uncertainty quantification (UQ), accelerated learning, and physics-informed learning; (3) the analysis of complex, multiphysics and multiscale systems and algorithms; and (4) demonstrated impact on applications in science and engineering. Algorithms developed within the applied mathematics program continue to be a critical component of ORNL's modeling and simulation capabilities and are widely recognized and used beyond ORNL. Applied mathematicians and theoretical computer scientists have developed key results for efficient and robust learning algorithms focused on dimension reduction and stochastic optimal control using reversible networks, upper quartile, and image classification, with a strong focus on scalable implementation targeting Summit. Several applications, such as medical imaging, neutron science, and materials design, have benefited from these algorithmic advancements. CNMS, MDF, and the National Transportation Research Center (NTRC) are among the experimental sites where the applied mathematics program develops supervised and unsupervised learning methods. This work builds on top quartile strengths such as optimum reconstruction from sparse and large amounts of noisy data; optimization, control, and design of high-dimensional physical and engineering systems; and linear and nonlinear solvers. Funding comes primarily from SC, DoD, the National Science Foundation (NSF), HHS, and other SPP sponsors.

Recent enhancements to this core capability include the following:

- Developed a stochastic approximate gradient ascent method that achieves designs with significantly improved confidence, avoids intractable overhead cost of Bayesian optimization, and has been demonstrated in problems of controlling Rabi oscillations for quantum optics.
- Developed a new mathematically well-posed, nonlocal Cahn-Hilliard phase-field model with a finite element discretization to allow sharp interfaces corresponding to the strict separation of a substance into pure phases, such as in solidification problems.
- Developed efficient data-driven approximations to replace expensive entropy-based closures in kinetic simulations. The approximations have been demonstrated on a neutron transport simulation and can be extended to problems in other applications, including plasma, charged particle transport, and radiative transfer.
- Designed new structure-preserving, multiscale methods for kinetic plasma simulations that are more efficient than direct methods in near-equilibrium regimes but still competitive in non-equilibrium settings. The methods have been demonstrated in high-fidelity boundary plasma simulations.

Biological and Bioprocess Engineering

ORNL brings substantial strength in fundamental biology to bioprocessing and bioengineering to address DOE mission needs in bioenergy production, carbon capture and long-term storage, and environmental contaminants processing. ORNL is (1) leading the Center for Bioenergy Innovation (CBI), a nexus for research on biomass utilization for biofuels and bioproducts (e.g., higher alcohols, esters, jet/marine fuel, and lignin coproducts); (2) characterizing the largest population of *Populus* genotypes for biomass deconstruction gene discovery and expanding that analysis to switchgrass; (3) developing new microbial platforms for the conversion of biomass to products; (4) coupling fundamental and applied research in biomass production and conversion (both thermochemical and biochemical conversion) for high-value materials and chemicals, fuels, and power; (5) making sustained contributions to assess biomass feedstock supplies at regional and national scales; and (6) automating design-build-test-learn cycles.

ORNL leverages its next-generation capabilities in chemical engineering, chemistry, materials science, AI, HPC, and systems engineering to accelerate the translation of research outcomes into demonstrable improvements in bioproducts and biofuels and to move research from the laboratory to the field or pilot level. ORNL uses integrated expertise in plant sciences, microbiology, molecular biology, molecular modeling, and bioinformatics—in combination with facilities such as the common gardens, high-throughput phenotyping equipment, neutron sources (SNS and HFIR), and computing resources (CADES and the OLCF)—to address the needs of the bioeconomy. ORNL continues to innovate in analytical technologies, from chemical imaging to multimodal small-angle neutron scattering (SANS).

ORNL is a recognized leader in multiple aspects and scales of bioenergy production, including biofeedstock sources and sustainability analyses, with emphasis on an integrated systems approach (e.g., landscape design) at multiple landscape scales (from hectare to nation) for applied impacts. This leadership has been leveraged to assess the potential for carbon management through bioenergy for carbon capture and long-term capture in soils. ORNL also leads in the use of a suite of biomass conversion processes: novel microbes and applied systems biology, computational chemistry and biophysics modeling for biomass conversion, and biofuels and bioproduct upgrading to advance bioenergy production. As part of this effort, ORNL is engaged in a range of efforts to advance the use of automation in design-build-test-learn cycles, from molecules to plant systems. In addition to using off-the-shelf robotics, ORNL is developing new interfaces between laboratory equipment and edge computing to facilitate these efforts.

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.

Recent enhancements to this core capability include the following:

- Developed a fluorescence biosensor for CRISPR-Cas that can detect the activity of gene editing machinery and that positions ORNL to develop drought-resistant bioenergy crops and engineer bacteria to efficiently convert plants into sustainable aviation fuels.
- Discovered a new biochemical pathway to cleave a lignin-derived aromatic dimer, which can be utilized in lignin valorization to commodity chemicals. Lignin is a waste product of biofuels production from plants, and its conversion to industrial chemicals makes biofuels production more economically viable.
- Co-developed with LanzaTech and Northwestern University a carbon capture technology that harnesses emissions from industrial processes to produce acetone and isopropanol, thus taking a major stride toward a circular carbon economy that can replace products made from fossil resources.
- Implemented nanocellulose in three-dimensional (3D) printing of advanced sustainable materials, a capability that uniquely expands the range of printable materials for manufacturing of durable goods and products.
- Designed and deployed a new robotic sample changer for Bio-SANS to increase measurement throughput by approximately 20% and accelerate analysis of the structural changes in plant cell walls during processing and conversion of biomass to biofuels.

Biological Systems Science

ORNL's core capability in biological systems science directly improves understanding of complex biological systems through (1) integration of plant sciences with synthetic biology, ecology, computational biology, and microbiology; (2) discovery of gene function; (3) foundational research in plant science that enables development of sustainable plant feedstocks for bioenergy and bio-derived materials; (4) the use of neutron science and exascale computing to characterize protein structure and interaction; (5) development of imaging and chemical measurement analytics at multiple spatial and temporal scales; and (6) development and application of data analytics, AI, and simulation for biology. The fundamental understanding delivered through application of this core capability is essential to solving challenging societal problems in bioenergy, nutrient cycling, climate change, carbon management, and environmental remediation.

ORNL has strategic strengths in plant biology that have largely focused on more than 1,000 genome-sequenced *Populus* lines and is the host institution for CBI, which is in its fifth year. ORNL has added a state-of-the-art Advanced Plant Phenotyping Laboratory (APPL), a multispectral imaging system that enables a new level of high-throughput phenotyping of plant systems. A robotic sampling system for APPL is under development. CBI continues to lead improvements in the economics and sustainable production of biomass and its conversion to bioproducts such as sustainable aviation fuel. ORNL's strengths in plant biology and microbiology support additional fundamental research in Science Focus Areas (SFAs), such as Plant-Microbe Interfaces (PMI), Secure Ecosystem Engineering and Design, and Biofuels. ORNL is also part of collaborative projects with other national laboratories (e.g., Ecosystems and Networks Integrated with Genes and Molecular Assemblies and Systems Biology Knowledgebase).

ORNL has launched a Biological Scales (Bio-Scales) effort to connect gene function with higher-order biological and ecosystem effects and create gold-standard data sets compatible with DOE Office of Science's Biological and Environmental Research (BER) program such as the National Microbiome Data Collaborative and for distribution via the APPL Public Interface. Integrated capabilities in biochemical sciences, neutrons, and computing benefit the Biofuels SFA and the Critical Interfaces SFA. ORNL research within the PMI SFA characterizes the soil and plant microbiome and elucidates fundamental aspects of plant–microbe signaling and symbiosis leading to chemical cycling in the terrestrial biosphere. These data-rich experimental efforts interface with bioinformatics expertise in microbial annotation and computational investigation, including AI approaches for modeling and design using complex systems biology and protein structure data.

ORNL's neutron scattering resources can be leveraged through the Center for Structural Molecular Biology, including the Bio-SANS instrument at HFIR. A BER-funded effort developed a prototype multimodal SANS instrument for the SNS Second Target Station (STS), with newly added robotic sample handling. 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.

Recent enhancements to this core capability include the following:

- Discovered a pathway that regulates C-lignin formation in plants that provides a good source of the building blocks and aromatic chemical compounds needed to produce clean bio-based fuels. This breakthrough could make possible the production of crops grown for sustainable jet fuels easier and less costly.
- Developed a HPC and ML pipeline using AlphaFold to predict protein folded structures and their functions across the proteome. Structure-based gene functional annotation can help connect genotype to phenotype in a range of organisms.

- Documented the sensitivity of plant-microbe interactions to disturbance and demonstrated how fire severity impacts plant microbiome assembly, diversity, and composition as a function of increasing plant fitness and ecosystem recovery after disturbance events.
- Designed diisobutylene maleic acid lipid nanoparticles to stabilize membrane proteins for structural characterization by neutron scattering. These scaffolds allow many challenging membrane systems to be visualized.
- Developed in situ liquid extraction mass spectrometry imaging for chemical analysis of exudates from living plant roots. This technique avoids the limitation of microfluidic ports by having a porous membrane through which exudates can be sampled at arbitrary locations.

Chemical and Molecular Science

ORNL's core capability in chemical and molecular science is focused on understanding how local environments and functional architectures can selectively control 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 carbon capture, removal, and conversion, for energy storage and conversion; for mitigation of environmental impacts of energy use; and for national security. The ORNL-led Fluid Interface Reactions, Structures and Transport Energy Frontier Research Center focuses on developing a fundamental understanding and validated predictive models of the atomic origins of electrolyte and coupled electron transport under nanoscale confinement that will enable transformative advances in capacitive electrical energy storage.

The design of new materials and processes for chemical separations and catalysis is a strength of the ORNL Chemical and Molecular Science core capability. Scientific underpinnings of direct air capture are demonstrated, including approaches that combine atmospheric CO_2 absorption by an aqueous oligopeptide (e.g., glycylglycine) with bicarbonate crystallization by a simple guanidine compound (e.g., glyoxal-bis-iminoguanidine). In catalysis, strengths in synthetic methods create metal nanoparticles encapsulated by strong metal support interactions to demonstrate approaches to enhance selectivity in hydrogenation reactions and stability in oxidation reactions. To overcome the bottleneck in the synthesis of new materials, Laboratory Directed Research and Development funding is being used to establish an autonomous chemistry lab underpinned by a robotic chemist guided by artificial intelligence to accelerate our understanding and discovery of new materials, such as catalysts for chemical conversion of CO_2 through our Interconnected Science Ecosystem (INTERSECT) initiative.

The neutron scattering expertise in combination with first-principle simulation provides fundamental understanding of the structural evolution of catalysts and porous rocks under reaction conditions and the solvation structure of ions. In geoscience, neutron and x-ray small- and ultrasmall-angle scattering in a combination with time-of-flight secondary ion mass spectrometry expertise enables the determination of how pore structures influence coupled dissolution, precipitation replacement reactions. In solution phase chemistry, neutron diffraction with isotopic substitution approaches are enabling the calibration of metadynamics rare event computational simulations relevant to solvation structures of ions.

The Chemical and Molecular Science core capability also develops novel characterization tools and data analysis methods to study reactive and dynamic interfaces over a range of time and length scales. For example, vibrational sum frequency generation spectroscopy and interfacial tension measurements are used to understand mechanistically how ion pairing, hydrogen-bonding, and oil phase solvation can be used to tune the organization at the liquid/liquid interface to impact extractions and self-assembly. This expertise is also used to probe the influence of nanomaterials on liquid/liquid interfaces relevant to tank waste remediation and other nonideal separations. This core capability is being strengthened by the development of unsupervised ML data analysis methods coupled with scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy. ML algorithms developed at ORNL are generally applicable to data analysis of any spectrum-imaging technique and for various material systems, revealing trace signals in complex local nanoenvironments at surfaces and interfaces in catalysis. Mass spectrometry is also being used in nuclear and radio chemistry in the quantitative characterization of stable and radioactive isotopes and for nuclear forensics, and it is the basis of the electromagnetic isotope separation capabilities established for the DOE Isotope Program. A new capability was developed for solid surface sampling with robotic particle manipulation and electrothermal vaporization system. This system employs a unique combination of laser-induced breakdown spectrometer/laser ablation with a newly developed surface microextraction system to locate; manipulate; and generate depth profiles and elemental maps of particles, bulk material, biological tissues, and nondigestible materials that were previously out of reach for inorganic mass spectrometry.

Funding comes primarily from BES. Applied programs sponsored by DOE's Office of Environmental Management (EM), NE, NNSA, FE, and EERE benefit from this research. Research in chemical and molecular sciences also has applications to BER, Office of Nuclear Physics (NP), and Isotope Programs.

Recent enhancements to this core capability include the following:

- Further developed and made investments in moving discoveries in dilute air capture of carbon dioxide to market by examining possible ways to scale the discoveries.
- Invested in new near-ambient-pressure x-ray photoelectron spectrometer to perform direct measurement of materials under near-real-world conditions, including materials to address energy conversion and efficiency challenges.
- Developed capabilities to investigate continuous flow chemistries and polymerization reactions under controlled temperature, pressure, volume, and multiphase conditions that can be guided by simulation and optimization algorithms.

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 fundamental research sponsored by the Office of Science in the following areas:

- research sponsored by BES in materials discovery, design, synthesis, and characterization;
- research sponsored by BES in chemical separations, catalysis, and computational modeling;
- research sponsored by BER in bio-based fuels and chemical production;
- research sponsored by the Office of Isotope R&D and Production in production of radioisotopes and stable isotopes;

- research sponsored by the EERE Vehicle Technologies Office and Bioenergy Technologies Office in applied chemical separations, fuels, pyrolysis, and catalysis development; and
- research sponsored by the Office of Fossil Energy and Carbon Management in CO_2 removal, capture, and conversion.

ORNL advances new chemical processes and develops new materials to improve efficiency, economy, and industrial competitiveness. For example, advancements in environmentally friendly and economical separations methods have been made at ORNL as part of the research at the Critical Materials Institute for recovering rare earth elements such as neodymium, dysprosium, and praseodymium from scrap magnets and as a means to improve methods for recycling batteries. ORNL has significant strengths in developing processes to produce carbon fibers.

Stable isotope research and production depend on the utilization of specialized or potentially novel feedstock chemicals not available commercially, including the reformulation of enriched stockpiles for use in processes to further increase enrichment of the desired isotope. We are pursuing the development of synthetic processes, enrichment processes, and physical property measurement. This includes the chemical process design for the first centrifuge production system for enriched stable isotopes at ORNL.

As the national steward of uranium science and processing technology, ORNL applies expertise in chemical engineering to advance the understanding of fuel cycle operations associated with processing, purifying, and enriching uranium. Related ORNL separations expertise in both electromagnetic and gas centrifuge techniques is also enabling advances in stable isotope enrichment that are being applied in the design and construction of the Stable Isotope Production Facility (SIPF) and the Stable Isotope Production and Research Center (SIPRC). Innovative chemical processes being developed for the recovery and recycling of nonnuclear materials from used nuclear fuel (UNF) assemblies have great potential for simplifying secure UNF disposition pathways and for reducing the mass and volume of the waste stream. Conceptual designs of processes for converting UNF into fuel for alternative reactor concepts are being developed. Established uranium chemical processes, operated at a range of scales, support ORNL's nonproliferation mission while providing learning opportunities for the next generation of radiochemical engineers and scientists. High-speed analytical capabilities usable in two-phase systems have been developed to elucidate separations and reaction mechanisms toward the control of residence time to improve separation efficiency and reaction yields.

In light of the current national interest in nuclear power plant technologies, ORNL has developed capabilities, laboratories, and systems for producing and characterizing molten fuel and coolant salts for fast and thermal molten salt reactor (MSR) concepts, including a chemistry laboratory for measuring molten salt properties and developing models to more accurately predict the behavior of candidate fuel and coolant salts. These facilities allow us to produce and characterize beryllium- and chloride-based salts in high-temperature environments to measure and understand thermophysical and chemical (e.g., corrosion) properties with various metal alloys. Additionally, ORNL has developed a new sensor for off-gas from molten salt processing to follow the chemical reactions occurring in the MSR.

Chemical engineering research at ORNL makes use of resources that span radiological laboratories and nuclear facilities, 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.

Recent enhancements to this core capability include the following:

- Made investments that could enable new approaches for mineral looping for carbon removal.
- Developed new AI/ML tools for new understanding of chemical and molecular processes.
- Standing up new automated laboratory for chemical process discovery.
- Expanded our capability through a new solid-surface sampling with robotic particle manipulation and electro thermal vaporization system.
- Combined sum frequency generation spectroscopy with interfacial tension measurements to show that organophosphorus-based extractants with branched or linear alkyl tails have similar adsorption energies but form disparate interfacial structures at the liquid-liquid interface.

Climate Change Science and Atmospheric Science

ORNL's core capability in climate change and atmospheric science is focused on improving understanding of the causes, impacts, and predictability of climate change by (1) conducting large-scale, long-term, complex ecosystem experiments and observations; (2) leading DOE Earth system model (ESM) development in biogeochemistry for the Energy Exascale Earth System Model (E3SM) project; (3) integrating multidisciplinary research connecting data, terrestrial and atmospheric sciences, and large-scale computing; (4) developing novel software to improve the credibility and scalability of next-generation ESMs in preparation for exascale computing; (5) developing model-data integration tools, ML methods, and synthesized data for model evaluation, diagnostics, and benchmarking; (6) performing data management for observations and large model output, and building tools for data discovery, distribution, and archiving; and (7) 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 subsurface hydrology dynamical cores.

ORNL advances next-generation integrated models of the Earth system by improving the characterization of ecosystem processes and land–atmosphere exchange of carbon, nitrogen, nutrients, water, and energy as well as human–climate–system interactions. ORNL leads in the use of knowledge derived from these long-term experiments to improve the representation of key plant and microbial traits in terrestrial biosphere models (e.g., spanning scales from genes to ecosystems) and their contributions to global 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 Facility. With over 3.2 petabytes of data from more than 11,000 data products, the ARM data center provides key atmospheric radiation measurements from around the world to improve understanding of atmospheric dynamics and cloud processes. During FY 2021, the ARM data center was recognized as a Public Reusable Research Data Resource by SC. Additionally, the team successfully deployed Site Data Systems, processing and archiving data for two new campaigns, the Surface Atmosphere Integrated Field Laboratory and the Tracking Aerosol Convection Interactions Experiment campaigns. ORNL advances high-resolution modeling, value-added data product generations, and AI-based data analysis by continuously deploying new HPC workflow capabilities and compute resources as part of the ARM Computing Environment. For example, during FY 2021 the ARM data center and OLCF successfully deployed a new HPC cluster Cumulus2 to support the Large-Eddy Simulation ARM Symbiotic Simulation and Observation expansion and other research proposals.

ORNL infrastructure supporting climate change science and atmospheric science includes a growing data storage facility and private cloud capacity for computing near data through the National Center for Computational Sciences; leadership-class computing through OLCF, which supports process-based and ML modeling and simulation and big data applications; state-of-the-art greenhouses; field and laboratory facilities; and SNS and HFIR, which enable characterization of soil organic matter and multimodal imaging of whole plant/soil systems and plant–water interactions.

SC is the primary sponsor for these efforts; NNSA, NASA, DoD, DHS, the US Geological Survey, National Oceanic and Atmospheric Administration (NOAA), and the US Department of Agriculture's Forest Service also sponsor or collaborate on activities that leverage and enhance DOE investments in climate change and atmospheric science to generate solutions for the nation.

Recent enhancements to this core capability include the following:

- Demonstrated a model-data intercomparison of land and ocean models from the fifth and sixth phases of the Coupled Model Intercomparison Project (CMIP), and quantitatively documented that community investments in land and ocean biogeochemistry model development yielded improvements in model performance for the sixth phase of the CMIP (CMIP6) models compared to earlier model versions from the fifth phase of the CMIP (CMIP5).
- Developed a data replication strategy to create a failsafe backup of 10 petabytes of model output from the Earth System Grid Federation at ORNL and Argonne National Laboratory, including simulation results from CMIP6 from modeling centers around the globe.
- Developed improved representation of Arctic vegetation within the E3SM Land Model (ELM) by measuring above- and below-ground tundra plant traits and implementing new plant functional traits (PFTs). The addition of the new Arctic PFTs enabled better representation of the variability in biomass across different plant communities, improved model projection of tundra vegetation carbon storage, and will ultimately enable more accurate projections of carbon cycling in high-latitude ecosystems.
- Developed a new tool by adding wetland processes to land surface models using model-experiment interactions involving lessons learned from the Spruce and Peatland Responses Under Changing Environments (SPRUCE) warming study and iterative interactions with the relevant models important to Earth System simulations. This new capability will enable improved model simulations of carbon cycling in high-latitude peatland ecosystems as well as other wetland systems.
- Developed a modified ELM subgrid hierarchy to improve simulations of tidal channels and rising and falling tides on hydrological conditions in coastal wetland systems and implemented these capabilities within the ELM. This new capability provides a foundation for new coastal wetland development in ELM, with future work focusing on biogeochemistry and extension to other coastal regions.

Computational Science

Computational science at ORNL is focused on the development and delivery of scalable computational applications that enable researchers to combine theory, experiment, data analysis, and modeling and simulation and thereby tackle science and engineering problems of national interest. It also provides foundations and advances in quantum information science (QIS) to enable quantum computers, devices, sensors, and networked systems. This core capability resides within the world's most capable complex for computational science, which comprises outstanding staff, infrastructure, and computers dedicated to a research portfolio that covers the full span of ORNL's interests. Integrated teams of domain scientists, computational scientists, computer scientists, and mathematicians provide scalable computational and analytical solutions delivered through the integration of algorithms, modeling and simulation, artificial intelligence, software technologies, computer and information sciences, and HPC infrastructure.

These solutions enable science and engineering insights and modeling of new quantum and nanomaterials with favorable and predictable properties; characterizing and closing the carbon cycle, predictive understanding of microbial, molecular, cellular, and whole-organism systems; simulation of existing and advanced light water reactors (LWRs); characterization of fusion systems; real time capture, prediction, and optimization of energy infrastructure and usage; reliable predictions, with uncertainties, of regional and community scale climate change, including extreme events and biogeochemical feedbacks; data-driven and simulation campaigns to tackle molecular, cellular, and human-scale health challenges; advanced software and algorithmic environments for enrichment of rare isotopes. Within the computing directorate, a synergistic, interdisciplinary computational capability also supports early-stage research for companies of all sizes—including SmartTruck Systems, GE, Rolls- Royce, Ford, Arconic, Polyceed/Dyenamics, and Boeing—to address problems that are tractable only by using HPC.

Example applications under active development for current and future leadership computing platforms include Lattice QCD for chemistry and materials applications; NWChemEx to address scientific challenges involved in the development of advanced biofuels; support for the GAMESS-US electronic structure code; QMCPACK for simulation of electron structure of atoms, molecules, and solids; E3SM-MMF to develop a cloud-resolving earth systems model for high-resolution climate simulations; and CANDLE, applying the latest deep learning techniques for information extraction from COVID-19 and cancer-related literature. ORNL is addressing critically important engineering problems and is supporting efforts in wind energy (ExaWind), energy grid optimization and workflows (ExaSGD), and combustion technologies (Combustion-Pele). In total, ORNL support for the ECP Applications Development focus area by leading projects that are building new simulation capabilities for small modular reactors (ExaSMR), additive manufacturing (ExaAM), and quantum materials (QMCPACK)—as well as having portfolio leadership of projects.

Multiple science and engineering disciplines have transdisciplinary connections, and they leverage our facilities and foundational mathematics and computer science that enables impactful insights and advances across projects, including materials design at the quantum to bulk scales, chemistry for polymers and scalable carbon capture, quantum computing and networking, electrical energy storage (batteries and supercapacitors) and resilience, microelectronics, new enrichment technologies and regimes, nuclear reactor efficiencies and lifetimes, fusion plasma containment, climate change science, weather prediction modeling, health and quantitative biology, and scalable analytics, networks, and workflows to address complex problems associated with DOE missions in instrument automation, and energy and national security.

Funding for this work comes from SC, NE, FE, the National Virtual Biotechnology Laboratory, EERE, and OE. Other offices and agencies, including the DoD, the Department of Veterans Affairs, HHS, and NSF, also sponsor or collaborate on activities that leverage DOE investments in computational science.

Recent enhancements to this core capability include the following:

- Demonstration of process intensification of chemical vapor infiltration for ceramics and simulations to enhance material properties during additive manufacturing using HPC at scale in preparation for using two ECP applications (ExaAM and Pele-Combustion) on Frontier.
- Developed and deployed a software framework for training Transformer deep learning models on OLCF's Summit in support of clinical text research for the DOE partnership with the National Cancer Institute.
- Co-developed with Duke University a method to characterize and then mitigate coherent noise in quantum circuits and demonstrate how these noise sources directly impact today's Noisy Intermediate Scale Quantum-era applications.
- Produced and demonstrated a scalable benchmark that can test a quantum computer's ability to produce large-scale entanglement, one of the most important quantum resources for quantum information tasks. The benchmark is portable to multiple architectures and has been demonstrated on both superconducting and trapped-ion devices.

Condensed Matter Physics and Materials Science

The scientific themes of ORNL's condensed matter physics and materials science portfolio include the following:

- mastering the origin of quantum phenomena;
- understanding and tailoring excitations and transport;
- harnessing quantum superposition, squeezing, and entanglement to enable QIS;
- elucidating how functionalities emerge at interfaces and phase boundaries; and
- understanding and controlling defects and disorder.

All of the themes aim to yield new materials and properties. These theme areas are based on ORNL's world-leading capabilities for predicting, synthesizing, characterizing, and controlling materials systems across temporal and spatial scales. They make it possible to ultimately design materials with specific functionalities by connecting the fundamental understanding of complex materials to applications in energy generation, storage, and use.

ORNL has specialized expertise in synthesis of single crystals, thin films, artificial heterostructures, alloys, nanophase materials, polymers, and polymer composites. The ability to manipulate orbital-driven interactions that direct handed-spin textures, such as nanometer-scale magnetic skyrmions, is important for discovering novel quantum materials that may be critical for the development of ultra-high-density information storage. ORNL has built up expertise in the autonomous control of atomic building blocks by strain applicable for various classes of materials to co-design multifunctional materials with novel or complementary physical properties.

QIS research focuses on leveraging quantum coherent, squeezed, and entangled quantum states to probe classically inaccessible material properties. Building of expertise in QIS, ORNL is accelerating the discovery of entangled and correlated quantum states through direct control of dopants, defects, and material geometry. A new realistic strategy has recently been proposed to explore various quantum phases by strain engineering and to achieve quantum anomalous Hall insulators, potential building blocks for topological quantum electronics and quantum computers, with high thermodynamic stability.

By developing quantum-enhanced microscopies, ORNL will offer the potential to provide new understanding of topological and superconducting order in emerging quantum devices.

ORNL has also expertise in energy materials focused on interfaces and solid-state transport. The presence of a stable and ion-conducting solid electrolyte interphase is key to stable, high-performance batteries. ORNL is expanding its expertise in microelectronics with the aim to close the knowledge gaps in neuromorphic computing architectures that prevent effective and on-demand design and implementation of analog, spiking, in-memory, and probabilistic computing paradigms. These efforts combine first-principles modeling, materials characterization, device physics, architecture design, algorithms, and whole-circuit implementation to enable bottom-up and top-down co-development of efficient neuromorphic algorithms and the physical models that can implement these algorithms. The development of effective compact models for hysteretic resistive devices based on binary oxides and metal-organic compounds are medium-term goals and will enable co-design in the absence of perfect knowledge of material parameters.

Leadership capabilities in materials imaging, including in situ electron microscopy and spectroscopy, scanning probe microscopy modalities, atom probe tomography, and chemical imaging, are in part made available through the CNMS user program. Developments in deep learning networks from STEM is advancing automated image analysis and recognition of the defects in solids and further strengthening this core capability. Additionally, ORNL has expertise in utilizing advanced neutron and x-ray scattering techniques to understand collective quantum phenomena, energy transport, and structure and dynamics in liquids.

ORNL's experimental condensed matter and materials science efforts are deeply integrated with theory, computation, modeling, and simulation. A hallmark of ORNL's theory, modeling, and simulation is the use of computation and data analytics to inform the design and discovery of novel structural and functional materials. Our efforts span electronic structure calculations of functional materials utilizing density functional theory and quantum Monte Carlo (QMC), model Hamiltonian studies of quantum phenomena such as topological insulators and magnons, and atomistic simulations of radiation-induced defects and damage. ORNL has strengths in the development and application of scalable computational approaches and codes (e.g., QMC and locally self-consistent multiple scattering) that take advantage of the OLCF. ORNL is developing approaches to apply codes to next-generation exascale computing.

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.

Recent advancements to this core capability include the following:

- Expanded QIS expertise, building off our foundational knowledge in quantum materials.
- Developed approaches to control room temperature magnetism in van der Waals magnets.
- Advanced unsupervised ML method that furthered our ability to detect and classify material defects.
- Developed chemically accurate pseudo-Hamiltonians for correlated elements that overcome localization errors in diffusion Monte Carlo.
- Demonstrated how to perform atomic-scale tailoring of nanophotonic properties of nanomaterials with electron beams.

Cyber and Information Sciences

ORNL's cyber and information science core capability includes expertise and resources in cybersecurity, cyber-physical security, identity sciences and biometrics, visual analytics, data analytics, AI/ML, database architectures, secure communications, signals analysis, QIS, data privacy, and information security.

These resources are used to (1) securely and resiliently collect, share, intelligently store/retrieve, transmit, analyze, and classify enormous and heterogeneous collections of data; (2) create knowledge from disparate and heterogeneous data sources; and (3) understand, assess, defend against, and defeat known or unknown adversaries to protect the nation's critical infrastructure, including energy, economic, and command and control systems; weapon systems; advanced manufacturing; biosecurity; and essential resource management and distribution systems.

Cybersecurity is a domain in which human-centric operations drive the efficacy of network security architectures. ORNL has substantial capability in developing science and technology that optimizes and enhances the security of cyber and cyber-physical systems and their operations. Our primary capabilities are in AI-enabled cybersecurity defense, cyber-physical security, and resilience with a focus on the power grid, manufacturing systems, transportation, and resilient/secure AI systems used in a national security context. ORNL has recently added new capabilities for the study of mathematical and ML methods applied to cybersecurity, including adversarial ML, the pragmatic evaluation of applications of ML in cybersecurity operations, and scalable vulnerability discovery for software and complex hardware/software systems. Finally, the often-underemphasized human component of cybersecurity vulnerabilities is being addressed via new technologies to identify those who interact with critical infrastructure (e.g., identity sciences) and to use physical and digital pattern-of-life data to identify and examine the intent of those who interact with cyber-physical systems.

Outcomes from the cybersecurity capability are translated from R&D to deployment through partnerships with operational cyber infrastructure and co-located expertise. ORNL is successfully transferring technologies to address cyber and information security challenges. Capabilities and tools such as scalable anomaly detection, ML-based network security, resilient AI methods, cyber-physical systems protection and resilience, and others have been licensed to multiple industry partners and/or operationally fielded within the US government. Multimodal biometrics technologies have been licensed to global companies that intend to deploy these technologies to enhance the safety of our nation and world. Information science and data play a crucial role in both scientific discovery and mission-oriented decision making. The grand challenge is how to securely collect, organize, and structure the complex and voluminous data so they are useful and informative for end-use scenarios and to establish privacy-preserving methods and systems as needed for sensitive data (e.g., personally identifiable information, personal health information, and classified material) for applications such as health records data analytics and biometrics data applications, in which ensuring the privacy of human subjects is paramount. Solutions to these problems require complex, sophisticated, and interdisciplinary approaches based on data science and data preparation. ORNL is among the national leaders in methods for heterogeneous big data management, open and sensitive data curation and processing, smart storage/retrieval, and feature engineering, which leverage resources such as the OLCF, Knowledge Discovery Infrastructure, and CADES. ORNL researchers apply strong mathematical rigor and computationally intensive methods to solve cybersecurity and information challenges at scale and/or in near-real time. ORNL's resources also allow for deep learning on HPC systems, providing unparalleled insights into the behavior of malicious and nefarious cyberspace actors.

In the information science domain, QIS R&D is providing game-changing capabilities for secure communications and control systems, especially in protection of the electric grid. These include programs in partnership with the Cybersecurity for Energy Delivery Systems R&D program of DOE's Office of Cybersecurity, Energy Security, and Emergency Response (CESER). For example, ORNL is participating in a project to develop photonic integrated circuits of larger optical systems, such as quantum random number generators and continuous-variable key distribution systems, to dramatically reduce the technology costs and ultimately make them manufacturable. The combination of these information science and quantum communication capabilities spans areas such as sensitive data analytics/distribution, cyber-physical systems protection, trusted and secure communication architectures, and persistent threat detection and mitigation in networks. This capability extends to supercomputing, where assurances in information and data integrity can guard against adversaries who attempt to influence policy by manipulating HPC processes, data, or results.

ORNL infrastructure supporting this core capability includes the Distributed Energy Communications and Control Laboratory (DECC); the Grid Research, Integration, and Deployment Center; classified HPC systems; the Center for Trustworthy Embedded Systems; the MDF; the Vehicle Security Laboratory; the Cyber Science Research Facility; and the Cyber Operations Research Range. This infrastructure - along with multidisciplinary staff proficiencies throughout ORNL in power systems, power electronics, nuclear power systems, and transportation - enables the laboratory to tackle cyber and cyber-physical security challenges for multiple systems that include the electric grid, smart transportation systems, vehicles and storage, and compute platforms for sensitive data and information.

Funding for this work comes from SC, OE, CESER, EERE, NNSA, the Intelligence Community, Intelligence Advanced Research Projects Activity, DHS, the Department of Veterans Affairs, the Centers for Medicare and Medicaid Services, and DoD.

Recent advances to this core capability include the following:

- ORNL has expanded its facilities to enable critical infrastructure security R&D over the last few years to include the Grid Research Integration and Deployment Center (GRID-C), the Vehicle Security Lab within the National Transportation Research Facility, the MDF to include manufacturing cybersecurity, an Embedded Systems Security Lab, and a new Cyber Sciences Research Facility with an industrial control systems security test bed.
- Completed the first demonstration of continuous variable quantum key distribution over a deployed optical network with a true local oscillator.
- Created a demonstration facility at GRID-C for reliable and resilient distribution of precision timing protocol using an alternative timing source for synchronization of grid devices in a substation to mitigate vulnerabilities and risks associated with GPS interruption.

Decision Science and Analysis

ORNL's decision science and analysis core capability assist a wide variety of decision makers who grapple with compelling local, regional, national, and global issues. Quantitative and qualitative social, institutional, and behavioral research is conducted on topics as diverse as technology acceptability, market transformation, societal implications of emerging technologies, linkages between science or technology and their intended users, and decision-making itself. ORNL's data-driven methods, models, analyses, and tools create knowledge and insights useful in anticipating, planning for, managing, and understanding responses to and impacts of numerous events and technologies.

In national security, ORNL's niche R&D areas in this capability are geographic information science, including human dynamics and geographic data science–driven decision support tools that aid national security sponsors in making decisions under uncertainty, data analytics for nuclear nonproliferation discovery and characterization, and data-driven cybersecurity operations research.

ORNL scientists operating at this nexus of technology and decision analysis have established critical capabilities and expertise in the practice of data-driven decision science, risk analysis, and 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 further refine and enhance ORNL's unique contributions to geospatial science, ORNL established three new research groups in FY 2021: Location Intelligence, Resilience Communications, and Autonomous Systems. ORNL's investment in these research areas follows careful evaluation of research opportunities and signals from both DOE and National Security sponsors of the criticality of these research areas to their mission needs.

ORNL uses geographic information science for decision and risk analyses of critical infrastructure expansion and human dynamics. For critical infrastructure, ORNL supports DOE and other agencies in strategic planning and program direction, policy formulation, and implementation. ORNL is a leader in performing risk analysis of extreme events to aid in siting critical infrastructure and in understanding population dynamics for emergency response, collateral damage assessments, and urban planning. In population mapping, ORNL is now mapping and modeling the environment in which humans occupy space (i.e., both built and natural environments) at unprecedented scale and resolution. ORNL has expanded its capability in human dynamics modeling to support DoD and humanitarian organizations. This work includes endeavors such as mapping polio vaccination distribution programs and conducting rapid assessments of population dynamics in crisis and conflict areas, which support collateral damage estimates. Researchers are now leveraging and coalescing these existing investments in geospatial technologies and data to develop and deliver global building intelligence that captures information about human occupancy, materials, geometry, morphology, and function with high spatial, temporal, and attribute detail for the world. These key pieces of information are critical to address broad issues, including vulnerability and resilience; they also can be used for assessing consequences, estimating shielding protection for a variety of hazards, understanding the implications of various land use configurations and urban morphologies for future growth scenarios, and generating new insights into the impact of human activity on changing energy and transportation behaviors.

ORNL is a demonstrated leader in a number of areas within this capability, including (1) spatial demography, geographic data analytics, and technosocial analytics; (2) data-driven decision science, risk analysis, UQ, design of experiments, and probabilistic risk assessment; (3) dosimetry and development of dose coefficients and cancer risk factors for human exposure to radionuclides; (4) nuclear power plant siting, reactor operations, fuel cycle performance, and lifetime extensions; (5) climate change impacts, adaptation, and vulnerability modeling and assessment; (6) energy economics; (7) learning for heterogeneous biomedical data with UQ; and (8) development of decision-support tools for a variety of national security challenges, including support of cybersecurity, identity science, and military missions.

The Transformational Challenge Reactor (TCR) project will enable a full demonstration of the potential for combining advanced manufacturing, data science, materials science, and advanced modeling and simulation to develop advanced nuclear energy systems. Cutting-edge data science and computation may allow autonomous sensor and control systems, as well as enable ML for robust component, system, and material design and optimization. ML has been heavily used to improve reactor performance, enabling new operational regimes, improved safety, and economics. Improved sensors and controls are also being developed to enable advances toward autonomous decision-making capabilities for the nuclear power industry.

Funding for this work comes from SC, NE, EERE, DHS, DoD, the Federal Emergency Management Agency, NRC, the National Cancer Institute, and the Food and Drug Administration.

Recent advances in this core capability include the following:

- Developed the MA3T model used for projecting the adoption of alternative fuel vehicle technologies, shared mobility, and vehicle ownership in the United States to 2050, considering heterogenous consumer behavior and systematically linked to a wide range of technology, infrastructure, behavior, and policy factors.
- Developed the REVISE model used to optimize the locations, capacities, and numbers of hydrogen refueling stations and electric vehicle (EV) chargers along a given regional or national road network in the United States to 2050.
- Developed the Automatic Building Energy Modeling (AutoBEM) to model and simulate over 125 million US buildings (bit.ly/ModelAmerica). Used to quantify energy, demand, emissions, and cost reductions for energy efficient building technologies under Intergovernmental Panel on Climate Change (IPCC) climate change scenarios.
- Developed VERIFI, a tool designed for industrial energy coordinators, plant managers, engineers, and personnel who are interested in improving system efficiency to help them benchmark, baseline, and visualize their energy and utility bills and use.
- Developed SecuRoute, a new web-based application for DOE to perform route risk analysis for radioactive material shipments within the United States and established a novel risk weighting approach called Temporal Avoidance to allow for user-customized risk profiles.

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 the following:

- linking a fundamental understanding of mercury biogeochemistry to engineering applications to develop transformational solutions for DOE legacy mercury contamination;
- developing novel, cost-effective, and time-efficient methods for measuring water quality in streams and rivers at a high spatial resolution;
- identifying and modeling ecological functions of rivers and streams within the site selection, design, and operational decision-support systems for hydropower;
- developing and assessing sustainability indicators and ecosystem services for bioenergy feedstock production and hydropower development through integration of landscape and aquatic ecological science and socioeconomic analyses; and
- producing downscaled future weather, hydrology, water availability, extreme events, and hydropower projections to support the evaluation of climate change-induced impacts, vulnerability, and adaptation strategies.

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, aquatic ecology, environmental informatics, data science, economics, 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), and CNMS. Funding comes from SC, EM, EERE, FE, NNSA, DoD, NE, and NRC.

Recent advances to this core capability include the following:

- Extended our comprehensive National Water-Energy digital platform of hydropower related data sets, data model visualization, and analytics tools by adding new data sets to support current and future US hydropower asset development.
- Developed a multi-model hydroclimate downscaling framework to provide ensemble projections of future meteorology, hydrology, and hydropower production based on the latest IPCC CMIP6).
- Initiated field measurements of greenhouse gas emissions, using our recently developed AquaBOT, in southeastern US reservoirs and a collaboration with the EPA SuRGE project (US-wide survey of greenhouse gas [GHG] emissions from reservoirs) to improve estimates of GHG emissions from US reservoirs.
- Developed a GPU-accelerated high-resolution inundation model on Summit supercomputer to support large-scale flood simulation and forecasting for critical US infrastructure.
- Converted the Policy Analysis System model to operate on CADES, an HPC environment. This conversion is enabling stochastic simulations to quantify supply uncertainty and to perform more detailed simulations.

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 export of carbon, nutrients, and metals in watersheds undergoing dynamic change (e.g., shifts in land-use/land cover change or hydrologic intensification). Examples of activities supported by this core capability include (1) catchment- to molecular-scale hydrology, geochemistry, and microbiology to elucidate the coupled physical and biogeochemical processes that govern the formation of "hot spots" for carbon, nutrient, and metal transformations along the stream corridor and within their surrounding watersheds; (2) state-of-the-art surface and subsurface hydrology and reactive transport model development; (3) delivering a deeper understanding of how hydrogeochemistry drive the day-to-day population shifts in surface and subsurface microbial communities; and (4) integration of neutron scattering, neutron imaging, and exascale computing to understand 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 carbon, nutrients, metals, and contaminants in environmental systems contribute to basic and applied R&D programs focused on delivery of freshwater by watersheds for human consumption and energy production, extraction of fossil fuels, disposal of nuclear waste, and cleanup of DOE legacy contamination. ORNL leads one of the world's largest ongoing efforts in trace metal biogeochemistry research. The Critical Interfaces SFA in collaboration with IDEAS Watersheds project, 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 trace metal biogeochemical transformations in metabolically active transient storage zones in low-order stream systems.

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

Recent advancements to this core capability include the following:

- Demonstrated that some methanotrophs incapable of producing methanobactin (MB), a copper scavenging chalkophore, can steal MB from others, enabling them to collect copper for methane consumption and to degrade toxic methylmercury. These findings suggest that coupled cycle of mercury and carbon at oxic-anoxic transition zones where methanotrophs thrive may be more widespread than previously thought.
- Performed high-resolution spatial-temporal groundwater and sediment sampling to determine geochemical and physio-chemical influences on the temporal flux of microbial communities and their respective role in denitrification.
- Implemented and demonstrated a novel multiscale model (Advective Dispersion Equation with Lagrangian Subgrid [ADELS]) to represent the effect of biogeochemical "hot spots" in the hyporheic zone of river corridors in the Advanced Terrestrial Simulator (ATS) community software. The ATS-ADELS capability will enable, for the first time, the effects of fine-scale biogeochemical processes that occur in the hyporheic zone to be represented at the societally relevant scales needed to predict downstream water quality.
- Developed a new ML approach to accelerate parameter estimation and uncertainty quantification for high-resolution watershed hydrology models, allowing this computationally expensive class of models to be calibrated over large sub-basins for the first time. This new capability will enable improved scale-aware predications of stream flow over large sub-basins.

Large Scale User Facilities and Advanced Instrumentation

ORNL has a distinguished record in developing and operating major facilities for DOE and in designing and deploying instrumentation. ORNL is noted for the breadth of the facilities and instrumentation it develops and deploys for DOE and for its integration of these assets to deliver mission outcomes. The user facilities at ORNL attract thousands of researchers each year and support the development of the next generation of advanced techniques and capabilities and skilled, scientific researchers.

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 among the best in the world. Thirty neutron scattering instruments are available to scientists at SNS and HFIR, in addition to the Fundamental Neutron Physics Beamline at SNS. Significant investments in instrument improvements, sample environment, remote access, and data reduction and analysis capabilities ensure that ORNL's neutron scattering instruments remain world-leading. Construction of the Versatile Neutron Imaging Instrument at SNS, in progress, will provide wholly new and unique capabilities for neutron tomography.

As part of a three-source strategy for ORNL, construction of a high-brightness, long-wavelength 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 FTS, thereby increasing scientific capacity and capability on currently oversubscribed instruments. The PPU Project also provides the platform for the STS. FY 2022 PPU planned Critical Decision 3 (CD-3) construction activities and fabrications are underway, including installation of technical equipment in the klystron gallery; fabrication and delivery of two superconducting RF cryomodules at the partner lab Jefferson Lab; fabrication of ring magnets at the partner lab Fermi National Accelerator Laboratory; fabrication and delivery of RF equipment from vendors including klystrons, high voltage modulators, and transmitters; as well as the use of the PPU test target 1 in operation and the fabrication of test target 2. Also, the initial installation of two cryomodules in the linac tunnel will occur in FY 2022.

The STS, which received CD-1 approval in November 2020 and is therefore in the preliminary design and R&D phase, will provide researchers from a wide range of disciplines with new experimental capabilities that can be used to probe the structure and dynamics of materials over extended length, time, and energy scales. The project leverages the capacity of the existing SNS accelerator, accumulator ring, and infrastructure and takes full advantage of the performance gains that will be delivered by the PPU Project.

HFIR's capabilities for radioisotope production, materials irradiation, neutron activation analysis, and neutrino research make it an asset for isotope R&D and production, materials and fuels testing, high-energy physics, and nuclear security science programs. HFIR also plays a critical role in the neutron scattering program, providing complementary opportunities for materials studies to those available at the SNS (including the STS). The capabilities in spectroscopy, diffraction, imaging, and small-angle scattering find applications in quantum materials, soft matter, and energy and engineering materials. In response to a BES Advisory Committee report issued in September 2020, DOE SC approved a CD-0 Mission Need Statement in December 2020 for replacement of the reactor pressure vessel and other major components to sustain HFIR operation through the end of this century. Conceptual work toward achieving CD-1 for the pressure vessel replacement project is now expected to start in FY 2023. Based on historical component lifetimes, the beryllium reflector surrounding the fuel element will need to be replaced after cycle 513, currently planned for August of 2025, as part of the HFIR Beryllium Replacement (HBRR) project, which also offers the opportunity to upgrade degraded instrument infrastructures such as neutron guides. Recent analysis has identified a path forward to extend the lifetime of the beryllium reflector, potentially allowing continued uninterrupted operation until replacement of the pressure vessel in 2029 or later. The prospect of starting planning toward CD-1 of the pressure vessel replacement in FY 2023 would allow us to incorporate the essential improvements currently foreseen as part of HBRR into the pressure vessel replacement project.

ORNL has a distinguished record in developing and operating major facilities for DOE and in designing and deploying instrumentation. The world-leading 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 its fourth year of full user operations. This pre-exascale, hybrid platform provides 200 petaflops of computing power for modeling and simulation and more than 3 exaflops of computational power for AI applications and research. Summit users are tackling scientific challenges across a wide variety of science domains, but one exciting contribution Summit made is to the study of the SARS-CoV-2 virus and COVID-19. At least 2,286,200 Summit node-hours have been allocated to 22 Covid-19 related projects to date. In 2021, researchers used Summit to model an aerosolized SARS-CoV-2 viral particle for the first time, while another team used Summit to peer inside the intricacies of how the SARS-CoV-2 virus reproduces itself. Scheduled to be the nation's, and likely the world's, first exascale supercomputer, the OLCF-5/CORAL-2 Frontier system, a 1.5 exaflops HPC Cray EX supercomputer, was delivered in 2021 by vendor partners HPE and AMD. Delivery began in August and was complete by the end of October 2021. The system is on track to be available for full user operations on January 1, 2023. ORNL also operates high-performance computers to support multi-agency cooperation and R&D partnerships that include the Gaea computer, operated for NOAA, the Fawbush and Miller computers operated for the US Air Force, and the Cumulus system for DOE's ARM program. Cumulus was upgraded in 2021 with a new system installed and brought on-line in November.

CNMS provides world-leading expertise in synthesis, characterization, nanofabrication, theory, and modeling and simulation to the greater user community. Synthesis capabilities at CNMS have been expanded as part of the BES Quantum Information Science and Research Infrastructure project, including recent deployment of (1) rapid synthesis and characterization via a pulsed laser deposition synthesis platform that will support ML approaches, rapid in situ diagnostics, high-throughput characterization using x-ray photoelectron spectroscopy and diffraction, and optical spectroscopies and (2) a cathodoluminescence (CL) scanning electron microscope that offers angle, polarization, temperature, wavelength, spatial, and time-resolved CL microscopy. Photon correlation measurements with superconducting nanowire single photon detectors and time-resolved experiments are possible with up to 30 ps timing resolution. Femtosecond pump-probe experiments that combine pulsed electron and laser beams are being advanced. In situ patterning of quantum emitters and plasmonic cavities is possible with environmental electron beam patterning and electron beam–induced deposition.

The CNMS user community will benefit immensely from the Nanoscale Science Research Center (NSRC) Major Item of Equipment project, which will recapitalize the five NSRCs and deliver new capabilities for the next decade of nanoscience. CNMS has prioritized a cryo-plasma focused ion beam and a liquid-helium–cooled monochromated aberration-corrected STEM. Users continue to take advantage of remote access capabilities developed during the pandemic.

CNMS and SNS are working together to develop coordinated research efforts in polymer science, biomaterials, AI/ML, and novel technique and capability development. For example, CNMS supports neutron studies of nanoscale structure in soft matter by providing site-specific deuteration capabilities.

ORNL is home to EERE-sponsored R&D facilities: MDF, which includes the pilot-scale CFTF; 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 and electrification of industry; energy-efficient homes, buildings, and manufacturing; and sustainable transportation and mobility systems, respectively. This suite of comprehensive and industry-facing applied energy 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.

Recent advancements to this core capability include the following:

HFIR

- Remote experiments were enabled on most HFIR scattering instruments, allowing users to fully control instruments remotely either for the entire experiment or portions of an experiment. Remaining instruments are on track for completion by the end of FY 2022.

SNS

- Neutron scattering experiment capability at SNS improvements include data reduction and analysis, creating common interfaces with instruments at HFIR, and providing methods to increase the speed of data reduction and of computed tomography. Enhanced sample environments, including those needed for quantum materials and for soft matter, are being deployed. Instrument upgrades are being pursued through improved detector coverage at the Nanoscale-Ordered Materials and Engineering Materials diffractometers (NOMAD and VULCAN, respectively). These detector improvements have led to higher throughput and better resolution for neutron experiments.
- Remote experiments were enabled on all SNS scattering instruments, allowing users to fully control instruments remotely either for the entire experiment or portions of an experiment.

OLCF

- Frontier's arrival will bring with it the new Orion center-wide storage system, which has been delivered and installed and is expected to be deployed in FY 2022. The portable operating system interface (POSIX) namespace file system is the world's largest and fastest single file system. Its massive scale and hard disk/NVMe hybrid nature features 40 Lustre metadata server nodes and 450 Lustre object storage service nodes, stretching the bounds of what is theoretically conceivable.
- Summit delivered 35 million hours of computation during calendar year 2021 despite the coronavirus pandemic, with an overall availability of approximately 98%. In 2020, Summit was one of the first significant supercomputing deployments in the war against COVID-19.
- OLCF launched the OLCF Quantum Computing User Program (QCUP) in conjunction with the Quantum Computing Initiative. The QCUP enables researchers from national laboratories, academia, and industry to access commercial, prototype quantum computers otherwise not available to the public. Current vendor subscriptions include IBM, Honeywell, and Rigetti Computing.

CNMS

- Awarded new 3-year project for "Precision Atomic Assembly for Quantum Information Science (QIS)" as part of the BES National Lab QIS Research and Infrastructure at the NSRCs funding opportunity announcement (LAB-21-2464). The overarching goal of this project will be the direct manipulation of individual atoms and molecules to create new quantum information structures via ML-assisted scanning tunneling microscopy (STM) integrated with atomically resolved STM and STEM characterization.
- Developed novel scanning ultrafast electron microscopy capable of probing optoelectronic materials at picosecond time scales and nanometer length scales and an ultrafast pump-probe spectroscopy microscope to reveal quasiparticle dynamics in micrometer-sized two-dimensional (2D) crystal heterostructures

- Acquired a fully automated large scanning atomic force microscopy (AFM) (DriveAFM, Nanosurf) equipped with hollow microfluidic probes for dispensing or aspirating individual droplets of liquid (down to femtoliter volume) with nm precision on a surface. To date, fluidic force microscopy (FluidFM) has been predominately used as a tool in life sciences for studying and controlling single cell function and dynamics. By incorporating automated positioning, microfluidic, and electrochemical control we will adapt FluidFM for a first of its kind platform for understanding applications in energy science, particularly related to catalysis.
- Developed an automated pulsed laser deposition facility that couples in situ plasma spectroscopy, in situ Raman spectroscopy, and laser processing to control the precision synthesis of Janus monolayers and other atomically thin 2D materials.
- Developed a novel chamber for the neutron reflectometer at SNS to measure time-dependent changes in polymer films in the presence of an applied electric field.
- Installed a Hyrel 3D printer on ORNL's small-angle/wide-angle x-ray scattering instrument to conduct in-situ x-ray characterization during 3D printing of polymers.

Mechanical Design and Engineering

ORNL deploys extensive expertise in mechanical design and engineering to support the development of a wide range of projects (e.g., reactors, accelerators, fusion experimental devices, enrichment technology) and instruments. For example, this core capability supports the US ITER project, the PPU and STS projects at SNS, the MAJORANA Demonstrator project, the MPEX project, and the neutron electric dipole moment (nEDM) experiment. In many cases, mechanical design and engineering efforts have drawn upon expertise across ORNL. For example, ORNL mechanical engineering staff used their expertise to design a new target for irradiation of Np-237 to produce Pu-238 at the Advanced Test Reactor at the Idaho National Laboratory. Expertise in the analysis of stress, strain, and thermal effects in composite materials, fluid dynamics, and dynamic analysis of rapidly rotating devices have been key to the development of advanced isotope separation devices. Further, ORNL capabilities in basic science and associated characterization tools have been exploited to provide innovative solutions in support of mechanical engineering applications. For example, HFIR’s neutron scattering capabilities have been applied to map residual stress in manufactured components, helping to improve material reliability in various devices, including additively manufactured heat exchangers and fuel injectors. Further, ORNL’s mechanical design and engineering capabilities provide breakthroughs in energy-efficient manufacturing; in the energy efficiency and durability of building envelopes, equipment, and appliances; and in transportation (including multicylinder combustion R&D and exhaust aftertreatment development).

Mechanical engineering capabilities at ORNL have been used to develop remote systems for SNS and nonreactor nuclear and radiological facilities, as well as production-level separation processes based on electromagnetic and gas centrifuge separation techniques that are being advanced for both radioisotopes and stable isotopes. The Centrifuge Manufacturing Capability, completed in FY 2021, supports the fabrication of Gaseous Centrifuge Isotope Separation machines for the SIPF and SIPRC. Also, ORNL combines its expertise in mechanical design and engineering with other disciplines to support a range of nuclear capabilities, including the thermal/hydraulic design of HFIR irradiation experiments, the HFIR closed-loop supercritical-hydrogen cold neutron source, a novel molten salt experimental loop facility, the SNS mercury target systems, and the high-heat-flux divertor components for the Wendelstein 7-X superconducting stellarator.[55] 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 has utilized its engineering expertise to rapidly advance the mechanical design of MPEX, which will be a unique facility that combines very high local heat fluxes (~ 10 MW/m2) with nearly steady-state operation. Unique designs of the helium antenna window, limiters, and target have been developed and are currently being tested to ensure they meet project requirements. ORNL is also pursuing the use of commercial software tools (e.g., ANSYS) in the analysis/design of complex blanket and first wall components for future fusion systems and exploring the capability to use these tools on next generation computing tools such as Summit

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.

Recent advances to this core capability include the following:

- Demonstrated the manufacturing of large-scale pieces of yttrium hydride free of cracks and flaws to meet TCR program requirements for a moderator that could be used inside small gas-cooled nuclear reactors.
- Linked efforts in additive, hybrid, and machine tool systems into metrology operations via the secure digital thread at the MDF to support AI and ML initiatives and digital twin generation and validation. An ORNL-led ECP application project (ExaAM) is focused on the development of an Integrated Platform for Additive Manufacturing Simulation (IPAMS), a suite of exascale-optimized capabilities that directly incorporate microstructure evolution and the effects of microstructure within additive manufacturing (AM) processes. IPAMS forms the digital side of the AM twin, with a focus on high-spec metal alloys in defense and other sectors, by integrating high-fidelity mesoscale simulations within continuum process simulations to predict the microstructure and properties of the final AM part. A key goal is to predict and ultimately control the microstructure of the final printed part via real-time feedback on the AM process to ensure the required specs are met. Current inabilities to match specs for new AM parts can be as high as 80%.
- Developed a wide variety of formulations with thermoplastic resins and different forms and concentrations of cellulose microfibrils, nanocrystals, and nanofibrils specifically including high specific strength foams for large-scale additive manufacturing. Targeted formulations will not only provide cost savings but will also improve processability and energy savings in feedstock life cycle (i.e., embodied energy) compared to their petroleum-based counterpart.
- Established a multidisciplinary laboratory focused on decarbonization including extensive capabilities around electrolysis, CO_2 capture/conversion, and catalyst synthesis.
- Developed an Advanced Construction Laboratory to support the synergistic development of advanced materials and assembly techniques to decrease embodied carbon and operational energy.
- Completed the Centrifuge Manufacturing Capability to provide enhanced capabilities and capacity for stable isotope enrichment system fabrication.

Nuclear and Radio Chemistry

Major focus areas for ORNL's nuclear and radiochemistry research are the nuclear engineering design of advanced targets for efficient production of isotopes and the development of highly selective separation techniques for the harvesting of isotopes after target irradiation for a broad range of applications, including cancer treatment, commercial uses, and research.

ORNL's nuclear chemistry and enrichment expertise is also critical in preserving and advancing US uranium enrichment capabilities. Production-level separation processes based on electromagnetic and gas centrifuge separation techniques are being advanced for both radioisotopes and stable isotopes. ORNL maintains and distributes the US inventory of enriched stable isotopes and radioisotopes for DOE's National Isotope Development Center.

In support of the DOE Isotope Program, ORNL has established routine production of high purity Pm-147, making us the world's only producer of this rare isotope used in nuclear batteries and to measure the thickness of materials. ORNL has developed and implemented gas trapping technology to minimize volatile radioactive materials emissions during tungsten and thorium irradiation, and we are developing emerging capabilities for ink-jet printing of thin-film targets, establishing ORNL as a supplier of thin film targets for isotope production and nuclear physics research. Funding provided by NASA supports the production of Pu-238 for use in radioisotope power supplies and heat sources for planetary science missions.

ORNL's unique facilities enable our innovative isotope research, development, and production. HFIR, which provides the world's highest neutron flux, is used to irradiate target materials for the production of various radioisotopes through the DOE IP and other sponsors. Separations are conducted in the Radiochemical Engineering Development Center, laboratories and hot cells in Buildings 4501 and 3047, and other radiological laboratories. ORNL is addressing long-term needs for satisfying the increasing demand for isotopes used in medical, industrial, research, and national security applications through investments in Radioisotope Processing Facility, SIPF, and SIPRC.

Funding in this area comes from several sources, including SC, NE, IP, NNSA, NASA, and other government agencies.

Recent advances to this core capability include the following:

- Established routine production of high purity Pm-147. ORNL is currently the world's only producer of this rare isotope used in nuclear batteries, thin film measurement instruments, and light sources.
- Established gas trapping technology to minimize emissions of volatile radioactive materials during processing of irradiated tungsten and thorium.
- Developing emerging capabilities for ink-jet printing of thin film actinide targets for isotope production and nuclear physics research.

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 toward acceleration of deployment of advanced nuclear technologies from concept to industry. This includes examining foundational concepts such as nuclear data and addressing engineering needs for the entire nuclear fuel cycle, development of new materials and systems for fission and fusion, and taking advantage of specialized facilities and core capabilities in materials science, chemistry, advanced manufacturing, chemical engineering, computing, artificial intelligence, and other areas. ORNL is also a leader in modeling and simulation for reactor physics and radiation transport, computational thermal hydraulics, reactor systems, nuclear criticality safety, and reactor safety; radiation detection and imaging; and radioisotope production.

Supporting all of these activities is the ability to develop, benchmark, and distribute validated modeling and simulation tools. ORNL has a wide range of specialized facilities for nuclear materials development and characterization. Capabilities include a complete "cradle to grave" suite, spanning materials irradiation capabilities at HFIR and post-irradiation characterization facilities at LAMDA, as well as hot cells facilities. Instrumentation and controls are another area of strength, with ORNL developing improved sensors and measurement techniques, which, when coupled with modern data science, enable advances toward autonomous decision-making capabilities for the nuclear power industry.

A leading example of applying modern, multidisciplinary science to nuclear energy is the TCR program (referenced in Section A.13). TCR leverages advances in manufacturing and computational science to deliver advanced nuclear technology at a reduced cost. To achieve this goal, TCR brings together advanced manufacturing with computational design and artificial intelligence. In addition, the program takes advantage of unique ORNL research facilities, including the SNS, OLCF, HFIR, and MDF. The TCR program has already demonstrated a number of significant achievements, including transfer of additively manufactured components to industry. Recently, ORNL partnered with Tennessee Valley Authority (TVA) and Framatome Inc., a TVA nuclear fuel supplier based in Richland, Washington, to introduce parts produced using additive manufacturing, or 3D printing, techniques into existing nuclear reactors. The key concepts of TCR have been incorporated into the DOE-NE Advanced Materials and Manufacturing Technologies program.

ORNL's nuclear engineering expertise is critical to the continued viability of the nuclear power industry, including improved operations and extended operations of the existing fleet.[3,4] ORNL's expertise in the design and post-irradiation examination of HFIR irradiation capsules is used to study reactor materials and accident tolerant fuels.

Recent advancements to this core capability include the following:

- Completed development and authorization for the HFIRCON (HFIR Controller) software for evaluating the safety basis of irradiation experiments. This software package couples neutron transport, variance reduction, and depletion capabilities to determine time-dependent isotopic content and heat generation rates of materials in HFIR, important for analysis of irradiated experiments.
- Initiated post-irradiation examination of lead-test assemblies of accident-tolerant clad materials following prototypical irradiation in commercial nuclear power plant conditions.
- Demonstrated successful integration and deployment of advanced nuclear technology bringing together advanced manufacturing with computational design and AI to produce and transfer additively manufactured components to industry.
- Provided critical experiment design, validation, and nuclear data testing activities, working with nuclear data and the NRC for licensee support. Also provided burnup credit and used nuclear fuel analysis for the DOE-NE and NRC.
- Developing emerging capabilities for reactor production of Th-229, further establishing ORNL's position as the primary worldwide supplier of active pharmaceutical ingredient Ac-225.
- Completed and published a new database on thermal properties for molten salt coolants, which is already being utilized by industry and regulatory partners.

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[3] A. Abd-Elssamd et al., *ACI Mater. J.* **117**, 265 (2020).

[4] R. Montgomery et al., *Nucl. Sci. Eng.* **193,** 884 (2019).

Nuclear Physics

ORNL's nuclear physics researchers lead a world-class fundamental symmetries program, enable experimentation at DOE's Office of Science Nuclear Physics (NP) program's user facilities, and make crucial contributions to the ORNL research portfolio in both discovery science and applied science. Work spans theoretical and experimental research that is relevant to DOE's NP mission of developing an understanding of nuclear matter and fundamental interactions that will help unlock the secrets of how the universe is formed.

In the area of fundamental symmetries, ORNL carries out an ambitious multi-pronged research program addressing the matter-antimatter asymmetry in the universe and completing the standard model of interactions. It has successfully concluded the MAJORANA Demonstrator project that has provided the foundation for the proposed ton-scale Large Enriched Germanium Experiment for Neutrinoless Double Beta Decay (LEGEND-1000) experiment to search for the hypothesized neutrinoless double-beta decay mode of nuclei. It also operates the Fundamental Nuclear Physics Beamline at the SNS, which is home to the ORNL-led search for the electric dipole moment of the neutron and the Nab experiment that will make precision measurement of the beta decay of the neutron. The analysis of the data from the n-^{3}He experiment, combined with the NPDGamma results, have provided the most precise measurement of parity violation in hadronic weak interactions.

ORNL has a very strong focus on enabling Day-1 physics experiments at the new Facility for Rare Isotope Beams (FRIB) and the future Electron Ion Collider (EIC). ORNL has assumed leadership roles for the FRIB Decay Station Initiator project and is delivering new experimental setups to the facility for the study of radioactive decays. The development of the gas jet target for nuclear astrophysics experiments using secondary beams at FRIB as well as aspects of the Separator for Capture Reactions is led by ORNL. Building on ORNL's highly valued contributions to the upgrade of the ALICE experiment at the Large Hadron Collider (LHC) at European Organization for Nuclear Research (CERN), ORNL has a leading role in the design, planning and management of the Day-1 collider detector at the EIC. ORNL expertise includes capabilities for analyses of aspects of the ALICE data, including jet shapes, jet substructure, photon-jet and jet-hadron correlations, and direct photons. In parallel, ORNL targets a leading role in the construction of the EIC detector and developing the tools for analyzing the EIC data using modern AI/ML techniques.

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 study the beta and beta-delayed neutron decays of very neutron-rich nuclei beyond doubly magic nickel-78 in unprecedented detail. ORNL has developed, in collaboration with Japanese laboratories, a novel experimental method for fast determination of the optimum heavy-ion beam energy for the synthesis of superheavy elements.

In nuclear theory, OLCF is used to investigate the structure and reactions of neutron-rich rare isotopes and nuclear astrophysical processes. ORNL develops world-leading approaches to relevant nuclei based on ab initio methods, HPC, and effective field theory. The highest-fidelity core-collapse supernova and neutron-star merger simulations are provided with cell-by-cell adaptive mesh refinement, coupled hydrodynamics, radiation transport, thermonuclear kinetics, and nuclear microphysics. These simulations will provide the capability to predict multi-messenger signatures of core-collapse phenomena.

ORNL has made breakthrough advances in resolving the computing problem for the detailed simulation of detector response for collider experiments in particle and nuclear physics using the ORNL HPC systems. This initiative aims to provide the ability to run full-fidelity Monte Carlo simulations of collider detectors to maximize utilization of the DOE leadership computing facilities (LCFs) to extract the ever-so-subtle physics results for new high energy and nuclear physics facilities.

ORNL's nuclear data program includes cross-section measurements, the development of evaluation and data analysis methods, and data processing. ORNL also leads the ENDF/B Formats Committee to standardize all nuclear data formatting. The goal is to coordinate all activities across the lab to provide input to the development of a national long-range strategy for nuclear data.

Leveraging the broad range of expertise across ORNL, advanced detector technologies are an area of strength with a focus on precision nuclear physics measurements and application to safeguards and nuclear material security. Novel germanium detector designs have been invented at ORNL and developed with NP support. 3D-printing methods are being developed to produce novel, background-free scintillator to support low-background measurements and interaction-resolving detectors for prevision neutron measurements and imaging.

Funding in this area originates from SC, DHS, DoD, and NNSA programs.

Recent enhancements to this core capability include the following:

- Delivered new experimental setups to FRIB for the study of radioactive decays.
- Expanded capabilities in detector simulations and nuclear data.
- Developing 3D-printing capabilities to produce novel, background-free scintillators to support low-background measurements and interaction-resolving detectors for precision neutron measurements and imaging.
- Provided the foundation for the proposed ton-scale LEGEND experiment to search for the hypothesized neutrinoless double-beta decay mode of nuclei.

Plasma and Fusion Energy Sciences

ORNL has a long history as a key player in the development of the knowledge base for plasma and fusion energy sciences essential for fusion energy deployment. With activities ranging from developing and testing innovative confinement concepts to delivery of large-scale fusion components, ORNL is the US leader, and in many cases the world leader, in several key areas of fusion development. ORNL's expertise coupled with its demonstrated abilities in large-scale project management, international collaboration, and computational simulation is applied to support the mission of the SC Fusion Energy Sciences (FES) program.

ORNL is DOE's lead laboratory for fusion nuclear science and fusion materials, which are required to fully enable fusion energy. Materials scientists at ORNL conduct experiments to support development of alloys and silicon carbide composites, that have been leveraged to develop a suite of economical high-strength, radiation-resistant steels that derive their properties from a fine dispersion of engineered precipitate nanoclusters.[5] The development of radiation-tolerant low-activation materials will be required to make a fusion pilot plant reliable and economical. Recent experiments have leveraged the capabilities of HFIR to expose candidate materials to high-energy neutrons to better characterize the response of these materials to fusion-like conditions. This capability is unparalleled in the world program with numerous international labs partnering with ORNL to develop data of interest for specific materials they are contemplating using in future fusion systems. Recent recommendations for the Fusion Energy

[5] B. Kim et al., *J. Nucl. Mater.* **545,** 152634 (2020).

Sciences Advisory Committee indicate that ORNL's aforementioned positioning in fusion nuclear science and materials will be a key capability in the FES program in the coming years.[6]

ORNL is the world leader in pellet fueling and blanket systems for fusion applications. This is evidenced by the recent development of the design basis for a steady-state pellet injector to be deployed on the W7- X stellarator in Germany.[7] These capabilities have positioned ORNL to play a key role in long-pulse particle transport and control experiments on W7-X. Leveraging this positioning, ORNL staff will carry out research to better understand long-pulse density control on ITER, validate particle transport models for stellarators, and connect stellarator and tokamak particle transport physics through comparisons with experiments on DIII-D. In addition, ORNL has delivered multiple shattered pellet injection (SPI) systems to devices around the world to support development of the technical basis of using SPI for disruption mitigation in ITER and future fusion devices.[8] The complementarity of these systems and ORNL strengths in disruption mitigation simulation will allow ORNL researchers to gain key insights in the implementation of SPI on ITER.

[9]In addition, ORNL is developing the technical expertise and capabilities to be a world leader in blanket technology. Combining a newly developed Helium Flow Loop to better understand helium flow and advanced computational tools, ORNL is well positioned to develop the foundational basis for optimizing the use of helium as a coolant of fusion blankets of the future.

ITER remains a key investment for US fusion goals, as noted in multiple reports from the National Academies of Science, Engineering and Medicine[10] and in the recently published DOE Fusion Energy Sciences Advisory Committee long-range plan for fusion energy and plasma science.[11] For a path to fusion energy—not just fusion science—US fusion leaders emphasize that it is essential to master both the science and the technology required for producing and controlling a plant-scale burning plasma. ORNL is well positioned to support the recommendations of these reports.

As directed by DOE, ORNL leads the US ITER project and executes the program in conjunction with its partner laboratories, Princeton Plasma Physics Laboratory and Savannah River National Laboratory. The project draws on ORNL's breadth of experience in fusion technology, radiation transport, high-power plasma heating systems, and advanced electronics for extreme environments. US ITER fabrication activities and participation in the project will lead to the capability for creating, sustaining, and studying burning plasmas, the next step toward fusion energy. US hardware contributions include the world's highest-stored-energy pulsed superconducting magnet; a superconductor for ITER toroidal field coils; a 1 GW cooling water system; high-power, long-pulse plasma heating systems; plasma diagnostics; parts of the tritium exhaust system; plasma instrumentation; and plasma disruption mitigation systems. The US ITER Project Office also works with the ITER Organization and other ITER domestic agencies to

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[6] Fusion Energy Sciences Advisory Committee Report, *Powering the Future: Fusion and Plasmas* (2020).

[7] S. Meitner et al., *IEEE Trans. Plasma Sci.* **48**, 1585 (2020).

[8] T. Gebhart et al., "Shear Strength and Release of Large Cryogenic Pellets from the Barrel of a Shattered Pellet Injector for Disruption Mitigation," submitted to *Fusion Sci. Technol.* (2020).

[9] C. Kessel and M. Wade, "A Strategic Framework for the U.S. Blanket and Fuel Cycle Program 2020," submittedto *Fusion Energy Sci.* (2020).

[10] National Research Council, *Burning Plasma: Bringing a Star to Earth* (2004); National Academies of Sciences, Engineering, and Mathematics (NASEM), *A Strategic Plan for U.S. Burning Plasma Research* (2019); NASEM, *Bringing Fusion to the U.S. Grid* (2021).

[11] FESAC Committee Report, *Powering the Future: Fusion and Plasmas* (2020).

achieve the required integration of management, design, and procurement activities. Much of the R&D is also executed at ORNL.

In parallel with US ITER efforts, ORNL continues to provide key capabilities in the understanding and demonstration of sustained magnetically confined plasma with the properties needed for a compact fusion pilot plant. ORNL scientists are world leaders in the application of state-of-the-art simulation tools toward the understanding of present-day facilities and design of future fusion facilities. Recently, an ORNL team of experts from applied math, computer science, HPC engineering, and fusion theory developed a new Adaptive Sparse Grid framework that enables solutions of high-dimensional PDEs typical to fusion. Initial applications of this tool delivered about a 100-times reduction in the number of elements required for Maxwell's equations in 3D compared with traditional methods.[12] ORNL scientists are also the world leaders in boundary modeling of present-day devices and the use of core modeling tools to simulate future devices. Of the multiple studies conducted along this line in the United States in recent years, ORNL scientists have played a key role in a large fraction of them.[13]

ORNL scientists and engineers are building Material Plasma Exposure Experiment (MPEX) to address the challenges associated with exposing materials to high-energy, high-density plasmas. As a testament to ORNL's capabilities in this area, both CD-1 and CD-3/a were successfully achieved in 2020, and significant progress has been made toward CD-2, expected in 2022. This engineering and design activity is exposing ORNL staff to the rigors required in operating a steady-state facility with megawatt-level heat sources and sinks. This experience will be invaluable in designing future fusion systems. Once operating, MPEX will provide world-leading capability for experiments in which power plant–level fluxes and fluences of particles will be incident on neutron-irradiated materials in prototypic geometries.[14,15]

Recent enhancements to this core capability include the following:

- Completed the delivery of the first and second modules for the ITER central solenoid, which will be world's highest stored energy pulsed superconducting magnet.
- Completed the design and documentation of the W7-X Continuous Pellet Fueling System extruder, accelerator, gas manifold, and injection line in support of a future Final Design Review of the complete system.
- Assessed the capability of the SPI system for use as the ITER baseline disruption mitigation system technology through experimental analysis.
- Provided simultaneous hydrogen/deuterium/tritium (H/D/T) and ^{3}He/^{4}He absolute concentration measurements during H/D/T operations on the Joint European Torus.
- Explored the potential of additive manufacturing of silicon carbide power plant components.

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-

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[12] E. D'Azevedo, et al., Comput. *Phys. Commun.* 256, 107412 (2020).

[13] J.M. Park et al., *Phys. Plasmas* 25, 012506 (2018).

[14] J. Rapp et al., Fusion Sci. Technol. 75:7 (2019).

[15] J. Rapp et al., Fusion Eng. Des. 156, 1115863 (2020).

performance inverters and converters for EVs and demonstrated the first wireless bidirectional charging and energy management system for a building and a vehicle operating as an integrated energy system. This core capability (1) delivers advances in high-temperature, high-power-density applications; (2) enables high-efficiency transportation and electrification systems to reduce US reliance on foreign oil; (3) develops technologies for power flow control, grid monitoring (e.g., FNET/GridEye), and grid protection that support the development of a secure and reliable 21st century electricity delivery system; and (4) creates advanced building sensors, communications, and controls for power management systems to maximize energy efficiency.

Through DOE's Grid Modernization Laboratory Consortium (GMLC), ORNL addresses the challenges of integrating conventional and renewable electric generating sources with energy storage and smart buildings while ensuring that the grid is sufficiently resilient and secure to withstand growing cybersecurity concerns. ORNL tests controllers in multiple environments, including both simulation and full hardware environments on different scales of power and voltage levels (24 to 480 V), as well as different grid configurations and communications protocols. A strong partnership with the Chattanooga Electric Power Board reinforces this core capability by providing real-world understanding and commercial-scale implementation of emerging technologies. ORNL's GRID-C combines and integrates electrification research activities across the utility, buildings, energy storage, and vehicle missions. Included in these research activities is the newly established Power Electronics Launch Pad to accelerate the development of power electronics components, subsystems and systems to improve reliability and reduce system costs.

ORNL leads in the creation of alternating-current power flow control systems for grid control and increased resilience. An advanced grid requires new materials for power electronics and energy storage devices. ORNL is a leader in power electronics R&D (serving as the Vehicle Technologies Office lead laboratory for power electronics) and is taking advantage of resources at NTRC to develop high-power devices to improve reliability and reduce costs. ORNL is leading the way in innovative wireless charging of EVs. In addition to providing an autonomous, safe, and convenient option for charging EVs, wireless charging, when applied to dynamic or quasi-dynamic scenarios, can provide virtually unlimited range to EVs. It can do away with "range anxiety" and long charging times because vehicles can be charged continuously while they are in motion. Recent achievements include the demonstration of bidirectional wireless charging on a medium-duty plug-in hybrid electric delivery truck.

ORNL designs, develops, and tests new materials capable of supporting cost-effective and higher-performing electricity control devices and systems. ORNL collaborates in developing power electronics from concept to prototype and applies its expertise in materials to develop innovative electronics and sensors.

Enhanced cybersecurity measures are required to prevent malicious attacks on energy infrastructure. ORNL's Acceleration Project for the Smart Grid is improving the efforts for securing smart grid systems.

Expertise gained in supporting a stable energy infrastructure for ORNL operations has been leveraged to facilitate large science experiments at other sites, such as LHC and FRIB. Current activities leverage broad expertise in electronics for extreme environments; compact high-voltage power supplies; pulsed power conversion; the Internet of Things, including connected sensor and internet frameworks; radio frequency; and communications capabilities for intelligent systems support.

ORNL supports DOE's energy mission by providing resources that can be used to catalyze the timely, material, and efficient transformation of the nation's energy system. Work in this area is conducted using the NTRC Power Electronics and Electrical Machinery Laboratory, the DECC microgrid, and the Powerline Conductor Accelerated Testing Facility; resources for thin-film deposition (i.e., inkjet printing, ultrasonic spray, sputtering, evaporation, low-temperature photonic curing); and tools for characterization of materials, devices, and communications. EERE, OE, and DOE's Office of Policy are the primary sponsors. SC also benefits from ORNL expertise in this area.

Recent enhancements to this core capability include the following:

- Established academic and industry consortium to support the Transformer Resiliency and Advanced Components program.
- Established and advanced core architecture for an alternative timing and synchronization system along with evaluation and deployment of high-fidelity sensors to support grid security as part of the Center for Alternate Synchronization and Timing.
- Peregrine, an AI-based quality control platform for powder bed additive manufacturing that assesses the quality of parts in real time was licensed to five industrial partners. This is the first time in ORNL history that a single product was licensed so many times in a single year.
- Fully operationalized GRID-C and developed new capabilities including an extreme-fast-charging test bed, building-to-grid controls, a Coordinated Management of Microgrids and Networked Distributed Energy Resources (COMMANDER) microgrid test bed, battery recycling, cyber-physical security, and power electronics applications.
- Established plan for carbon reduction and electrification of manufacturing systems including electric power heating, chemical process scalability including microreactors, carbon capture, novel reduction technologies, and sustainable manufacturing processes.

Systems Engineering and Integration

ORNL's core capability in systems engineering and integration takes advantage of the full range of capabilities across the laboratory. Solutions to pressing scientific and technical challenges are developed by integrating expertise in fundamental science, technology, and project management in multidisciplinary and multi-institutional teams. This approach allows us to accelerate research innovation in managing scientific projects of various sizes through partnerships across ORNL and with universities, other national laboratories, and private industry. Examples of recent accomplishments in working with private industry include modeling combustion processes, understanding materials properties for advanced manufacturing, improving technology to advance fusion energy systems, and modeling the energy use of buildings at the community scale.

ORNL's strength in pursuing solutions from concept to implementation and in spanning fundamental to applied research ensures the success of national and international projects, such as SNS, OLCF, MPEX, the Pu-238 process development project, the LEAD project, the Nab and neutron electric dipole moment experiments, ALICE at CERN, the ECCE detector at the EIC, 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 (Consortium for Advanced Simulation of Light Water Reactors and the Critical Materials Institute), the Institute for Advanced Composite Materials Innovation, and other multi-institutional collaborations (Fuels/Engine Co-Optima, GMLC, Lightweight Innovations for Tomorrow, Clean Energy Smart Manufacturing Innovation Institute).

Additionally, ORNL's EERE R&D facilities (NTRC; BTRIC, including MAXLAB and DECC; MDF; and CFTF) build on ORNL scientific systems infrastructure to develop and deliver market-driven solutions for energy-saving homes, buildings, and manufacturing; sustainable transportation; and power generation (fuel cell and wind) and storage. Capabilities and scientific expertise available within these facilities are highly sought after by industry and other sponsors.

Adding to ORNL's deep systems engineering and integration capabilities is GRID-C which became operational in FY 2021. GRID-C is a multipurpose research facility that houses several research laboratories in support of OE and EERE initiatives. GRID-C offers industry, academia, and other agencies the opportunity to access state-of-the-art technologies, equipment and instrumentation, and computational resources to advance technologies in support of modernizing the electric delivery system. These resources will assist in buildings-to-grid integration research and development, extreme charging of electric vehicles, development of next generation energy storage systems and modeling of energy interdependencies.

The primary sponsors for these efforts include SC, EERE, OE, FES, NE, and NNSA. Some support is also provided by DHS, NRC, DoD, and other SPP sponsors.

Recent advances to this core capability include the following:

- Leveraged the digital thread to connect new additive and hybrid systems with a state-of-the-art metrology suite to better understand and validate both additive and subtractive processes via more accurate digital twins, moving closer to full component certification.
- Established machine tool research in MDF on sensors, data analytics, visualization, difficult-to-machine materials, and development of hybrid additive-subtractive systems and ML algorithms for the automation of machining processes.
- Developed the Residential Scale Grid Laboratory for home and neighborhood emulation, transactive controls, and grid integration test beds as well as developed, instrumented, and operationalized eight new electric grid infrastructure laboratories in GRID-C.
- Developed alternative timing infrastructure for synchronizing energy systems and mitigating cybersecurity risks associated with current synchronization systems.
- Developed, instrumented, and operationalized eight new electric grid infrastructure laboratories in GRID-C.

Science and Technology Strategy for the Future

With the same sense of urgency and purpose that drove the laboratory's original mission, ORNL is advancing and stewarding an ambitious strategic vision that builds upon its 23 core capabilities, diverse user facilities, key partnerships, a rich portfolio of projects, and a world-class staff to tackle some of the most pressing and complex challenges facing humankind. ORNL is distinguished within the DOE system of national laboratories for excelling at the translation of fundamental discoveries and applied research into solutions having national scale and impact. Translational research and convergent science have long been deeply engrained into ORNL's ethos and modalities. With signature strengths in neutron sciences, computational science, materials science, nuclear technologies, and isotopes R&D and production—and through the convergence of these strengths with deep expertise in biological and environmental sciences, advanced manufacturing, energy technologies, and security science—ORNL continues to advance world-leading capabilities that enable ORNL, and those who partner with it, to improve the world. Recognizing that DOE's ambitious decarbonization goals require a whole-of-innovation "Earthshot" approach, ORNL is drawing on its extensive resources to advance new ideas, strategies, and solutions important for contributing to this urgent mission.

The ORNL mission of delivering scientific insights, technical breakthroughs, and unique facilities to accelerate solutions in clean energy and national security is being addressed through an S&T strategy that is underpinned by nine ambitious ORNL S&T objectives, which are listed in Table 4.1. Successfully meeting these objectives requires continued stewardship of several critical elements, including a talented workforce, a unique ecosystem of facilities and major projects, core programs, strategic investments, and key partnerships. The key elements are summarized in the following text and further discussed in the sections that follow, which focus on objective-specific strategic goals.

Table 4.1. ORNL S&T Objectives
4.1. Maintain and strengthen global leadership in neutron sciences
4.2. Deliver exascale computing from system to ecosystem
4.3 Discover and design next-generation materials and chemical processes for clean energy
4.4. Advance the fundamental science, engineering, and integrated technologies to accelerate deployment of fusion and advanced fission energy
4.5. Unlock complexity in biological and environmental systems
4.6. Provide strategic capabilities in isotope R&D and production
4.7. Deliver transformational R&D for integrated energy systems to accelerate decarbonization
4.8. Elucidate the principles of fundamental physics and particle interactions
4.9. Address complex national security challenges through advancements in science and technology

ORNL's most valuable resource is its extremely creative, dedicated, and mission-ready workforce of more than 5,800 researchers and professional staff. As part of its scientific reorganization in 2020, ORNL took the opportunity to position itself for a vibrant future through implementing several measures. With diversity in mind, ORNL made significant investments in world-class scientists and scientific leaders. For example, ORNL recruited 78 senior researchers in FY 2021. Today, ORNL is led by the most diverse leadership team in the institution's history, with 35% female representation and 30% minority representation. To support recent growth, and with a focus on early-career staff and new leaders, ORNL is developing comprehensive talent development programs and is fostering an ecosystem for cultivating research and operational careers. ORNL is also strengthening its organizational culture and engaging staff through focused inclusivity efforts.

ORNL staff continue to be recognized nationally and internationally. Examples this year include recognitions of seasoned scholars for prestigious awards such as National Academy of Engineering (Nancy Dudney), Turing Award (Jack Dongarra), AAAS Fellow (Shaun Gleason, Mark Lumsden, and Mircea Podar), APS Fellow (Larry Baylor and Andrew Lupini), Materials Research Society Fellow (Jagjit Nanda), Microanalysis Society Fellow (Lawrence Allard), Microscopy Society of America Fellow (Miaofang Chi), and Neutron Scattering Society of America Fellow (Larry Anovitz, Valeria Lauter, Alan Tennant, and Volker Urban) among others. ORNL early-career scholars also continue to be recognized, including a Minerals, Metals & Materials Society Award for Young Innovator in the Materials Science of Additive Manufacturing (Michael Kirka), American Chemical Society Young Investigator Award (Xi Chelsea Chen), Heinrich Award from the Microanalysis Society (Jordan Hachtel), Albert Crewe Award from the Microscopy Society of America (Jordan Hachtel), and five new SC Early Career Research Program recipients (Matthew Beidler, Melissa Cregger, Fankang Li, Kiersten Ruisard, and Daisuke Shiraki).

ORNL's remarkable ecosystem of user facilities, major projects, and key centers provides a cornerstone for ORNL's S&T strategy as well as a unique resource that enables researchers throughout the world to contribute to the DOE mission. ORNL is stewarding and advancing world-leading capabilities at four DOE SC user facilities, which enable scientific breakthroughs in neutron scattering (SNS and HFIR), nanoscience (CNMS), and computing (OLCF). ORNL's strategic plan is anchored by its facilities. For example, a key S&T objective is to deliver exascale computing from system to ecosystem. ORNL is deploying the Frontier system at the OLCF in 2022. Frontier will provide a vast resource for the community. Frontier, the world's first open science exascale system and the first exascale system in America, is the next leap forward in the development of supercomputers. Frontier promises to be at least a 1.5-exaflop system, exceeding speeds of 1.5 quintillion calculations per second—more than 10^{18} operations per second. With an ability to analyze data considerably faster than today's most powerful supercomputers, Frontier will help scientists use leading-edge capabilities to solve some of the world's most complex scientific research problems in fields such as engineering, physics, climate, and nuclear energy. Although it is still being tested and stabilized, it is already more powerful than Summit, which is currently ranked as the fastest supercomputer in the United States and is also at ORNL. As another example, HFIR and SNS serve as a basis for ORNL's neutron science strategy, which aims to continue to advance world-leading capabilities in neutron science and simultaneously offer the scientific community game-changing tools for scientific discovery.

ORNL operates several unique applied energy facilities that complement the SC user facilities. These facilities are critical for fostering deep engagement with industry and delivering technical breakthroughs that address challenges posed by decarbonization, electrification, advanced mobility, and integrated energy systems. Examples include the MDF, which is a unique DOE open innovation center where subject matter experts work with users to advance materials and manufacturing; and the CFTF, which is an export-controlled facility enabling production of carbon fiber and new materials for clean energy applications and defense programs. The National Transportation Research Center (NTRC), the BTRIC, and the Grid Research Integration and Deployment Center (GRID-C) similarly offer unique resources that are critically important for industry partners and key stakeholders to simultaneously enhance the pace and scale of clean energy solutions, regional innovation, and US economic prosperity.

While each facility mentioned above individually provides a critical resource for the research community, the co-location of SC facilities and key centers with applied energy facilities at ORNL offers a vast ecosystem for synergistic development and investigations that does not exist elsewhere. For example, advances at the SNS connect strongly with synthesis and characterization capabilities at the CNMS as well as with QSC efforts to unblock roadblocks in quantum state resilience and controllability. The exascale computing, AI, and integrated ecosystem capabilities being developed by the OLCF are being deployed to advance capabilities and discoveries at the SNS, CNMS, MDF, and CBI (which is advancing bioenergy and products for a cleaner bioeconomy). OLCF is also providing unparalleled scientific instruments to support the quantum community in the discovery and development of quantum science and technology and advancing quantum devices. More than a dozen quantum communications-related technologies have been developed by lab researchers and are available for study or commercial licensing. OLCF capabilities are also helping to ensure US scientific leadership and national security, as well as enabling the Climate Change Science Institute (CCSI) to develop climate models and weather forecasting important to determine net-zero pathways and climate mitigation strategies.

ORNL's extensive project management expertise is enabling the development of new large-scale capabilities for the nation and world. ORNL is executing America's first exascale computing system (Frontier) as well as the SNS STS and Proton Power Upgrade (PPU) projects. ORNL is also leading ECP for DOE, which is advancing key elements important for the exascale revolution: critical applications, an integrated software stack, and close partnerships to drive the development of advanced computer system engineering and hardware components. ORNL leads US ITER for DOE, an international effort focused on demonstrating the scientific and technological feasibility of fusion energy through assembling and operating a burning plasma experiment.

Strategic investments are urgently needed to accelerate basic science discoveries and their translation into solutions. ORNL is advancing four ambitious crosscutting LDRD initiatives as well as eight core LDRD initiatives important for advancing strategic goals associated with the objectives shown in Table 4.1 and urgent national needs. The LDRD initiatives draw upon, enhance, and integrate core capabilities and take advantage of key facilities and centers at ORNL. As described in Section 3 and Appendix C, the INTERSECT crosscutting initiative is integrating edge computing, AI, Summit and Frontier, and scientific instruments to enable steerable, smart, high-throughput "lab of the future" environments. Key INTERSECT aspects include scalability, reusability, and interoperability of the architecture, tools, and software services across scientific disciplines. The crosscutting AI Initiative is developing core AI research capabilities to support ORNL's science and engineering mission with use cases in materials, chemistry, biology, and manufacturing. TDI is developing novel yet scalable approaches for carbon capture and conversion to address the nation's decarbonization challenge. TDI takes advantage of ORNL core capabilities and facilities to codesign the permeability, selectivity, reactivity, and chemical/electrochemical stability of carbon capture and conversion materials and to enhance soil carbon storage. The Enzyme Engineering Initiative seeks to develop and deploy advanced DBTL capabilities to modify enzyme function. The capability will enable scientists to introduce specific mutations into the coded enzyme (as predicted by computational design and genetic recombination) to optimize enzyme functions.

ORNL values diverse collaborations with national laboratories, universities, industries, and communities that lead to new discoveries, significant impacts, and economic development. ORNL collaborates with its core universities (University of Tennessee [UT], Georgia Tech, Vanderbilt, Duke, Florida State, North Carolina State, Virginia Tech, and University of Virginia), as well as other universities through major projects and initiatives and through joint faculty and student engagements. Leveraging a 75-plus year partnership between ORNL and UT, the UT-Oak Ridge Innovation Institute (UT-ORII), established in 2021, is preparing the next generation of scientists and engineers to create a strong, diverse pipeline of talent for our nation. ORNL has established workforce development and other programs with more than 15 historically Black colleges and universities (HBCUs) and 10 minority-serving institutions (MSIs). As the only SC laboratory in the southeastern United States, and located within a Southern Appalachian laborshed that is categorized as distressed, at-risk, or transitional, ORNL is investing deeply in enhancing new partnerships toward the development of a vibrant regional innovation ecosystem. ORNL is home to Innovation Crossroads, a Lab-Embedded Entrepreneurship Program, and launched the Techstars accelerator in 2022. With Tennessee as a leading electric vehicle manufacturer, the potential to support an emergent nuclear power industry in the region, and a recent memorandum of understanding with Tennessee Valley Authority (TVA), a federally owned utility corporation that provides electricity for Tennessee and six surrounding states, ORNL is enthusiastic about galvanizing regional economic growth associated with clean energy.

ORNL is a world-leading research institution by many measures. With a vision to be the world's premier science and energy research institution, ORNL is extremely intentional in its development of its S&T Strategic plan and the nourishment of key elements critical for reaching that vision, including a world-class workforce, a unique ecosystem of facilities, strategic investments, diverse partnerships, and an inclusive culture. The nine objectives listed in Table 4.1 represent the S&T pillars of our strategic plan.

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). Traditionally (before the pandemic), ORNL hosts approximately 35,000 people annually, comprising UT-Battelle's roughly 5,800 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. On ORNL's main campus, work is performed in 192 operational buildings (4.5 million gross sq. ft. [GSF]) owned by SC and 78 operational buildings (0.45 million GSF) owned by DOE's Office of Environmental Management (EM). Fifty-seven buildings in shutdown/decommissioning/stabilization status, owned by SC and EM, represent 1.15 million GSF of ORNL's building inventory. A total of 22 buildings owned by SC (0.71 million GSF) are awaiting disposition, having been excessed to DOE. Nine buildings owned by SC, 1 owned by DOE NE, and 2 owned by EM (0.06 million GSF) are in standby status, awaiting repurpose or reuse. All SC mission-unique facilities (1.0 million GSF) have an adequate condition rating. Of SC's facilities that are not mission-unique facilities, 93% are rated adequate; the balance is rated substandard. Building 4500N (363,758 sq. ft.) is the largest substandard building on campus, with $2.3 million in operating costs and repair needs of $17 million. That facility and aging plantwide utility systems (i.e., substandard Other Structures and Facilities) are important focus areas for modernization.

Research requiring ready access for industrial partners is conducted in 10 off-site leased facilities totaling 0.32 million GSF. ORNL's Hardin Valley Campus, about 7 miles from the main campus, hosts the MDF, GRID-C, and NTRC. The Carbon Fiber Technology Facility is located at a separate site in Oak Ridge about 5 miles from the main campus. In pursuit of optimal support for mission needs, ORNL's leased space portfolio is evaluated frequently to identify opportunities for consolidation. The 2021 evaluation indicated there were no opportunities to consolidate. Therefore, no change was made to the leased space portfolio. ORR land use is governed by the current *ORR Land Use Plan*[16] and ORNL's *Site Wide Master Plan*.[17]

Campus Strategy

ORNL's campus strategy is to develop new assets, revitalize existing assets, sustain facilities, and enhance infrastructure to advance scientific missions. The success of this strategy relies on achieving four primary objectives:

1. Support science missions, initiatives, and critical programs.
2. Establish a modern, adaptable support infrastructure.
3. Reduce excess facility liabilities and footprint.
4. Evaluate and implement technologies to ensure carbon footprint reduction.

These objectives will be accomplished, in part, by successfully addressing critical infrastructure needs identified through ORNL's Mission Readiness process, culminating in the planned investments shown in Fig. 6.1. At ORNL, space is an institutional resource and a strategic asset managed for delivery of ORNL's campus strategy. Clear understanding of design, limitations, and utilization is leveraged to provide

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[16] *Oak Ridge Reservation Planning: Integrating Multiple Land Use Needs. FY 2012 Update*, DOE/ORO/2411, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

[17] https://services.ornl.gov/ronweb/Media/ORNLswmp.pdf

efficient solutions. Space utilization in support of scientific initiatives is maximized by co-locating and consolidating scientific disciplines, thus creating synergies in support of ORNL's science missions.

The figure below illustrates ORNL's vision, which combines DOE and institutional investments needed to advance the laboratory's scientific and technical capabilities and continue transforming the ORNL campus into modern research space. Over the last two decades, ORNL has implemented sustainable designs and has built LEED-certified buildings as integral components of campus modernization.

Proposed Facility and Infrastructure Investments 2022–2032

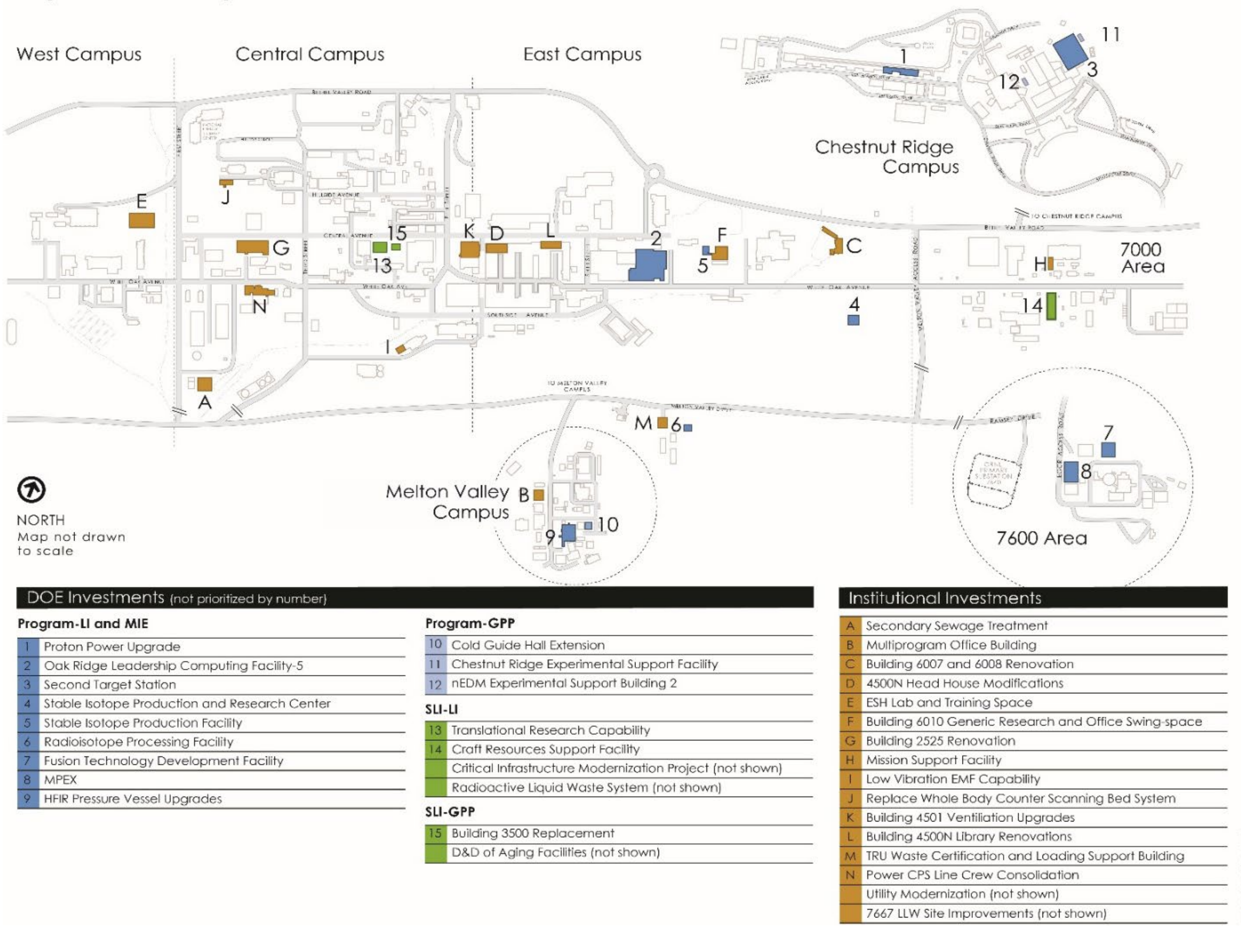


Figure: Proposed facility and infrastructure investments

ORNL's planned programmatic line items and GPPs for the ORNL campus are shown in Table 6.3. The table shows the importance of utility systems (Science Laboratories Infrastructure line item [SLI-LI] Critical Infrastructure Improvement Project) to the delivery of major science and technology projects. No new programmatic line item starts are planned for West Campus.

Key facility and infrastructure investments are crucial for successful delivery of ORNL's science strategies. These investments are shown in Figure 6.1 and summarized in the following list:

Six programmatic line item construction projects:

- Spallation Neutron Source (SNS) Proton Power Upgrade (PPU) project, supported by DOE SC Basic Energy Sciences (BES) (CD-2/3 approved)

- SNS Second Target Station (STS), supported by BES (CD-1 approved)
- HFIR Pressure Vessel Upgrades, supported by BES (CD-0 approved)
- Stable Isotope Production and Research Center (SIPRC), supported by the Office of Isotope R&D and Production (IP) (CD-1/3a approved)
- Radioisotope Processing Facility, supported by the IP (CD-0 approved, CD-1 in process)
- Fusion Technology Development Facility, supported by DOE SC Fusion Energy Sciences (FES) (proposed for FY 2025)

Three Major Item of Equipment (MIE) projects:

- Stable Isotope Production Facility (SIPF), supported by IP (PD-2/3 approved)
- Material Plasma Exposure Experiment (MPEX), supported by FES (CD-3a approved)
- Oak Ridge Leadership Computing Facility (OLCF)-5 (Frontier), supported by DOE SC Advanced Scientific Computing Research (CD-3 approved)

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

- Translational Research Capability (TRC) (CD-2/3 approved, construction in process)
- Craft Resources Support Facility (CRSF), (KD-3 approved)
- Radioactive Liquid Waste System (CD-0 approved)
- Critical Infrastructure Modernization Project (CD-0 approved, CD-1in process)

Three programmatic General Plant Projects (GPPs):

- High Flux Isotope Reactor (HFIR) Cold Guide Hall, supported by BES (proposed for FY 2024)
- Chestnut Ridge Experimental Support Facility, supported by BES (proposed for FY 2026)
- nEDM Experimental Support Building (EB-2), supported by NP (proposed for FY 2023)

Two SLI GPPs:

- Building 3500 Replacement (proposed)
- Decontamination and Decommissioning (D&D) of Aging Facilities (proposed)

These projects, as well as numerous smaller projects supported through Institutional GPP (IGPP) funding, are discussed in the following sections.

Objective 1: Support Science Missions, Initiatives and Critical Programs

Our campus strategy focuses on five areas of infrastructure investment to advance ORNL's science and energy leadership and enable accomplishment of major initiatives.

Maintain and strengthen global leadership in neutron sciences

Continued operation of SNS and HFIR as world-leading neutron scattering user facilities requires two major programmatic investments. The PPU project at SNS will increase power delivered to the First Target Station to 2 MW, increase neutron flux on available beamlines, and provide additional proton pulses to support operation of the STS. The addition of the STS will provide ORNL with three complementary neutron sources, ensuring US leadership in neutron sciences into the foreseeable future. HFIR has operated for 55 years and is a key scientific asset. In response to the September 2020 Basic Energy Sciences Advisory Committee (BESAC) report,[18] DOE-SC has approved the mission need

[18] *The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility*, Report of the Basic Energy Sciences Advisory Committee, July 2020.

statement for the replacement of the reactor pressure vessel and other major components for long-term sustainment of HFIR capabilities. Upgrading HFIR with a new pressure vessel and making strategic facility improvements will improve and extend the reactor's capabilities for at least another half-century at a fraction of the cost of construction of a new reactor.

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. Additionally, NP-funded GPP resources are necessary to construct a new experimental building to house the neutron Electric Dipole Moment (nEDM) research experiment at SNS. ***Computing to enable convergence of experiment, theory, simulation, and data for science and engineering.*** Leadership-class computing underpins nearly all scientific disciplines. Thus, continued development of ORNL's HPC infrastructure as part of the OLCF is a high priority. DOE's well-defined path to maintain leadership in HPC includes continued operation of the pre-exascale Summit machine (OLCF-4) and acquisition, installation, and operation of an initial exascale system, Frontier (OLCF-5), located in the former Titan location in Building 5600. To leverage significant prior investments in power and cooling systems, a new mechanical plant, located in Building 5800, and new power feeders from the 7640 substations were constructed that increased power and cooling to the computing complex. Construction of the TRC facility will provide additional resources for housing novel capabilities in quantum and neuromorphic computing.

To support SC's goal of delivering exascale computing and data curation for scientific instruments and sensors, ORNL has created INTERSECT. This initiative includes the capture, storage, curation, and transport of information from various sources in scalable fashion. Scalability relies heavily on the ability to move large data sets from the instrument to the edge and from the edge to a supercomputer requiring a high bandwidth network capability. ORNL has also initiated the replacement of older router technology and core fiber technology to be installed in FY 2022. The ESNET 400G project will address campus redundant border routers for business continuity, fiber optic cables, and border firewalls. Investments are also planned for high-bandwidth network capability.

Discover and design next-generation materials and chemical processes for energy

Accelerating design, discovery, and deployment of new materials and manufacturing processes requires specialized instrumentation and facilities. Over the past 5 years, ORNL has made discretionary investments to secure new, world-class tools for materials science, including a secondary ion time-of-flight mass spectrometer, a MAC-STEM, an x-ray tomography system, and a low-temperature four-probe scanning tunneling microscope. To support increasingly sensitive imaging equipment, institutional funds have been allocated to provide a low-vibration, low-electromagnetic field space as an extension to the Advanced Microscopy Lab. ORNL has successfully completed CD-2/3 approval with construction in process for the TRC facility, a $93.5 million SLI-funded facility.

Advanced manufacturing is an important component of our materials portfolio. The MDF houses integrated capabilities to assist industry in adopting new manufacturing technologies, including a focus on decarbonizing the industrial sector, and provides a gateway to expertise in materials synthesis, characterization, and process technology.

Advance the fundamental science, engineering, and integrated technologies to accelerate the deployment of fusion and advanced fission energy

ORNL's nuclear capabilities support a broad range of efforts: several SC programs (IP, FES, and BES), other DOE programs (NE and NNSA), and other sponsors in areas that span fission energy technologies, fusion R&D for plasma-facing materials and fuel cycle, radioisotope production and R&D, and nuclear security. These capabilities are dependent on the following:

- *HFIR operation as a high-flux irradiation source.* Continued success in this area depends on sustained programmatic operations support, new fuel fabrication, spent fuel shipment, and annual funding to perform necessary planned maintenance and life extension projects. Investments above fixed operating costs will be required to address fuel fabrication and inspection process improvements implemented at BWX Technologies. In addition, a new permanent beryllium reflector, four new beam tubes, and other core components are being fabricated in preparation for the beryllium reflector replacement outage. A mission need has been approved for replacement of the HFIR pressure vessel, which will extend the reactor life for at least another half-century.
- *Operation for radioisotope production and for processing and handling of irradiated and nuclear materials*. ORNL's isotope complex 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 these facilities. Consistent funding of ORNL's nuclear facilities is needed to ensure long-term sustainability and compliance with DOE's nuclear safety standards.
- *The Material Plasma Exposure Experiment (MPEX) project*. MPEX has received CD-1 and CD-3A approval, and a preliminary design has been completed. MPEX will be a key tool in understanding plasma-surface interactions, and ultimately, the performance of divertor and plasma-facing materials. ORNL continues to place high priority on the execution of the MPEX project, which is on track for construction and commissioning. Resources are being prioritized to assist project execution as needed. Institutional investments, including replacement of the cooling water tower, are planned to support MPEX and other experimental facilities in the immediate area.
- *Fusion prototypic neutron source.* A fusion prototypic neutron source has been identified by the American Physical Society's Division of Plasma Physics Community Planning Process as a high-priority facility for fusion energy and has been endorsed by the recent FESAC report (2020).[19] Options to repurpose existing ORNL facilities are being evaluated, but utilities would be required. ORNL is ready to support a mission need statement and identification of potential approaches when the sponsor is ready to move forward.
- *Fusion Technology Development Facility.* ORNL is developing plans for the Fusion Technology Development Facility (proposed for 2025), enabling advancement in several key fusion technology areas. This plan will require investment in a facility with multiple flexible laboratories, high bay space, and sufficient utilities to support a diverse R&D program. A DOE-funded preconceptual design study of a small, multipurpose building is ongoing. This building would provide much needed near-term lab space for fusion technology activities and serve as the first step in the buildout of the Fusion Technology Development Facility.

Providing strategic capabilities in isotope R&D and production

DOE IP makes extensive use of ORNL's research and production facilities: HFIR, the Enriched Stable Isotope Prototype Plant, REDC, and other radiological facilities.

[19] *Powering the Future: Fusion and Plasmas*, A Report of the Fusion Energy Sciences Advisory Committee, 2020.

- *Stable isotope portfolio.* To meet demand for critical isotope production and reduce national dependence on foreign suppliers, ORNL proposes to complete the SIPF MIE by 2025 and to continue to expand stable isotope research and production capabilities through several major initiatives. SIPRC, which received CD-0 approval in FY 2019 with CD-1 in process, will greatly expand research and production capabilities for stable isotopes using several different enrichment technologies. In close association with SIPRC, ORNL plans to optimize all aspects of the stable isotope portfolio, including electromagnetic, gas centrifuge, and other isotope enrichment technologies; R&D and other supporting laboratories; stable isotope storage and dispensing operations; and technical services for preparing special isotope forms through physical and chemical conversions.
- *Radioisotopes.* Continued growth in demand for ORNL radioisotope production is anticipated to meet multiple needs in areas such as basic science, applied R&D, and medical applications. The proposed Radioisotope Processing Facility (CD-0 was approved on April 29, 2021) will eliminate the capacity gap introduced with increased demand and will provide wider availability and improved quality assurance for multiple emerging reactor-produced radioisotopes. Eliminating this capacity gap allows for increased radioisotope production in support of the entire DOE complex and other needs.

Objective 2: Establish a Modern Adaptable Infrastructure to Support Research

The cornerstone of this objective consists of strategic investments that optimize, modernize, and sustain facilities and utility systems to best accomplish current and future ORNL missions. ORNL fosters safe, efficient, reliable, and environmentally responsible operations through targeted investments.

Modernization of ORNL's utility systems: Reliable, efficient, and maintainable utility infrastructure provides the foundation for successful scientific achievement. Uninterrupted reliable operation of ORNL utilities underpins modern scientific tools used to support cutting-edge research that drives technological breakthroughs. ORNL has consistently provided a high level of service through routine preventive maintenance and continued institutional investments. However, many of ORNL's core utilities were installed as part of the Manhattan Project and are becoming increasingly inefficient and difficult to maintain. Aged infrastructure requires more frequent emergency repairs, which are complicated by the need to secure obsolete parts. These factors ultimately culminate in decreasing reliability, increasing inefficiency, and escalating costs. To correct the highest-risk utility system deficiencies identified by utility system stewards through condition assessments and inspection, ORNL proposed an SLI-LI (CD-0 approved, CD-1 in process). As part of this project, ORNL will implement both enabling structures and technologies to drive adoption of ML/AI capabilities. The IGPP-funded secondary sewage system, slated for completion in FY 2024, will provide much-needed increased capacity and improve operational efficiency by reducing costs associated with outdated and deteriorated equipment. Additional institutional investments are being made in the 7600 area and Central Campus to support research activities and improve utility distribution systems, thus providing interconnections for redundancy.

Revitalization of mission support campus: ORNL's 7000 area is a centralized craft asset supporting research and laboratory operations. This campus area hosts multiple craft shops and services, centralized and co-located security and fire response personnel, and 600 craft personnel. Institutional investments are funding the construction of the Mission Support Facility, which will provide an environmentally controlled, conditioned workspace. Additional infrastructure modernization, funded by IGPP, will address roads, parking, and sidewalks.

The CRSF, which received KD-3 approval, will provide modern facilities to include vehicle garage and shops for sheet metal workers, carpenters, mechanics, and electricians. This new facility will eliminate current infrastructure capability gaps such as inadequately designed aging infrastructure, insufficient storage capacity, and poor environmental controls needed to maintain high-value equipment and materials. The CRSF will also enable the D&D of 10 or more 1950s vintage facilities, eliminating the high cost required to maintain and operate aging buildings.

Repurposing space to maximize utilization: ORNL continues to maximize utilization by repurposing and modernizing existing facilities. Repurposing Building 2719A, the old biomass facility, will consolidate power operations from Buildings 2500 and 2621 while freeing up 5,000 ft^2 of space within Building 2621 for research. Building 6010 modernization work is ongoing. Additional institutional investments planned to modernize and maximize space utilization in Building 4500N include modernization of the headhouse and renovation of the library and Wings 1 and 2.

Management of radioactive waste: Historically, ORNL has relied on EM infrastructure for management of gaseous, liquid, and transuranic waste from nuclear and radiological facilities. EM infrastructure is 30 to 60 years old, oversized, and not designed for the waste generated by today's isotope production and nuclear R&D missions. EM plans to shut down portions of existing infrastructure once legacy waste missions are completed. With this in mind, ORNL is developing independent waste management capabilities to achieve self-sufficiency. IGPP investments have created a remote-handled waste loading station at REDC. Investments to construct a local high-efficiency particulate air filtration system and exhaust ventilation stack in Building 3525 will enable independence from the EM-operated central stack in 2022. However, Buildings 3047 and 3025E will still be reliant on the EM-operated central stack. As EM completes its transuranic mission in Oak Ridge, ORNL SC needs to acquire storage facilities from EM and adapt that space for packaging transuranic waste. Institutional investments will be needed to construct a TRU waste Certification and Loading Support Building to support Waste Isolation Pilot Plant campaigns and to provide loading capabilities, dose-to-curie measurements, and flammable gas analysis.

Objective 3: Reduce Excess Facility Liabilities and Footprint

ORNL currently expends approximately $2.5 million annually to address environmental and safety risks associated with excess SC facilities. ORNL's rationale in prioritizing facilities for demolition is based on:

- removing significant risks and liabilities;
- enabling future development by clearing aging facilities from prime locations; and
- eliminating assets which are unlikely candidates for renovation due to age, condition, and deferred maintenance (DM).

Working with DOE's Excess Contaminated Facilities Working Group, ORNL has prioritized excess facilities into four groups: (1) ORNL-managed SC and NE facilities at Y-12, (2) SC facilities in ORNL's Central Campus, (3) 7000-area facilities, and (4) balance of buildings for demolition.

SC and NE facilities at Y-12: Due to deteriorated condition and size, ORNL facilities at Y-12 represent the highest ORNL cost risk. EM has demolished 9207, 9207A, 9210, 9743-02, 9767-06, 9767-07, and 9770-02. At present, EM is preparing to demolish Buildings 9201-2, 9204-1, 9401-1, 9422, and 9732-2.

SC facilities in ORNL's Central Campus: A prime location for future development, the Central Campus houses several excess facilities awaiting demolition. The presence of these aging facilities hinders mission delivery and modernization while increasing liabilities and risks. Modernization of this campus area will be most quickly enabled when facility demolition is accompanied by associated contaminated soil removal, allowing for immediate redevelopment. Continuation of a strong EM funding profile is key to ensuring ORNL's ability to deliver on its mission. EM actions to complete the cleanup of the Central Campus, in parallel with investments in modernization by SC and ORNL, are enabling future mission assignments. ORNL has transferred operational responsibility of several SC-owned buildings to EM in preparation for demolition (Buildings 3003, 3010A, and 3080 in 2019; Buildings 3034 and 3036 in 2020). EM is currently removing the 3026 C&D hot cells and is working toward the removal of Isotope Row facilities and the research reactors (Buildings 3005, 3010, and 3042) in Central Campus. ORNL actively coordinates with EM contractors to enable the D&D activities. ORNL's long-term plan for this campus is the construction of a series of modern facilities built upon a revitalized utility infrastructure. Planned actions include (1) construct TRC, (2) replace aging facilities, and (3) vacate and demolish 1940s-era facilities.

- *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 in support of fusion and high-energy physics. ORNL has received CD-2/3 approval.
- *Replace aging facilities:* A proposed SLI GPP investment will provide modern space for staff currently housed in Building 3500, a 1950s-era facility in the Central Campus area. Demolition of Building 3500 will also eliminate $2 million in DM.
- *Vacate and demolish aging mission support facilities:* Upon completion of the Research Operations Support Center, ORNL vacated both the Protective Force and Fire Stations (Buildings 3037 and 2500). During the pandemic, Building 2500 was temporarily reoccupied for COVID testing.

7000 area facilities: Demolition tasks were performed in FY 2021 to make way for construction of the CRSF. Facilities demolished in FY 2021 to clear space for construction of the CRSF include Buildings 7033, 7035, 7035A, 7035B, 7035C, 7035E, 7035F, 7062, 7070, and 7082. Extensive underground utilities will also be removed for utility upgrades.

Balance of buildings for demolition: SC transferred operational responsibility of Buildings 7600, 7609, 7610, and 7014 to EM to prepare for demolition. Building 5505 transfer to EM is also in process. Buildings 7914, 7914A, and 7915 have been demolished at the Melton Valley campus. ORNL continues to clean up and dispose of abandoned facilities and experiments throughout its campus. For example, Building 2644 has been demolished to support the construction of the new Sewage Treatment Facility. Building 7067 has been demolished to support the construction of the Mission Support Facility. Building 7615 has been demolished to allow for future site development. Structures 7077C, 7849, and 7867 have been removed to eliminate the liabilities associated with aging structures. Facilities 7964C, 7981B, 7981C, 8940, XF1304, XG1410, XG1415, and XG1416 are slated for demolition in FY 2022.

Objective 4: Evaluate and implement technologies to ensure carbon foo

The ORR (inclusive of ORNL and Y-12) constitutes a small city, ideal for demonstration and deployment of a carbon-neutral testbed. ORNL's Net-Zero Carbon Campus efforts will include approaches that demonstrate a variety of technologies such as electrical storage, carbon capture, integration of renewables, transition to an all-electric vehicle fleet, and efficiencies gained through infrastructure modernization that reduce or eliminate carbon emissions. Carbon capture research will be conducted in a phased manner, developing prototype technologies, with potential implementation planned across campus. Disposition of captured carbon will also be evaluated for potential re-use, conversion to fuel, or disposal.

In addition to these efforts, deployment of new nuclear generation will help ORNL to reach net-zero. TVA has approved up to $200 million to prepare for the potential construction of a small modular reactor (SMR) at its Nuclear Regulatory Commission (NRC)-licensed site, which could provide carbon-free electricity for the reservation and the region. To further ORNL's progress towards net-zero, UT-Battelle has established a memorandum of understanding (MOU) with TVA focused on decarbonization technologies. Activities considered under this MOU include:

- Point source and direct air carbon capture
- Carbon utilization
- Hydrogen generation and utilization
- Electric vehicle charging and vehicle to grid interaction applications
- Light water small modular reactors and 4th generation advanced nuclear reactors
- Long duration energy storage
- Electrification of parts of economy that are currently fossil fuel
- Grid resiliency and security

Net-zero carbon campus projects will require programmatic and institutional investments. Traditional energy conservation measures (ECMs) such as lighting improvements, HVAC, and temperature setbacks are being implemented to reduce energy consumption, also resulting in greenhouse gas (GHG) footprint reduction. The SLI-LI Critical Infrastructure Modernization Project (CD-1 in process) will contribute to resiliency, GHG reduction, and energy/fuel efficiency.

Future Infrastructure Gaps within a 10-Year Window

The following future infrastructure gaps are anticipated:

- New space will be required to support secure biosystems design, biodesign goals, robotics systems for automated sampling, mass spectrometry, and advanced, high-throughput imaging equipment important to advance the bio-scales initiative.
- To advance ORNL's goal to remain a global leader in innovative isotope research, development, and production, additional space will be required to optimize all aspects of the stable isotope portfolio by consolidation of existing small-scale enrichment science, engineering, and technical services activities across the ORNL campus into the 6000 area to enable more efficient enrichment research and production.
- New isotope engineering, maintenance, and support capabilities will be required to replace current capabilities in Central Campus Buildings 3025M, 3104, and 3502 that are to be turned over to DOE-EM in the 2030 timeframe. Addition of the RPF will require expanded manipulator capabilities because the existing Building 7935 manipulator shop will be fully utilized by REDC. A mix of conventional and radiological space will be required.
- Additional space will be needed to house classified computing, laboratories, and additive manufacturing.
- The 3025E facility is required to prepare irradiated samples for MPEX exposure but is expected to be turned over to DOE EM in the early 2030s. A project to relocate these capabilities needs to be completed to avoid a mission capability gap.

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 19 years, institutional investments have been the predominant funding mechanism for continued site modernization. Since FY 2002, when ORNL began using IGPP for core infrastructure improvements, 103 projects have been completed at a total cost of $258 million. Over the next decade, there is a need for continued investment in infrastructure to recapitalize and sustain aging assets, some of which are 75 years old.

Maintenance and repair investments are between 2% and 4% of the replacement plant value. Thirty-nine percent of ORNL's operational non-mission-unique facilities, representing approximately 45% of the total gross square footage, are more than 50 years old and carry nearly 62% of DM. ORNL will continue to demolish shutdown assets that carry a high DM.

Site Sustainability Plan Summary

The ORNL Site Sustainability Plan (SSP), submitted in December 2021, 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:

- GHG emissions have been reduced by 26% from the FY 2008 baseline.
- Energy use intensity (EUI) has decreased by 33.8% since FY 2003. The FY 2021 non-High Energy Mission Specific Facility (HEMSF) energy consumption increased 1.6% from the previous year. However, updates to ORNL's energy-consuming gross square feet, demolition of 15 buildings, and improved reporting methodologies yielded an overall 4.5% increase in the EUI (in thousands of British thermal units per gross square foot) compared with the EIU for FY 2020. ORNL continues to look for ways to reduce the non-HEMSF energy consumption for ongoing progress toward achieving an annual reduction to the EUI.
- Water use intensity (WUI) has decreased by 23.2% since FY 2007. The FY 2021 total water consumption decreased 4.8% from the previous year. However, improvements in identification of water-consuming facilities yielded a reduction in gross square feet, resulting in a 2.2% increase in the WUI (gallons per gross square foot) compared to FY 2020. The WUI calculation does not permit exclusion of process usage (like HEMSF). Changes in HPC and associated mission-specific growth are expected to increase ORNL's total water consumption by 15% by FY 2030, further increasing the WUI. ORNL will continue to aggressively identify and repair leaks and seek creative solutions for ongoing progress toward achieving an annual reduction to the WUI.

ORNL has an opportunity and a responsibility to lead by example and integrate climate and sustainability into all aspects of its operations. Accordingly, ORNL is taking the following actions:

- Energy studies and audits per the Energy Independence and Security Act are core efforts for ORNL to identify projects for energy and water conservation.
- ORNL is also using energy conservation tools such as Resource Advisor, DOE 50001 Ready, and SkySpark to build energy awareness, provide robust data analysis, assist with data visualization, and utilize fault detection and diagnostics to help identify opportunities for improved performance and energy savings.

- Guiding principles can be used to incorporate best practices into new construction and modernization efforts to continue to expand ORNL's energy efficiency facilities.
- The development of the Vulnerability Assessment and Resilience Plan will help ORNL to manage risks to critical missions and utility infrastructure from disruptions for operational resiliency.

High Performance Sustainable Buildings (HPSBs)

ORNL's on-site HPSB inventory included a total of 21 buildings that are certified by either being grandfathered through LEED certification or having attained 100% of the HPSB Guiding Principles.[20] Building 3137 has been transferred from DOE SC to DOE EM, reducing ORNL's HPSB inventory. According to the new 2020 Guiding Principles Guidance requirements, all certified Guiding Principles buildings must be reassessed every 4 years. ORNL will need to recertify 21 buildings and identify and certify other existing buildings as candidates for the HPSB inventory, which will impact available resources.

Energy Savings Performance Contracts (ESPCs)

The ESPC with Johnson Controls is in its tenth performance period. DOE, Johnson Controls, and ORNL regularly meet to review performance. The Year Nine Performance Period identified annual savings of 335,169 million BTUs of electricity, natural gas, and fuel oil and 187 million gal of water, all of which contribute to lower EUI and WUI.

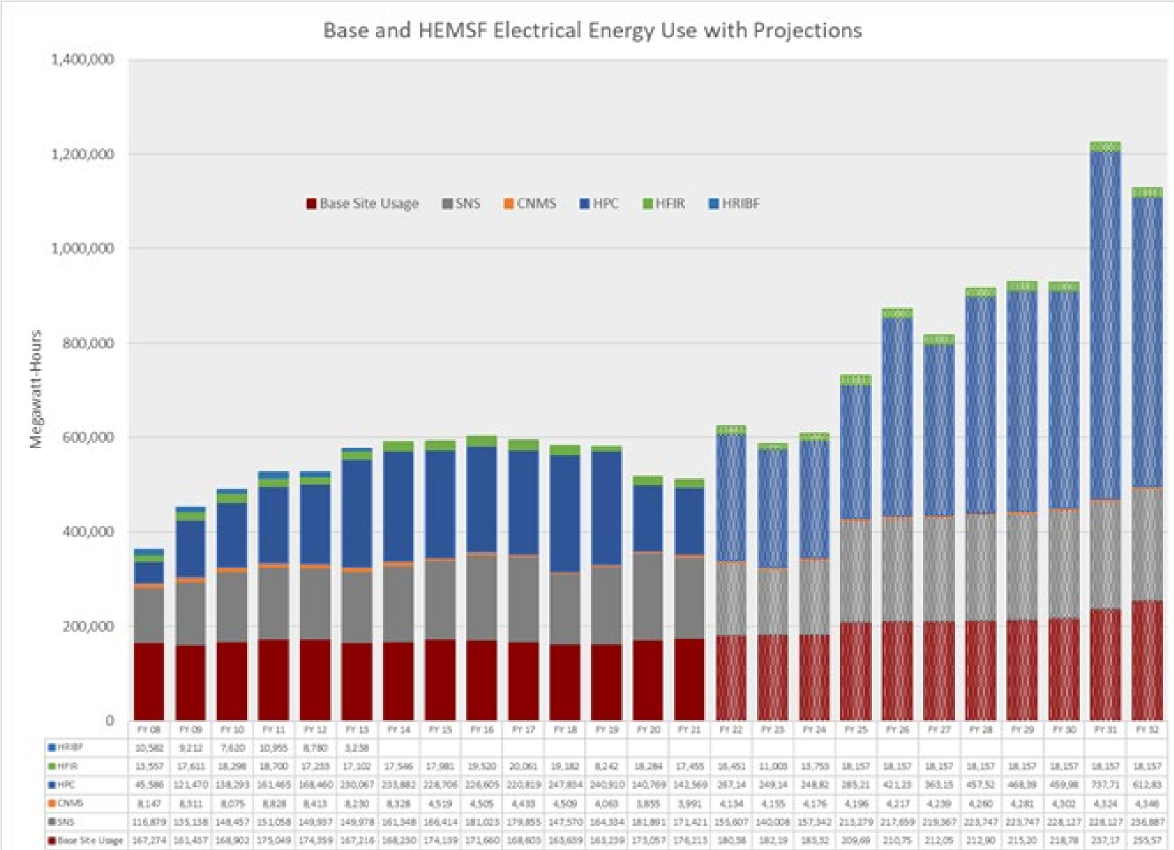
High Energy Mission-Specific Facilities (HEMSFs) Electrical Use with Projections

The historical (FY 2008 Baseline), current (FY 2021), and projected electrical energy consumption for ORNL's base facilities and HEMSFs are shown in Fig. 6.2. Each year, ORNL reviews its mission plans to estimate energy consumption for utility costs and to anticipate energy reduction goal impacts for the next 10-year period. These projections are updated throughout the year as the mission scope changes.

HEMSF electrical energy consumption accounted for 66% of ORNL's electrical use in FY 2021. HEMSF electrical consumption is expected to grow to approximately 77% of total electrical energy use by FY 2032 based on projections for HPC expansion and STS.

The electrical energy and water consumption for SNS and HFIR are expected to slightly decrease for FY 2022 through FY 2024, returning to normal research levels in FY 2025 (figure below). The power use increases in FY 2025 with the SNS PPU. Beginning in FY 2022, energy consumption will increase because multiple HPC systems will be running concurrently while one system is decommissioned, and a new system is installed. The forecast assumes no large increase in power due to non-HEMSF projects.

[20] Council of Environmental Quality, *Guiding Principles for Sustainable Federal Buildings and Associated Instructions*, December 2020.



	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
HRIBF	10,582	9,212	7,620	10,955	8,780	3,258							
HFIR	13,557	17,611	18,298	18,700	17,233	17,102	17,546	17,981	19,520	20,061	19,182	8,242	18,284
HPC	45,586	121,470	138,293	161,465	168,460	230,067	233,882	228,706	226,605	220,819	247,834	240,910	140,769
CNMS	8,147	8,311	8,075	8,828	8,413	8,230	8,328	4,519	4,505	4,433	4,509	4,060	3,855
SNS	116,879	135,138	148,457	151,058	149,937	149,978	161,348	166,414	181,023	179,855	147,570	164,334	181,891
Base Site Usage	167,274	161,457	168,902	175,049	174,359	167,216	168,230	174,139	171,660	168,603	163,639	163,239	173,057

	FY 21	FY 22	FY 23	FY 24	FY 25	FY 26	FY 27	FY 28	FY 29	FY 30	FY 31	FY 32
HRIBF												
HFIR	17,455	16,451	11,008	13,753	18,157	18,157	18,157	18,157	18,157	18,157	18,157	18,157
HPC	142,569	267,14	249,14	248,82	285,21	421,23	363,15	457,52	468,39	459,98	737,71	612,83
CNMS	3,991	4,134	4,155	4,176	4,196	4,217	4,239	4,260	4,281	4,302	4,324	4,346
SNS	171,421	155,607	140,008	157,342	213,279	217,659	219,367	223,747	223,747	228,127	228,127	236,887
Base Site Usage	176,213	180,58	182,19	183,32	209,69	210,75	212,05	212,90	215,20	218,78	237,17	255,57

Figure: Base and HEMSF electrical energy use with projections

Renewable Energy Credit (REC) cost projections

In FY 2021, ORNL purchased 48,400 MWh of RECs or certificates to supplement on-site renewable energy generation, representing 9.4% of the laboratory's electrical energy consumption, exceeding the current DOE target of 7.5% renewable energy as identified in the Energy Policy Act of 2005. As ORNL's mission grows, specifically in HPC and neutron scattering (PPU and STS), the quantity of RECs purchased will increase to meet or exceed targets of the DOE or the US Environmental Protection Agency (EPA) unless ORNL develops significant on-site renewable energy generation capabilities. ORNL continues to look for renewable energy projects and research opportunities.

PACIFIC NORTHWEST NATIONAL LABORATORY

Lab-at-a-Glance

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

- **FY 2021 Lab Operating Costs:** $1,205.7 million
- **FY 2021 DOE/NNSA Costs:** $830 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $294 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 24.4%
- **FY 2021 DHS Costs:** $81.7 million

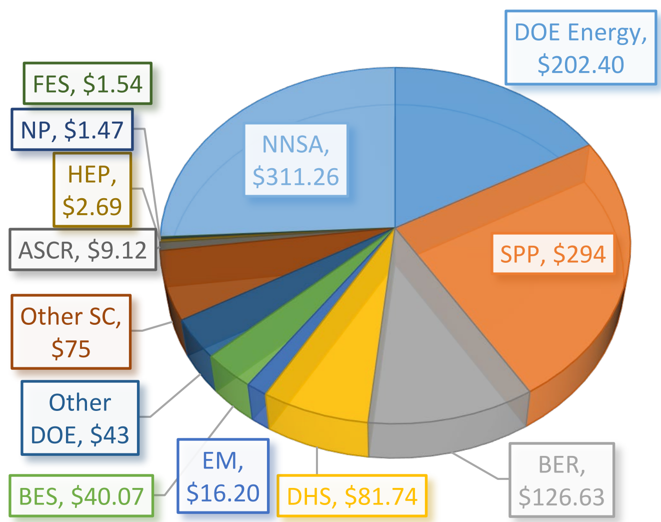
Physical Assets:

- 554 acres and 86 buildings (DOE & Battelle Facilities)
- 1,297,460 GSF in buildings
- Replacement Plant Value: $1.272B
- 982,508 GSF in 29 Leased Facilities
- 65,849 GSF in 13 Battelle Buildings

Human Capital:

- 5,310 Full Time Equivalent Employees (FTEs)
- 90 Joint Appointments
- 342 Postdoctoral Researchers
- 487 Graduate Student
- 416 Undergraduate Students
- 166 Facility Users
- 228 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Mission and Overview

Pacific Northwest National Laboratory (PNNL) draws on signature capabilities in chemistry, Earth sciences, biology, and data science to advance scientific discovery and create solutions to the nation's toughest challenges in energy resiliency and national security.

A Department of Energy (DOE) Office of Science (SC) laboratory, PNNL focuses on discovery science. In chemistry, we design catalysts and chemical pathways for new fuels, feedstocks, and energy storage materials. In Earth sciences, we build the predictive power of DOE's Earth system models, emphasizing Earth systems in transition. In biology, we seek to understand, predict, and control phenotypes of biological systems to produce desired functions and products. In data science, we combine machine learning (ML), data visualization, and modeling to create machine reasoning capabilities that interact with scientific instruments and generate data yielding new theoretical insights and physical models. PNNL operates two DOE user facilities—the Environmental Molecular Sciences Laboratory (EMSL) and the Atmospheric Radiation Measurement (ARM) user facility.

PNNL research enhances decarbonization of the national energy system through the development and deployment of large-scale energy storage and advanced grid control technologies. We apply deep knowledge of the North American grid to design, test, and evaluate technologies for security and optimization. We apply our chemistry and materials science capabilities to develop advanced energy storage solutions for grid resiliency.

We integrate expertise in data sciences, chemistry, biology, and nuclear science to detect weapons of mass effect, accelerate nuclear materials characterization, advance nonproliferation and nuclear forensics, automate threat analysis, secure our borders, and protect critical infrastructures from cyberattack.

PNNL is proposing a new 10-year $1.2B facilities recapitalization goal and is committed to becoming a net-zero (NZERO) emissions DOE laboratory.

Core Capabilities

PNNL's ability to meet changing DOE needs relies on the strength of 19 core S&T capabilities resident at the Laboratory. Eighteen of these core capabilities are discipline-based and are grouped into four categories—Biological and Earth Sciences, Chemical and Materials Sciences, Engineering, and Computational and Mathematical Sciences. The nineteenth capability, User Facilities and Advanced Instrumentation, supports two BER user facilities managed by PNNL—EMSL and ARM.

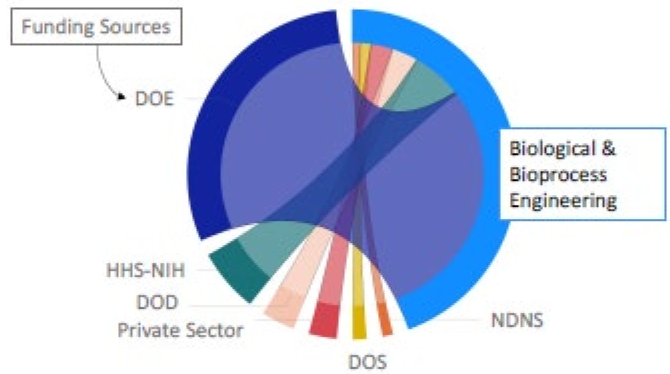
PNNL's *Integrated Capability Management (ICM) Program Description Document – April 2021* provides a complete description of our capability health assessment process and the underlying data sources. Wherever possible, PNNL has chosen indicators that are quantifiable and comparable across laboratories. A brief summary of relevant highlights of this assessment is included as the last paragraph discussion of each core capability below.

The figures below made possible by our ICM approach to core capability stewardship, illustrate how our core capabilities are drawn upon to support each of the Major Initiatives described in Section 4.0 of this Annual Laboratory Plan, and illuminate the extent of the integration across sponsors and capabilities necessary to position the Laboratory for a successful future.

In the figure below, the width of each core capability (gray boxes along the bottom of the figure) is based on the number of staff equivalents (not headcount) mapped to each core capability. This data is generated by the ICM system using a mapping that each year codes all researchers (as determined by their manager) according to the percentage of time they spend working on a core capability. Managers can partition staff time toward up to three core capabilities. The connection between each Major Initiative and the core capabilities on which it relies is determined by the authors of the Major Initiatives, as requested by DOE guidance. For the purposes of creating this graphic, we have assumed that core capabilities equally support all the Major Initiatives to which they are connected.

One of the most important functions served by a DOE national laboratory within the U.S research ecosystem is that of integrating a diverse set of scientific disciplines, sponsor needs and funding streams, and practical problems requiring S&T solutions. It is at the intersection of these that the most significant breakthroughs occur, and from which discoveries with the most far-reaching impact originate. One way to illustrate the vibrancy of this interaction of ideas, capabilities, and research at PNNL is through the lens of sponsor support for our core capabilities. The figure below, for example, shows how our work for non-DOE sponsors contributes to the strength of the capabilities on which the laboratory depends.

Each of the core capability descriptions provided in this appendix is accompanied by a graphic (similar to the image on the right) that illustrates the cross fertilization of sponsors in that area (i.e., who contributed to the funding of that core capability and the relative amount of funding), color coded to match the figure below.



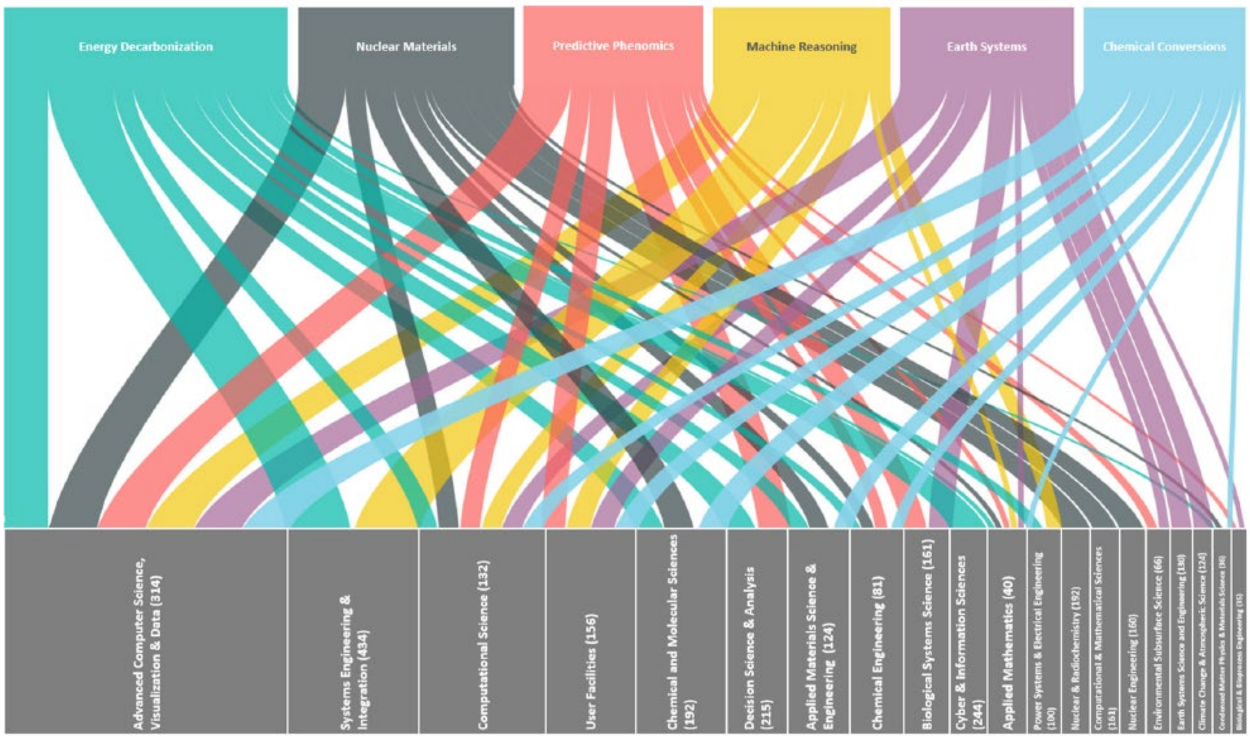


Figure: ICM mapping of PNNL core capabilities to 2021 Major Initiatives; the number of FTEs (not head count) in each capability is provided in parentheses

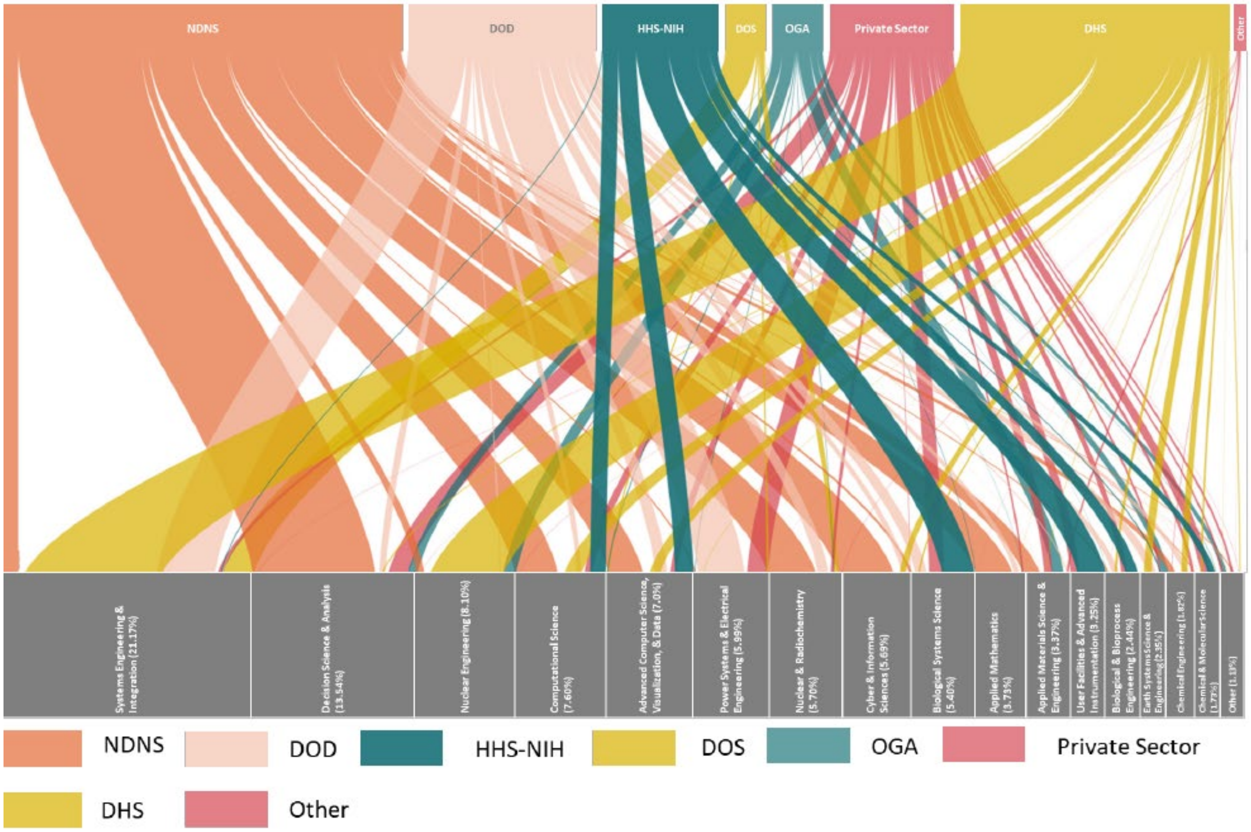


Figure: ICM mapping of all active non-DOE sponsored projects to core capabilities, weighted by the size of the authorized investment; the numbers in parentheses reflect the percentage of non-DOE funds contributing to each core capability

Chemical and Materials Sciences

Chemical and Molecular Sciences

Chemical and Molecular Sciences advance the understanding, prediction, and control of chemical and physical processes in complex, multiphase environments. PNNL has significant domain expertise in condensed phase and interfacial molecular science, chemical physics, catalysis science, chemical separations, geochemistry, theoretical and computational chemistry, physical biosciences, and heavy element chemistry. This core capability has strong ties to the Condensed Matter Physics and Materials Science, Computational Science, and Applied Mathematics core capabilities, leveraging expertise in those areas to advance our understanding of complex phenomena at interfaces and produce high-fidelity simulations of molecular processes controlling macroscopic phenomena. A key strength of our Chemical and Molecular Sciences capability is the close and purposeful integration of experiments and theory, achieving rapid feedback for understanding and control of interactions, transport, and reactivity in multiphase, multicomponent systems. Connections to data science are growing as well, which increase our rate of predictive learning.

PNNL 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 are essential for the upcoming renewal of the Center for Molecular Electrocatalysis Energy Frontier Research Center (EFRC) from DOE's BES program. Further, recent new programs in direct air capture and plastic upcycling awarded by BES built on these strengths.

The Laboratory also has significant strength in geochemical sciences, which contributed to the successful renewal of the iDREAM EFRC. Contributing to PNNL's strength in this area is EMSL's computational chemistry software suite (NWChem), which is used worldwide to efficiently address large molecular science problems on computing architectures ranging from workstation clusters to high-performance leadership class computer architectures. A major redesign of the architecture of NWChem is under way (in the NWChemEx project, funded by ASCR) to dramatically improve its scalability, performance, extensibility, and portability to take full advantage of exascale computing technologies. NWChemEx will target the development of high-performance computational models for the ground states of complex systems that will be used to produce advanced biofuels and other bioproducts. Further computational capabilities targeting excited states are being designed in the Scalable Predictive Methods for Excitations and Correlated Phenomena project, recently renewed 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. These capabilities are also appropriate to interpret the signals obtained at DOE's light source facilities. Novel computational chemistry tools for catalysis, photo-induced charge transfer, and actinide chemistry studies are also utilizing emerging QIS technologies, which enables optimal design of accurate many-body frameworks that will take advantage of the evolving quantum and classical resources to describe complex electron correlation effects in molecular systems. Capability stewardship efforts, such as those proposed in the ESC project, will accelerate scientific discovery in chemical transformations by enabling close integration of synthesis with dynamic characterization capabilities and real-time computational capabilities.

This capability receives support from programs in BES, BER, ASCR, DHS, EERE (geothermal, biomass, and hydrogen; fuel cells; and infrastructure technology), the Office of Fossil Energy (FE; carbon- and co-sequestration), OE (battery chemistries), the Office of Environmental Management (EM; environmental remediation), NNSA (nonproliferation), the Department of Health and Human Services (DHHS), and DoD. In addition to our primary DOE-SC sponsor (programs in BES chemical sciences, geosciences, and biosciences), a number of applied programs rely on our Chemical and Molecular Sciences capability for improvements in sustainable energy technologies, catalysis and reaction engineering, hydrogen storage, biomass conversions, environmental remediation, and carbon capture/sequestration. BER's support of EMSL capabilities also greatly enhances this core capability through the continued focus on molecular transformations that occur in complex systems (including biocatalysts), as well as at complex interfaces.

Health: The predominant sponsor is BES, with very long-term stable programs. This core capability is benefiting from strong partnerships (joint appointments and three joint institutes). A majority of the staff have been at the Lab less than five years, bringing new vitality to this important area. Some existing space shortfalls will be addressed with the construction of the ESC. ESC related equipment will significantly enhance this capability. Issues remain with respect to replacing aging workhorse research equipment.

Condensed Matter Physics and Materials Science

PNNL is an emerging leader in Condensed Matter Physics and Materials Science, a core capability that provides the knowledge base for discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for development of new materials for energy generation, storage, and conversion, as well as manipulating electronic and quantum effects and mitigating materials degradation due to environmental factors and substituting low-abundance elements without the loss of functionality.

The Laboratory has domain expertise in the synthesis of inorganic and biomolecular nanostructures and heterointerfaces, interfacial dynamics of solid-solid and solid-solution liquid interfaces, electrical energy storage, in situ electron and scanning probe microscopy, radiation effects and degradation in materials, and computational materials science. This core capability has strong ties to the Chemical and Molecular Sciences, Applied Materials Science and Engineering, Computational Science, and Applied Mathematics core capabilities. In combination, these capabilities advance our ability to understand and manipulate complex phenomena at gas-solid, 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 materials transformation under operating conditions. Capability stewardship efforts enabled by the ESC project will strengthen the strategic link with our world-class efforts in the predictive design and understanding of chemical transformation processes. The ESC project will provide close integration with the Chemical and Molecular Sciences capabilities through emphasis on predictive synthesis of hierarchical and atomically precise materials and understanding the coupling between external stimuli and chemical processes. This strategic link will enable translating an understanding of catalytic processes into multifunctional catalytic materials.

PNNL has a distinctive strength in the emerging science of materials synthesis, to which it brings synthesis of hierarchical and atomically precise materials, both inorganic and organic; the most advanced imaging, tomography, and spectroscopy tools, many of which are applied in situ and operando; and computational approaches that draw on PNNL's long-standing leadership in computational chemical physics, as well as new capabilities in condensed matter theory and computation. PNNL's capability is particularly strong in understanding the complexity at interfaces, specifically their role in synthesis and their control of electronic, optical, electrochemical, and quantum properties, as well as transfer of matter and energy. These strengths have advanced PNNL's research at the JCESR, an Energy Innovation Hub led by Argonne National Laboratory that was renewed at the end of FY 2018, and in the Fundamental Understanding of Transport Under Reactor Extremes (FUTURE) and Center for the Science of Synthesis Across Scales (CSSAS) EFRCs led by Los Alamos National Laboratory and UW, respectively, that were awarded in late FY 2018. FUTURE includes a thrust that brings together PNNL's capabilities in the synthesis of structures with precisely positioned chemical and isotopic tracers and multimodal imaging to reveal mechanisms of mass redistribution in radiative environments, while CSSAS includes a thrust that brings together deep learning approaches for data analytics and modeling machine learning for molecular design. Most recently, this core capability—which includes measuring the materials properties, such as coherence times, that are key to the performance of quantum sensors—has enabled PNNL to play a significant role in the Co-Design Center for Quantum Advantage, a new Quantum Information Science Research Center led by Brookhaven National Laboratory.

This capability forms the basis for PNNL's sponsor-funded, fundamental science programs in synthesis and processing, biomolecular materials, QIS, electron and scanning probe microscopy, mechanical behavior, radiation effects, and materials chemistry. 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, legacy waste forms, accelerator technology, development of extremely radiopure materials for detection of dark matter and neutrino experiments, and nuclear nonproliferation research. This capability receives support from programs in BES, BER, OE, DOE Office of Nuclear Energy (NE), EERE, and NIH. BER's support of EMSL capabilities (e.g., Quiet Wing and the high-resolution mass accuracy capability) greatly enhances this core capability. Staff members are housed primarily in the Physical Sciences Laboratory, EMSL, and LSL2.

Health: This core capability is stable; however, the condensed matter physics portfolio is smaller than optimal and is being addressed. Some existing space shortfalls will be addressed with the construction of the ESC.

Applied Materials Science and Engineering

PNNL's capability in Applied Materials Science and Engineering emphasizes the development and validation of materials synthesis, manufacturing, and component fabrication concepts that are relevant to DOE mission needs and readily scalable for industry adoption. PNNL has made significant contributions over the years to the commercialization of automobile catalysts, organic light-emitting diodes, new battery technologies, tailor-welded blanks, and many other zero-carbon emission energy technologies. PNNL holds domain expertise in materials characterization, and especially in situ characterization; solid phase processing approaches for the production of alloys and composites as well as the fabrication of semi-finished products; development of scalable materials synthesis approaches; design and fabrication of electrodes and electrolytes for emerging battery systems; materials theory and simulation, including data management and machine learning approaches to accelerate the materials discovery, development, and scaleup cycle; solid oxide reactors for fuel cells and/or electrolysis; durable polymers and composites for hydrogen infrastructure; and materials performance in hostile environments, including the effects of radiation. This capability includes the ability to engineer enabling nanostructured and self-assembled materials, as well as tailored thin films, ceramics, glasses, cements, polymers, metal alloys, and composites.

The Laboratory leverages its Applied Materials Science and Engineering capability to develop new materials and strategies to enable a variety of technology areas, including grid- and transportation-scale energy storage, renewable hydrogen production via solid oxide water electrolysis, solid-state lighting, absorption cooling, lighter-weight vehicles, next-generation reactors, tritium production, separations, and nuclear waste management. PNNL also leverages this capability to develop advanced waste forms (e.g., glass, glass-ceramic, ceramic, metallic, and cementitious), key process control models, and tactical processing strategies to assure safe and successful immobilization and processing of nuclear wastes around the DOE complex. To support these R&D efforts, PNNL has built unique laboratory capabilities, including high- and low-dose radiological facilities, laboratories for materials synthesis and deposition, the Solid Phase Processing Demonstration Facility, the Advanced Battery Facility, Battery Reliability Laboratory, Redox Flow Battery Prototyping Laboratory, and the Solid-State Lighting Test and Analysis Facility. PNNL is currently in the early construction stage for a new OE-funded battery development facility, the GSL. Working in collaboration with academia, industry, and other national laboratories, PNNL plays a critical role in high-impact national programs, such as BES's JCESR; FE's XMAT; HFTO's Hydrogen Materials Compatibility, H2NEW, HMAT, HyBlend, and Million Mile Fuel Cell Truck consortia; and VTO's Battery500 Consortium, Lightweight Metals, and LightMat consortia.

The Applied Materials Science and Engineering capability forms the basis of PNNL's sponsor-funded research programs in metals manufacturing; electrochemical energy storage; radiation effects in materials; multiscale behavior of structural materials; integrated computational materials engineering; gas and liquid separations; electric and lightweight vehicle technology; nuclear reactor safety assessment, regulatory criteria, and life extension; and legacy waste forms. These efforts are funded by a variety of DOE programs, including the DOE-SC (BES and FES), many of the DOE Applied Energy Offices (EERE, OE, NE, FE, EM), Advanced Research Projects Agency – Energy (ARPA-E), NNSA, and the Nuclear Regulatory Commission (NRC). This capability is also leveraged in support of research programs for DoD and for the private sector through SPPs.

Health: This capability continues to be strong, with multiple publications in high-impact journals and multiple national awards. Staff continue to be recognized for their technical impact by sponsors and by the professional community. However, realizing full business growth potential is hampered by difficulties in hiring staff in rapidly growing areas, such as machine learning and electrochemical energy storage, and hiring senior leaders. There is a shortage of office and lab space, especially those dedicated to export-controlled tasks, though these will ease as staff move into ESC and GSL is completed and brought online. A high bay space that can accommodate growing capabilities in advanced manufacturing remains a need that will be relieved when the Laboratory Support Warehouse (LSW) is converted in FY 2023.

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 focused ion beam and state-of-the-art measurement systems such as the Aberration-Corrected Nuclear Scanning Transmission Electron Microscope. Mission-ready instrumentation includes suites of microscopy, mass spectroscopy detection, magnetic resonance, and specialized ultra-low-background radiation detectors; numerous specialized wet chemistry laboratories; and ultratrace radio analytical and radiometric facilities, including a shallow underground lab, providing one of the largest collections of instrumentation and expertise at any single institution in the world.

At the core of PNNL's Nuclear and Radiochemistry capability is leadership in plutonium production and waste processing knowledge (specifically in Hanford's legacy waste), forensic signatures of plutonium production, post-irradiation examination of materials, and tritium target fabrication. This includes the development and deployment of the world's most sensitive radionuclide detection systems. A system called Xenon International won awards for its engineering accomplishments and international impact. Through mitigation of the nation's nuclear waste legacy, PNNL researchers are developing new real-time sensors and radiochemical insights to enable the EM to expand waste processing operational windows, enable new treatment alternatives, and accelerate the waste processing timelines at Hanford waste treatment facilities. PNNL is also leading two international teams, one on glass corrosion and another on ancient analogs, to predict the long-term performance of glass waste forms, which are the basis for high-level waste disposal.

PNNL stewards a set of facilities unique to the DOE complex. These facilities include a Hazard Category II non-reactor nuclear facility (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 (High Energy Physics program [HEP], NP, and BES) in the search for dark matter and neutrino mass. EM depends on PNNL for rapid understanding of legacy waste behaviors, pilot-scale testing and validations, and the development of new processing options. The NNSA Office of Defense Nuclear Nonproliferation R&D relies heavily on these capabilities for next-generation nuclear detection systems, along with the Defense Threat Reduction Agency.

Health: Aggressive hiring over the last 12 months has resulted in new, high-quality staff at all levels. This portfolio is strong in applied research and operational projects; leadership emphasis now is on growing the more fundamental aspects of the research portfolio. PNNL will be upgrading the infrastructure in 325RPL to support operations with special nuclear materials. Some short-term facility gaps exist (insufficient ventilation and glove boxes to support research). Options to address shortfalls in high bay and limited purpose space are being considered as part of the new federally owned facility in the higher hazard zone of the PNNL-Richland campus.

Biological and Earth Sciences

Climate Change Science and Atmospheric Science

PNNL has extensive experience and strengths in measuring, modeling, and understanding atmospheric and climate system processes from molecular to global scales, as well as the interactions between human activities and Earth system processes. This core capability includes activities ranging from laboratory and field measurements to multiscale numerical simulations to integrated analyses of climate impacts and response options. PNNL has domain expertise in atmospheric aerosol chemistry, cloud physics, boundary layer meteorology, land-atmosphere interactions, extreme weather, climate analysis, hydrology, biogeochemistry, ecosystem science, coastal system science, energy-water-land interactions, multisector dynamics, and adaptation and resilience. We leverage expertise from related core capabilities, including Chemical and Molecular Sciences; Biological Systems Science; Earth Systems Sciences and Engineering; Decision Science and Analysis; Power Systems and Electrical Engineering; Advanced Computer Science, Visualization, and Data; and User Facilities and Advanced Instrumentation.

PNNL’s climate change and atmospheric science research focuses on improving our basic understanding of and ability to project changes in the Earth system and related human systems, and on developing the measurements and data-driven modeling frameworks needed to do so. Key facilities include the ARM user facilities, AAF, Atmospheric Measurements Laboratory, EMSL, PNNL-Sequim campus, and the JGCRI (a partnership between PNNL and the University of Maryland focused on understanding the interactions among climate, natural resources, energy production and use, economic activity, and the environment). These facilities house a wide range of world-class equipment, such as a flow-through environmental chamber, cutting-edge radar systems, and manned and unmanned aerial observational systems. PNNL is also a leading developer of atmospheric, climate, land surface, coastal, and integrated human-Earth system models, including the Global Change Analysis Model, the Weather Research and Forecasting model, and the E3SM, as well as in integrating modeling and observational systems to yield new insights into the evolution of the coupled human-environment system).

PNNL’s capability includes programs in atmospheric process research, regional and global Earth system modeling, multisector dynamics, coastal and Arctic systems research, coastal system science, and atmospheric wind energy, along with advanced computation and data management techniques. Our observational and modeling capabilities are deployed to develop a more robust understanding of how extreme events and long-term stresses influence the Earth system and human systems, especially the energy sector and national security. This core capability is funded by programs in BER, ASCR, EERE, NASA, EPA, NOAA, and other sponsors.

Health: Key leadership gaps and staffing needs continue (e.g., JGCRI Director, expertise in machine learning and artificial intelligence, and a Senior Atmospheric Scientist), and there are several open positions that are being filled. The portfolio is very strong, and equipment is good. Office space shortages are being addressed and reviewed in light of Hybrid Workplace efforts.

Earth Systems Sciences and Engineering

PNNL's Earth Systems Science and Engineering capability involves research of the impacts of energy production, storage, and use on valued environmental resources and functions; develops and deploys technologies to mitigate the impacts of past, current, and future energy production systems; and develops and deploys technologies that improve the performance of energy generation and minerals extraction. This capability spans terrestrial, aquatic, and coastal ocean systems, both biological and abiotic. Applications of our expertise include Arctic and deep-ocean oil and gas, hydropower, wind power, marine and hydrokinetic generation, algal biomass production, nuclear energy, and legacy waste.

PNNL has scientists and engineers in a variety of fields, including aquatic and terrestrial ecosystems science, oceanography, biogeochemistry, hydrology, environmental engineering, and microbiology, with domain expertise in molecular-to-field-scale biogeochemistry, laboratory-to-field-scale hydrology, multiphase flow modeling, integrated (e.g., biogeochemical, physical, and ecological) aquatic modeling, aquatic acoustics and tracking technologies, ecosystem-level adaptive management, biofouling/bio-corrosion, climate-simulating culturing of algae and higher plants, minerals extraction, ecosystems modeling and restoration, human health and environmental risk assessment, and environmental systems technology development and deployment.

PNNL's marine research laboratory in Sequim, Washington, provides coastal locations and facilities that enable studies of anthropogenic impacts on marine species and systems; a controlled study area for development and testing of marine energy systems; biogeochemical, ecotoxicological, and biotechnology investigations with ambient seawater; and a platform for development and testing of autonomous and in situ marine technologies. In addition, PNNL's distinctive Aquatics Research Laboratory supports fisheries research focused on sustainable hydropower operations and development. Advanced environmental monitors and ecological sensors for conventional hydropower, wind, marine, and hydrokinetic renewable energy systems are developed and tested at PNNL's nationally accredited Bio-Acoustics and Flow Laboratory. 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. This capability improves our fundamental understanding, model representation, and predictive capacity of critical Earth systems. PNNL is leading the COMPASS program advancing scalable, predictive understanding of the fundamental biogeochemical processes, ecological structure, and ecosystem dynamics that distinguish coastal terrestrial-aquatic interfaces (TAIs) from the purely terrestrial or aquatic systems to which they are coupled. This effort will develop predictive understanding of the causes, mechanisms, and consequences of the shift between aerobic and anaerobic conditions at both saltwater and freshwater TAIs. The Earth Systems Science and Engineering capability is funded through DOE programs in BER, BES, EM, NE, EERE, as well as NRC, EPA, DHS, Bonneville Power Administration, Department of Interior, NOAA, and the U.S. Army Corps of Engineers.

Health: The scholarly output trend has increased. The majority of staff have been at the Lab for less than 10 years. Leadership in this core capability benefits from strong partnerships, but attention is needed on leadership recruitment and development. The portfolio is moderately diverse, but risks exist, and diversification is being pursued. Significant infrastructure needs, including renovations and new laboratory spaces at the PNNL-Richland campus and the PNNL-Sequim campus, 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, biogeochemistry, multiphase flow and transport analyses, computational geochemistry, subsurface technology development and deployment, advanced geophysical and geomechanical modeling and monitoring, isotopic analyses, and high temperature and pressure geochemistry. Potential applications include enhanced oil recovery systems, the design and operation of carbon sequestration reservoirs and enhanced geothermal systems, technology development for nuclear waste repositories, and remediation of contaminant plumes.

For DOE-EM, PNNL applies an integrated experimental and modeling approach to resolve technical issues necessary to inform decisions for environmental remediation, waste management, adaptive site management, and long-term stewardship. PNNL leads the Deep Vadose Zone-Applied Field Research initiative, providing the technical basis to quantify, mitigate, and monitor natural processes and contaminants in the vadose zone and groundwater. Outcomes include advanced understanding of complex systems and the processes, features, and events controlling long-term behavior and risk, engineered solutions to remediate contaminants, and systems-based monitoring approaches for ensuring long-term performance and protection of human and ecological health.

This capability is also applied to numerous energy and water challenges, including sustainable energy generation, production, and use. PNNL led one of the world's first carbon storage projects into basalt formations, completing a 1,000-ton injection into the Grande Ronde basalt formation, and is exploring potential carbon storage in the sub-seafloor Cascadia basin basalt offshore of Washington State. PNNL has key roles in DOE-FE's National Risk Assessment Partnership and in the new Enhanced Geothermal Stimulation 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, NE, NNSA, DHS, EPA, NASA, and DoD, and have numerous active collaborations with other national laboratories and universities nationwide. Staff are located across the PNNL campuses in Richland and Sequim, including EMSL, LSL1, LSL2, the Information Sciences Building 2 (ISB)2, 331, Environmental Technology Building (ETB). Some staff on those campuses directly support capabilities, such as the Marine and Coastal Research Laboratory (MCRL).

Health: The scholarly output trend has improved. Management has actively recruited and grown new leaders and increased diversity. Portfolio diversification continues to increase. Infrastructure needs remain, including renovations and new laboratory spaces at the PNNL-Richland campus, and new equipment is needed.

Biological Systems Science

Through PNNL's Biological Systems Science core capability, the Laboratory is developing a predictive understanding of complex multicellular systems and their response to perturbation to enable improved predictions of the impacts of environmental change, energy production, and emerging technologies and biothreats on ecosystem sustainability and human health.

PNNL has made significant contributions in deciphering mechanisms of microbial community metabolic interactions and dynamics, understanding multiscale terrestrial biogeochemistry, predicting contaminant behavior and microbial ecology of the subsurface, quantifying the effects of renewable energy devices on aquatic ecosystems, and applying a systems biology approach to plant, microbial, and algal systems relevant to DOE's missions in science, energy, and environment. PNNL's Soil Microbiome SFA aims to achieve a systems-level and predictive understanding of the soil microbiome's phenotypic response to changing moisture through spatially explicit examination of the molecular and ecological interactions occurring within and between members of microbial consortia. Capabilities in microbiome science, multi-omics measurement, and computational biology are used to understand functional interactions across biological kingdoms, as well as how metagenomic information is translated to the function of microbial communities to influence the resilience and sustainability of ecosystems, bioenergy crops, and human health. Investments in synthetic biology have expanded into programmatically supported capabilities to identify novel functions of gene products within soil microbe and plant rhizosphere environments and develop strategies for the secure biodesign of engineered functions in these systems to advance BER bioenergy missions. PNNL's expertise in fungal biology has generated an in-depth understanding of the biological processes underlying efficient fungal bioprocesses that produce fuels and other chemicals. In addition, PNNL is providing insight into the development of medical countermeasures and early diagnostics, characterizing emerging pathogens, and advancing human exposure assessment to improve health and biodefense. This is particularly true for toxins with a growing capability to assess the threat from bacterial and viral pathogens.

In combination with other core capabilities—including Chemical and Molecular Sciences; Environmental Subsurface Science; Advanced Computer Science, Visualization, and Data; and User Facilities and Advanced Instrumentation—this core capability delivers expertise in microbial ecology, microbiome science, fungal biology and biotechnology, pathogen biology and biological threat prediction, systems toxicology, plant science, biochemistry and structural biology, trace chemical analysis, biomolecular separations, advanced in situ and dynamic imaging, computational biology and biophysics, and signature discovery through data analytics. PNNL's role in BER's NMDC program is also accelerating data analytics expertise for multi-omics data integration and workflows, which also enhances the EMSL User Facility capabilities. PNNL's integrative omics capabilities, widely used by the BER programs (e.g., the phenotypic response of the soil microbiome to environmental perturbations), leverage this broad suite of expertise to provide unprecedented molecular to mesoscale resolution of the function of biological systems. BER investments in advanced bioimaging capabilities at PNNL (e.g., cryo-EM, nanospectroscopy), including a program to develop a first-of-kind quantum bioimaging capability, further strengthen PNNL's effort to elucidate the structure and functions of proteins and other gene products needed to advance predictive modeling of biological systems.

This capability is funded through programs in BER, ASCR, BES, EERE, EM, DHS's Science and Technology, DoD, NIH, and NASA. Key capabilities (MCRL) and facilities supporting this capability include the Biological Sciences Facility (BSF); the Computational Sciences Facility (CSF); the Bioproducts, Sciences, and Engineering Laboratory (WSU-BSEL); the Aquatic Research Laboratory; Life Sciences Laboratory 1 (Gnotobiotic Animal Facility); the Microbial Cell Dynamics Laboratory; EMSL; and Building 331. PNNL partners with the JGI to provide large-scale genome sequencing and analysis for DOE missions. EMSL and JGI now issue an annual joint call for user projects focused on synergistic use of capabilities at both facilities, targeting collaborative science projects in biogeochemistry, carbon cycling, and biofuels.

Health: Scholarly output grew significantly. The capability has grown by 20 staff; seniority and pipeline have a good distribution. The portfolio is growing through increased programmatic support by both BER and NIH, as well as new funding from the Defense Advanced Research Projects Agency and the Defense Threat Reduction Agency. Capital equipment through internal and programmatic investments (e.g., x-ray nanotomography, Cryo-EM, quantum imaging) is expanding the bioimaging capability. Workhorse equipment that supports multiple sponsors (e.g., mass spectrometers and NMRs) is aging, and the path for replacement is unclear. Laboratory space in Building 331 is being upgraded to accommodate growth; however, space is lacking to expand toxin and opioid work, and facility modifications are required to support ventilation for biosafety cabinets.

Computational and Mathematical Sciences

Advanced Computer Science, Visualization, and Data

PNNL has depth and breadth of expertise in advanced data analytics and artificial intelligence; energy-efficient computing; performance, power, and reliability modeling; exploration and design of novel computing architectures; and runtime and system software. Specific domain areas include machine learning and artificial intelligence, predictive modeling and simulation of complex architectures, programming models, resiliency, architectural testbeds, fault tolerance, image processing, information visualization, data analytics, and data management. Our work is recognized internationally by scientific peers in areas of performance, power and reliability modeling for co-design of systems and applications, design space exploration and optimization, human-centered computing and visual analytics, and artificial intelligence. PNNL is also advancing the state-of-the-art in QIS and its application to address problems in various domains, including computational chemistry, energy resiliency, and materials science. Research that supports quantum computing, simulation, communication, and sensing is at the core of PNNL's QIS capability.

PNNL has advanced the state-of-the-art in machine learning algorithms and in their application to DOE missions such as biology, the power grid, and cybersecurity, and has developed new approaches for domain-aware machine learning to accelerate training and interpretability of classifiers as well as few-shot learning to accelerate scientific discovery. PNNL also develops new methods to characterize the robustness and security of artificial intelligence algorithms. Through the Center for Artificial Intelligence-focused Architectures and Algorithms (ARIAA), PNNL is collaborating with other research institutions to co-design core technologies to apply artificial intelligence to DOE mission priorities, such as cybersecurity and electric grid resilience. PNNL is making investments in artificial intelligence to increase scalability and interpretability, including advances in the mathematical foundations of artificial intelligence for automated reasoning, large-scale multimodal machine learning models, and research in data/model convergence to integrate the historically distinct computing platforms for HPC (particularly for its use in physical simulation), data analytics, and machine learning. Our expertise in programming models for extreme-scale computing is demonstrated through toolkits such as Global Arrays, which powers NWChem and other important scientific applications, including subsurface flow modeling code Subsurface Transport Over Multiple Phases (STOMP) and power grid modeling code GridPACK™. PNNL data scientists lead research in data exploitation, workflow, and provenance at extreme scales for science, energy, and security domains (i.e., ARM, Livewire, A2e, Project 8, and Cooperative Protection Program efforts). In the field of visualization, PNNL has developed new techniques to improve human interfaces to artificial intelligence systems, enhance situational awareness and discovery in high-throughput streaming data analytics, and interactively train and evaluate machine learning algorithms. PNNL is also making significant advances in graph analytics, including hybrid architectures for exploiting large graph datasets and algorithms for scalable graph query on multithreaded systems. Finally, PNNL has deep expertise in scientific data management, including workflow, system architecture, and database architecture; PNNL's DataHub provides secure, timely, efficient, and open access to all laboratory, field, and benchmark model data produced in the course of research, while the Data Stewardship Board and Living Laboratory provide controlled access to risk-sensitive data sets (including internal PNNL data) for use in PNNL research.

Special facilities in support of this core capability include the CENATE, an advanced architecture testbed capability for measuring performance, power, thermal effects, and cyber vulnerabilities to assess their overall potential and guide their designs; computing resources, such as the Tahoma supercomputers, the Constance institutional computing cluster, the Marianas cluster (including Tonga, an NVIDIA DGX-2 system, and Deception, a state-of-the-art NVIDIA A100 system) optimized for machine learning workloads, an experimental IBM Power9 testbed for on-ramping codes to Oak Ridge National Laboratory's Summit, and a SambaNova testbed for advanced artificial intelligence architectures; private research cloud and public cloud access through Amazon's AWS, Microsoft's Azure, and Google's Cloud Platform; testbeds for internet of things (IoT) devices and new FPGA and ARM processor-based hybrid architectures; laboratory-scale scientific data management platforms and services; and human-computer interaction research laboratories for visual interfaces, including emerging virtual reality environments. These resources are housed primarily in CSF and EMSL. This capability receives support through programs from ASCR, BES, BER, HEP, EERE, FE, NNSA, DHS, and other sponsors, including DHHS and DoD.

Health: Recruiting and retention is strong with good gender diversity; however, market competitiveness for computing talent, particularly in artificial intelligence, continues to be a challenge. Demand remains extremely high, thus hiring and retention are anticipated to remain among leadership priorities. Infrastructure and equipment are good, and recent investments in machine learning hardware have provided up-to-date capabilities.

Computational Science

Computing permeates all research domains at PNNL. The Laboratory actively employs HPC and AI/ML to solve compelling, extreme-scale scientific problems, and has a long history of developing computational tools and application codes built collaboratively by multidisciplinary teams composed of domain scientists, computer scientists, data scientists, and applied mathematicians. PNNL maintains strong capabilities across many computational science domains, including computational chemistry, computational materials science, high energy physics, computational engineering, computational biology, computational geochemistry with subsurface flow, and computational fluid dynamics, as well as climate, including participation in developing community climate codes and management of the ARM user facilities. This capability uses the state-of-the-art computing infrastructure and services provided by PNNL's Research Computing, which includes CPU/GPU supercomputers (Tahoma), computing and AI/ML clusters (Constance, Deception, Marianas), and onramp systems to optimize computational codes for DOE Leadership Computing Facilities. PNNL also has cloud access to advanced quantum systems with different qbit configurations through IBM's Quantum Network.

Multidisciplinary teams of domain and computer scientists and applied mathematicians have long been a key part of the research and innovation process at the Lab. In the area of computational chemistry, PNNL developed and maintains NWChem, a unique molecular modeling capability that dramatically advances the state-of-the-art through the development of scalable predictive methods for excitation and correlated phenomena and directly ties to experiments at DOE light sources. The software is continuously updated to incorporate new theoretical approaches and to adapt to the changing computing landscape through efforts such as the Exascale Computing Project, which includes developing NWChemEx. The exceptional scalability of PNNL's chemistry codes has resulted in DOE grants providing significant computing time and resources on Leadership Computing Facility systems and at the National Energy Research Scientific Computing Center. This Computational Science capability will be a key component of the nascent Computational and Theoretical Chemistry Institute (CTCI), a multidisciplinary effort aimed at positioning PNNL as a world-leader in scalable computational chemistry. The Northwest Quantum Nexus partnership and PNNL's participation in three of the new DOE Quantum Information

Science Centers also provide new leadership opportunities at the intersection of quantum computing with quantum chemistry with the goal of applying quantum computing in computational chemistry and materials science.

The same integrative, co-design-based approach is now being employed to develop advanced computational models at multiple length and time scales for the power grid, high energy physics, materials science, health, and climate, to name only a few. Internal LDRD investments have focused on bringing together interdisciplinary teams of data scientists, computer scientists, applied mathematicians, applied statisticians, and domain scientists to work on a wide range of DOE-relevant problems in microbiology, soil science, climate sciences, materials, renewable energy, and nonproliferation. Recently, these investments have focused on the development of novel software and hardware architectures to support scalable scientific machine learning methods that can be applied to a wide range of DOE problems.

This capability leverages PNNL's Applied Mathematics and Advanced Computer Science, Visualization, and Data core capabilities. The core capability supports sponsor-funded research by DOE-SC, including BES, BER, ASCR, HEP, FE, and NP. In addition, internal LDRD support across multiple initiatives and Agile investments also contributes to further develop this core capability.

Health: Solid project portfolios exist for all DOE-SC sponsors. The focus is now on expanding the project portfolio to include sponsors outside of DOE-SC. Workforce development efforts should focus on mid-senior hires and on continuing to improve diversity metrics. Research computing provides adequate infrastructure; however, hardware requires continuous update/upgrade plans to ensure state-of-the-art resources. Office space has been reorganized to improve collaboration, absorb planned growth, and to accommodate new modes of work resulting from the new Hybrid Workplace model.

Applied Mathematics

PNNL is a leader in applied mathematics and statistics, using mathematical models to predict the behavior of dynamic, complex systems and quantify associated uncertainty to accelerate scientific discovery. Our researchers develop novel mathematical methods for predictive modeling, uncertainty quantification, risk and decision analysis, physics-informed AI/ML, complex information modeling, data analytics, and control of complex systems. A strength at PNNL is the seamless integration of applied mathematics with computer science, data science, and domain expertise to make major impacts in national problems, such as the reliability and security of critical infrastructures.

PNNL has broad expertise in multiscale mathematics, including dimension reduction, mesoscale Lagrangian particle methods, and hybrid methods for coupling multi-physics models operating at different scales. Building on our strength in multiscale modeling, we develop capabilities in domain-aware machine learning, as well as physics-informed methods for parameter estimation and uncertainty quantification. These techniques focus on solutions for nonlinear and high-dimensional systems and include surrogate and multi-fidelity modeling for both forward prediction and inverse models. In addition, PNNL develops strategies to generate scientifically interpretable mathematical models that are capable of reasoning over numerous complex scenarios defined by partial information and partial model understanding. The integrated use of mathematical or statistical techniques—such as uncertainty quantification, machine learning, signature discovery, causal reasoning, and game theory—enables domain scientists to generate novel hypotheses in both static and streaming applications.

PNNL develops operational models focused on resource utilization and risk assessment via simulation, optimization, and mathematical programming. In addition, PNNL is growing capabilities in distributed and hierarchical decision systems, reinforcement learning, verifiable machine learning based control, and concurrent system and control design for safety-critical systems.

PNNL pursues innovative research in the analysis and integration of complex, high-dimensional data. Our mathematicians also advance computational methods rooted in topology, algebra, geometry, hypergraph theory, and applied category theory. We use these methods to build novel representations of tabular, relational, and time-series data, aimed at synthesizing quantitative and qualitative information with complex, multi-way dependencies. Applications include sensor fusion, anomaly detection, and visualization of complex data for critical problems in cybersecurity, computational biology, geolocation, and open-source data analysis. PNNL also has an emerging capability in the applications of discrete mathematical techniques to a range of problems in the DOE mission space to solve crosscutting problems of national interest. PNNL is heavily invested in solving issues related to large-scale graph analysis, time evolution of discrete structures, and the development of network invariants and their applications. PNNL researchers leverage emerging capabilities in QISs to develop algorithms for combinatorial optimization.

This core capability supports sponsor-funded research by DOE-SC, including BER and ASCR, as well as government funded innovation and technology transfer programs such as Small Business Innovation Research/Small Business Technology Transfer. Most of the applied mathematics research related to AI/ML is currently funded by internal LDRD investments, such as Data-Model Convergence (DMC) and Mathematics for Artificial Reasoning in Science (MARS), as well as from external sponsors, such as DOE-ASCR, DoD, and NNSA.

Health: A solid project portfolio, which is focused on DOE-SC with an emerging presence of other sponsors such as DoD and NNSA. There are well-established national partnerships; the focus is now on expanding collaborations to include international partners to increase visibility and leadership. Research computing provides adequate infrastructure to support computational mathematics research; however, hardware requires continuous update/upgrade plans to ensure access to state-of-the-art resources. Office space has been reorganized to improve collaboration, absorb planned growth, and accommodate new modes of work resulting from the new Hybrid Workplace model.

Cyber and Information Sciences

The Laboratory conducts research and develops technology that brings scientific approaches to cyber operations and defense, giving the United States a strategic advantage in the cyber domain. PNNL's work enables cyber resilience for U.S. critical infrastructures, based on expertise in the development and implementation of advanced sensing techniques, analytic algorithm development to increase automation and machine speed defense, and the design of resilient control systems. Research, engineering, and analysis staff are nationally and internationally recognized in cybersecurity resiliency theory, the development of secure design principles for control systems, cyber analytics, graph theory, machine learning, text and multimedia analytics, statistics, and emerging techniques for human-machine teaming.

PNNL's cybersecurity expertise spans IT, industrial control systems, operational technology, and the IoT. The Laboratory's cybersecurity portfolio is based on the intersection of its data science and threat intelligence capabilities, including work to develop cybersecurity sensors for wide-scale network intrusion monitoring and situational awareness (this includes the operation of the Cooperative Protection Program for DOE complex cyber defense and CRISP, a voluntary information sharing and threat intelligence program for the energy sector). PNNL has developed unique expertise in the scientific and mathematical foundations of cybersecurity, including leadership in biologically inspired cybersecurity, multiscale graph methods for active cyber defense, critical infrastructure resiliency analysis and modeling, supply chain security, vulnerability assessment, and integrated cyber and physical security. An emerging area of focus is in autonomous resilience in cyber systems through the convergence of PNNL's artificial intelligence and cybersecurity expertise, including predicting and mitigating the consequences of failures across linked cyber and physical systems. PNNL has also developed a research-to-operations model for cybersecurity, in which its cybersecurity research staff and internal cybersecurity operations staff partner closely to use PNNL-developed analytic and security solutions to defend PNNL from cyber threats, as well as use PNNL's operational expertise to inspire the next generation of cybersecurity technologies.

PNNL's information science expertise is in areas of data acquisition and management (e.g., experimental design, analytic pipelines, provenance, and quality assurance), analytics and algorithms (e.g., streaming and graph analytics and scalable machine learning), and decision support (e.g., novel visual interfaces, 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 and natural language processing to improve analytic quality and efficiency. PNNL maintains a world-class capability in natural language processing and computer vision. PNNL has significant expertise in developing effective data science/domain science partnerships to apply machine learning to accelerate discovery across all its missions.

Major computing resources that support this capability include research computing resources, such as 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, IoT Common Operating Environment, the Visualization and Interaction Studio, the Machine Learning Studio, and the Electricity Infrastructure Cyber Security/Resilience Center support this capability. External collaborations include industry, academic, and governmental partners from across the nation and around the world. Primary sponsors for PNNL's Cyber and Information Sciences research include ASCR, OE, DoD, DHS, and Strategic Intelligence Partnership Program sponsors.

Health: Demand for this core capability remains very strong. Aggressive hiring among early-career cyber and data scientists has improved the staffing situation; however, additional attention is still required for mid- to senior-level hires. The demand, coupled with continued strong competition for talent with relevant hot skills and the associated high compensation levels, makes this core capability one of several being addressed through intensive recruiting and cross-training. Currently, there is insufficient federally owned office and laboratory space for research in data science and cybersecurity.

Decision Science and Analysis

PNNL maintains strong capabilities in modeling, analyzing, communicating, and mitigating crosscutting impacts at the interface between science, technology, policy, and society. Working collaboratively with scientists and engineers across the Laboratory and with external partner organizations, our experts continue to develop and implement innovative, resilient, and holistic solutions to complex decision problems on the front lines of the nation's energy, environment, and national security challenges.

PNNL's staff expertise is focused on the areas of decision science, risk analysis, economics, systems engineering, decision support systems, operations research, policy analysis, social and behavioral science, statistics, and safety analysis. This capability enables the development and application of cutting-edge decision and risk analysis; safety, impact, and risk assessments; resilient decision-making under uncertainty; alternatives analysis; strategic process/systems improvements; and operational decision support. Additional modeling and analysis capabilities include socioeconomic modeling, market and policy analysis, techno-economic modeling and analysis, regional and national energy simulation, and cost-benefit analysis and uncertainty analytics. The team's breadth and depth of decision and risk analysis expertise fosters flexibility in assembling dynamic, multidisciplinary teams to develop science-based strategies for minimizing risks to individuals or the public, program life cycles, facility designs and operations, and the environment at the local, state, regional, national, and global levels.

Staff that support this capability at the Laboratory are located in several locations in Richland, including ISB1, ISB2, the Engineering and Analysis Building, MATH, and the National Security Building, as well as the PNNL offices in Portland, Oregon, and Seattle, Washington. They are recognized in the areas of nuclear and alternative energy; operational safety review and risk assessment; technology testing, evaluation, and performance assessment; technical and programmatic risk assessment; geo-spatial decision analytics and visualization; geointelligence; nuclear proliferation risk modeling; knowledge management and data reuse; multi-organizational collaboration decision support; distributed decision-making for power grid reliability; energy policy and regulatory development/deployment; appliance and commercial equipment energy efficiency codes and standards; and feasibility analyses of technology, siting, policy, and tax structures for energy technology deployment. Leadership in safety assessment, probabilistic risk assessment methodology development and application, environmental impact assessment, and analyses and feasibility assessments for nuclear, geothermal, hydropower, and other sustainable energy technologies, such as hydrogen-powered vehicles, are specific strengths. Current stakeholders that primarily use our capabilities include DOE (EERE, OE, EM, FE, and NE), NNSA, DHS, DoD, EPA, Bonneville Power Administration, and NRC.

Health: Portfolio and equipment are good. However, 33 percent of staff are early career, and another 17 percent are retirement eligible; recruitment and retention remain a matter to watch.

Engineering

Biological and Bioprocess Engineering

PNNL is developing technologies and processes that create opportunities from ecological and economic liabilities by leveraging the capabilities in Biological and Bioprocess Engineering. These capabilities are critical to realizing energy and industrial decarbonization by sustainably converting biomass and carbon-containing waste materials into fuels and chemicals. Potential carbon feedstocks include food wastes, sewage sludge, municipal solid wastes, polymers, industrial wastes, lignocellulosic materials (e.g., agricultural residues and wood wastes), and algae. This capability is strengthened through collaboration with Laboratory expertise in our Earth and Biological Sciences Directorate for biological processes and PNNL's unique approach to integrating biological processing with catalysis and reaction engineering from the Institute for Integrated Catalysis; separations, process engineering, and process flow and system analysis; materials science; and techno-economic modeling. The capability also benefits from strong collaboration with external partners through the WSU-PNNL Bioproducts Institute and several Bioenergy Technologies Office (BETO) and BER consortia, including the Chemical Catalysis for Bioenergy Consortium, Feedstock-Conversion Interface Consortium, Bioprocessing Separations Consortium, Agile BioFoundry, and the Joint Bioenergy Institute.

PNNL successfully leverages cross-directorate capabilities in multi-omics and computational biology combined with fungal genetic engineering and bioprocess engineering to enable dramatic improvements in organisms and process conditions to achieve industry-relevant rates for the production of renewable bioproducts and chemical precursors. In addition, we have advanced hydrothermal liquefaction for conversion of wet feedstocks to products, catalytic hydrotreating of bio-oils to fuels, conversion of renewable carbon-derived alcohols to jet fuels, and conversion of intermediates to chemical products. PNNL's capabilities for processing of biomass and wastes span from high-throughput catalyst screening, to benchtop reactors, to foundry-scale reactors for next-generation conversion technologies. PNNL houses unique indoor, climate-controlled raceway ponds and photobioreactors that can cultivate microalgae strains under conditions that simulate outdoor ponds at any geographic location in the world. The capability also includes a unique Biomass Assessment tool that can quantify potential resource supplies, infrastructure connectivity, and biomass production from microalgae and waste feedstocks.

This capability primarily supports the research mission of BETO and is also utilized by BER, AMO, and others. Current applied research focuses on fungal genetic and bioprocess engineering to produce desired bioproducts from lignocellulosic or organic wastes. This pursuit is accelerated by implementation of the design-build-test-learn approach, which also leads to a fundamental understanding of biological conversion processes captured in a genome-scale modeling framework. Scaling bioprocesses up to pre-pilot volumes demonstrates the bioprocess technologies, paving the way for technology transfer to industry for commercial application.

A recent example of the Lab's success in technology transfer leveraging this capability is the PNNL-developed alcohol-to-jet process that has been licensed to LanzaTech to enable the production of jet fuel from alcohol derived from industry flue gases using fermentation followed by thermochemical processing. Through the PNNL-LanzaTech partnership, the jet fuel has been certified by the American Society for Testing and Materials for commercial use, and the first transatlantic flight utilizing a waste-gas derived jet fuel was flown by Virgin Atlantic.

Health: This capability remains strong, and technical accomplishments such as the development of the alcohol-to-jet process continue to receive national attention (2020 IRI Technology Achievement Award). The Biological Processing portfolio grew in FY 2021, and we expect it to continue to expand in FY 2022. Publication and patent records are solid. The pending retirements of several senior technical experts requires thoughtful succession planning, and a hiring plan to address this challenge has been developed. Although this capability is primarily supported by one DOE office, there are an increasing number of potential research sponsors.

Power Systems and Electrical Engineering

PNNL has internationally recognized capabilities spanning the entire electric power grid. Staff at PNNL have deep expertise in the grid's transmission and distribution networks, reliability and resilience, smart grid and intelligent systems, distributed energy resources, market systems, and energy demand. PNNL develops innovative solutions to addressing emerging challenges facing today's power industry through better planning, operating, and controlling of modern power grids for enhanced resilience and reliability as well as decarbonization. Primary supporting disciplines include power system, electrical, and control engineering; computational science and software engineering; cybersecurity; data analysis; and mechanical engineering. With a focus on system-level issues, PNNL is the national leader in defining a decarbonized, resilient power grid of the 21st century, delivering innovative tools to enable unparalleled grid performance (resilience, reliability, security, transparency, efficiency, and sustainability) and new control and architecture paradigms spanning future demand and supply for unprecedented consumer engagement.

Key research areas include grid architecture, transmission and distribution system reliability and control analysis, power system protection, advanced grid data applications, computing and visual analytics, renewable resource integration, energy storage, distribution system modeling, power system economic analysis, and grid cybersecurity. PNNL's expertise in grid simulation and analytics enables high-performance grid monitoring and control at an unprecedented speed, from minutes to sub-seconds. For over a decade, PNNL has led the world in the development and application of transactive systems that combine economics and controls to enable distributed optimization and integration of distributed energy resources, including controllable loads, batteries, and renewable generation. PNNL's expertise in advanced control theory, application, and testbeds supports advancements in the development of new, distributed controls for the electric power system. PNNL's leadership in phasor measurement technologies supports broader national deployment, enabling unprecedented grid visibility and enhanced situational awareness. PNNL's one-of-a-kind, utility-grade control center infrastructure supports research in grid visibility, control, and resiliency, with the largest national repository of grid data and models to inform research.

This research is made possible with the use of the EIOC, the Interoperability Laboratory, and the Power Electronics Laboratory. These laboratories and facilities support world-class commercial tools, as well as PNNL-developed tools, including the following: the GridLAB-D™ open-source simulation and analysis tool for designing and operating power distribution systems, the GridAPPS-D open-source platform for advanced distribution system planning and operations application development, the GridPACK open-source package for parallelizing power grid simulations, the VOLTTRON™ open-source software platform enabling grid-interactive efficient buildings, the R&D 100 award-winning Dynamic Contingency Analysis Tool 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, water power, solar energy, wind energy, hydrogen storage, building technologies, and fuel cell technology); DOE Office of Cybersecurity, Energy Security, and Emergency Response (CESER); ARPA-E; DHS; ASCR; DoD; the U.S. Department of State; and private industry.

Health: Aggressive hiring will continue for the foreseeable future, with 30 staff hired over the past 12 months to support a diverse and growing portfolio of sponsors. PNNL continues to be assigned leadership roles on major DOE initiatives, such as NAERM, GMLC, and the Energy Storage Grand Challenge. While senior hires are helping to backfill key thought leaders who have retired, there is a continued need for both mid-career and additional senior hires. Office space pressure has been reduced by planned acquisition of additional space in Seattle and temporary work-from-home orders; future space sufficiency depends upon effective space management and implementation of lab-wide flexible work strategies. The EIOC continues to be a distinguishing capability to attract leadership roles in DOE programs, as does the transactive campus with the addition of thermal storage and new battery installations. Additional distributed grid assets (e.g., photovoltaics, energy storage, inverters, smart building loads, and advanced metering infrastructure) are needed to advance next-generation controls work at scale.

Systems Engineering and Integration

PNNL is internationally recognized for systems engineering and integration through the implementation of technology in real-world complex systems focusing on smart and robust nuclear and radiological security and energy systems optimization and integration. This core capability has solved some of the most challenging national problems by defining and interpreting complex technical requirements and translating them into fieldable solutions that address economic, social, policy, and engineering considerations. Using a structured approach to understand complex systems throughout their life cycle, PNNL applies its domain knowledge and experience in engineered systems simulation and modeling; system architecture and design; test, evaluation, and optimization; technology assessment, integration, and deployment; policy assessment and economic evaluation; and regulatory analysis, risk assessment, and decision support. This allows our staff to effectively take early-stage research through the development and technology maturation processes and to deploy technical solutions that address our sponsor's most critical challenges.

PNNL proactively engages with other national laboratories and industry to define best practices for applying systems engineering in early-stage R&D, and applies a graded approach to our systems engineering discipline that enables us to deliver solutions in a highly efficient, effective way. PNNL is known worldwide for effectively field-deploying international nuclear materials safeguards, nuclear and radiological security, and complex radiation detection systems. PNNL is also known for leadership in integrated building energy technologies, including advancing solid-state lighting, advanced building control, and building-grid integration technology. Further, PNNL is recognized nationally for the rigorous analyses that support building energy code development and enable DOE to fulfill statutory requirements related to appliance standards. Lastly, PNNL is widely known for advancing national power grid reliability and smart grid technologies.

Staff members are housed in facilities that include the Systems Engineering Building (SEB), EIOC, System Engineering Facility, 2400 Stevens, Engineering Development Laboratory, APEL, Radiation Detection Laboratory, and the Large Detector Test Facilities. The Systems Engineering and Integration capability is funded through programs in BES (design and operation facilities), BER, HEP, NP, EERE (buildings and transportation), EM (waste processing and nuclear materials disposition), OE (infrastructure security and energy restoration), FE (carbon and co-sequestration), NNSA (nonproliferation and safeguards), DHS (radiation portal monitoring and critical infrastructure and analysis), NRC, EPA, and DoD.

Health: Staff, portfolio, infrastructure, and equipment are all healthy. Increased recruiting support is needed to meet aggressive hiring targets in this space. There is some need for additional high bay space and dedicated facilities for testing and evaluation.

Chemical Engineering

PNNL's Chemical Engineering capability translates scientific discovery into innovative, first-of-a-kind processes to solve tough energy and environmental challenges for DOE and other stakeholders. PNNL develops materials, catalysts, unit operations, and integrated chemical processes at scales ranging from molecular interactions to engineering-scale experiments to full-scale demonstrations that can be transferred to the sponsor or to industry for commercialization. The processes are designed for industry-relevant geometries and scales with typical operations over extended periods of time. PNNL's competency in this area includes chemical engineers and related disciplines specializing in catalysis and reaction engineering, gas and liquid phase separations, heat exchange, process intensification, fluid dynamics and mixing, thermal-mechanical modeling, electrochemistry, flowsheet development and modeling, and techno-economic analyses. Nuclear waste treatment (from milligram to ton-scales) is another area of expertise, encompassing slurry transport and mixing, glass melting, advanced rheology, and fluid dynamics for complex multiphase systems.

Examples of how PNNL successfully applies its Chemical Engineering capabilities include the invention and development of affordable, scalable processes for CO_2 capture and utilization, biomass and waste carbon conversion to fuels and products, hydrogen production and liquefaction, liquid organic hydrogen storage and release, catalytic automobile emissions control, novel heat pumps to increase energy efficiency, magnetocaloric liquefaction of hydrogen and other industrial gases, micro-channel-based reactors and separations systems for high-efficiency chemical conversions and solar-aided natural gas reforming, solid oxide electrolyzers and fuel cells, and the development and application of software to predict the thermal and structural performance of spent nuclear fuel storage and transportation systems. Working in collaboration with academia, industry, and other national laboratories, PNNL has a leadership role in high-impact national programs, such as DOE AMO's Rapid Advancement in Process

Intensification Deployment (RAPID) Institute, BETO/VTO's Co-Optimization of Fuels and Engines Consortium, H2@Scale, H2NEW, HyMARC, FE's Carbon Capture and Simulation Initiative (CCSI2), and VTO's Cross-Cut Lean Exhaust Emission Reductions Simulation (CLEERS) initiative.

This core capability supports sponsor-funded research by DOE-SC (BES), as well as many of DOE's Applied Energy Offices (EM, EERE, FE, and NE), NNSA, and ARPA-E. PNNL's Chemical Engineering core capability is also leveraged in support of research funded by DHS and DoD. Current research focus areas include CO_2 capture and utilization from point and distributed sources; large-scale clean hydrogen production, storage, and liquefaction; biomass, carbon waste, and fossil fuel conversion to fuels and chemicals, as well as subsequent fuel upgrading; nuclear waste processing and immobilization; and cost-effective startup and operation of the Hanford Waste Treatment Plant.

Health: Publication record continues to be strong, with increasing numbers of articles in high-impact journals. Equipment is adequate, though appropriate lab space, to include high bay space, continues to be tight and puts future capability growth (e.g., the development of a catalysis process development unit) at risk. The new ESC building will upgrade and expand catalysis development labs, but high bay space continues to be a challenge. Attracting diverse and qualified candidate pools to fill job vacancies is a challenge in this area, though the quality of new hires remains high.

Nuclear Engineering

PNNL has expertise in complex irradiation systems that support materials science, tritium production, advanced fuel modeling, and reactor production analysis. Research staff members have broad and deep technical skills across the full spectrum of nuclear engineering disciplines, including reactor physics, mechanical design, thermal-mechanical analysis, fluid dynamics, heat transfer criticality safety, nondestructive evaluation, and robotics, as well as materials science and microscopy. PNNL applies these skills in radiological facilities (e.g., 325RPL) to characterize and understand irradiation effects on materials through post-irradiation examination, and to make precise measurements and analyses that enable nuclear archaeological assessments. In addition, PNNL has experimental testing capabilities that enable the design, development, and fabrication of advanced, accident-tolerant fuel for commercial reactors and low-enrichment fuel for research reactors, as well as the design, modeling, fabrication, and deployment of complex irradiation tests to evaluate nuclear materials.

PNNL is specifically recognized for the development of the Graphite Isotope Ratio Method, which is the world's most accurate estimation tool for graphite reactor operational history, and has a deep expertise in proliferant plutonium production, from reactor irradiation to plutonium metal. This year, a significant effort went in to expanding our support for NNSA's defense programs. PNNL is the design authority for tritium production targets, and this year we successfully addressed significant quality assurance program concerns that could impact tritium supply. The combination of thermal, nuclear, and structural skills is also used to evaluate spent nuclear fuel storage and transportation options. PNNL is currently testing high burn up spent nuclear fuel to assure the continued safe dry storage at nuclear power plants across the nation.

A wide range of sponsors rely on PNNL's Nuclear Engineering capability. These include BES, who relies on PNNL to understand the benefits of modeling interfacial dynamics in radioactive environments and materials. The NRC relies on PNNL expertise to evaluate and confirm the thermal performance of nuclear systems as well as develop new techniques for nondestructive evaluation to extend the life of existing reactors. This strong knowledge base and expertise in the commercial nuclear industry enables the design of targets for isotope production and fuel performance modeling to develop or evaluate fuels for use in NRC-regulated commercial or research reactors. PNNL's Nuclear Engineering capabilities also support NE's missions and objectives, including the Versatile Test Reactor program, based on our historical expertise with the fast reactors. NNSA's defense programs rely on nuclear engineering to understand the production of materials for the nuclear deterrent, most notably tritium. NNSA's Office of Defense Nuclear Nonproliferation supports the understanding of future reactors and their impact on nuclear proliferation.

Health: Aggressive hiring over the last 12 months has brought on high-quality staff at all levels; however, we still have demand for more, especially with enhanced clearances. The current portfolio, while strong, is operationally focused and needs to be expanded and/or balanced with more research. Equipment is of high quality but is operating at full capacity. Some additional infrastructure needs at 325RPL (e.g., recapitalizing acid-compatible glove boxes and fume hoods, general building maintenance) have been identified.

User Facilities and Advanced Instrumentation

Environmental Molecular Sciences Laboratory

As one of BER's national scientific user facilities, EMSL leads molecular-level discoveries for BER and DOE that translate to predictive understanding and accelerated solutions for national energy and environmental challenges. Our vision is to provide a predictive understanding of dynamic molecular transformations underpinning biological and ecosystem functions. Research in EMSL focuses around three science areas: 1) Functional and Systems Biology; 2) Environmental Transformations and Interactions; and 3) Computing, Analytics, and Modeling. Within each of these thematic areas, EMSL scientists partner with users from around the world to explore critical questions in BER relevant science.

The Functional and Systems Biology area focuses on understanding and harnessing enzymes and biochemical pathways that connect genotypes to complex phenotypic responses through a deep understanding of interactions within cells, among cells in communities, and between cellular membrane surfaces and their environment for microbes, fungi, and plants. This understanding encompasses experimental observations, metabolic reconstruction, and biosystems modeling leading to improved strategies for designing plants, fungi, and microbes for biofuels and bio-based products, as well as unraveling the complexities of carbon, nutrient, and elemental cycles within cells and their immediate environment.

The Environmental Transformations and Interactions area focuses on the mechanistic and predictive understanding of environmental (physiochemical, hydrological, biogeochemical), microbial, plant, and ecological processes in above- and below-ground ecosystems, the atmosphere, and their interfaces. EMSL provides the experimental, data analytics, modeling, and simulation expertise to investigate and model the cycling, transformation, and transport of critical biogeochemical elements, contaminants, and atmospheric aerosols. Coupled experimental and modeling approaches will accelerate understanding of the mechanisms and dynamics of processes, their interdependencies, and feedbacks at molecular to ecosystem scale.

The Computing, Analytics, and Modeling area focuses on combining advanced data analytics and visualization and computational modeling and simulation with state-of-the-art experimental data integration to develop a predictive understanding of biological and environmental systems. Our cohesive approach to integrating experimental and computational methods advances predictive approaches to biodesign for biofuel/bioproduct production and accelerates research to understand the molecular mechanisms underlying biological and hydro-biogeochemical processes controlling the flux of materials (e.g., carbon, nutrients, and contaminants) in the environment.

PNNL is recognized for its ability to conceive, design, build, operate, and manage world-class scientific user facilities, and is known internationally for its advanced instrumentation designed to accelerate scientific discovery and innovation. As an example, PNNL demonstrated this ability with the development, design, construction, and deployment of the 21T Fourier-Transform Ion Cyclotron Resonance (FTICR) mass spectrometer. As new capabilities are developed, special calls for first science applications promote rapid and effective utilization of these new tools. EMSL is active in leveraging its capabilities with other DOE user facilities to maximize the scientific community's ability to address critical challenges in biology, environment, and energy. As an example, EMSL jointly sponsors user calls with JGI and ARM through BER's FICUS initiative. The EMSL-JGI FICUS calls have been used to maximize DOE's genomic/transcriptomic and other omics capabilities, as well as EMSL's chemical and physical measurements for breakthroughs in systems biology. The EMSL-ARM FICUS call enables investigation of aerosol processes or aerosol-cloud interactions by studying the physical, chemical, optical, and microphysical properties of aerosols, including biological particles to develop a process-level understanding of the formation, transport, and evolution of aerosols and their impact on warm and cold cloud formation, and ultimately improve Earth system models. EMSL also partners with other user facilities via the FICUS initiative, such as the BES-funded Bio-SANS beamline at the High Flux Isotope Reactor and the National Ecological Observatory Network (NEON). In addition, EMSL collaborates with other user facilities through the new Society for Science at User Research Facilities.

Health: The quality of staff and the research portfolio are both strong. Research equipment health remains strong. A strategic science plan is guiding future equipment acquisition and scientific capability development efforts. The EMSL roof is nearing the end of its useful life and plans for replacement are in process. Planning is in process for the use of space that will be available when Physical and Computational Sciences Directorate staff move to the ESC. Additional planning for renovations to the HPC space for future expansion of BER computing capabilities are in process and are focused on cooling and electrical upgrades to accommodate the increased demands.

ARM User Facility

The world's premier ground-based observations facility for atmospheric science research, ARM is a DOE user facility that provides a global network of instrumented fixed-location, mobile, and aerial observatories for obtaining cloud and aerosol measurements, as well as precipitation, solar and thermal radiation, surface heat and moisture, and meteorological conditions. ARM observatories are deployed to diverse meteorological regimes around the world where there are critical science questions and deficiencies in global-scale models. Fixed-location observatories are in the U.S. Southern Great Plains, the North Slope of Alaska, and Graciosa Island in the Eastern North Atlantic. Diverse data sets are being incorporated into integrated products for evaluating high-resolution atmospheric process models and large-scale Earth system models, such as the DOE E3SM Model.

To accelerate model development and associated atmospheric process studies, ARM is working to bridge the scale gap between ARM observations and global Earth system models by expanding capabilities at ARM observatories. The first test of this new strategy has been at the Southern Great Plains observatory, where ARM has developed a framework that combines high-resolution model simulations with ARM observations. The ARM observations provide three-dimensional constraints to the model as well as a test of model output. The combination of the ARM observations with the high-resolution model output and associated diagnostics provides a more complete representation of the ARM site domain, enabling broader use of the data by the scientific community. ARM has now begun to apply this modeling framework to study deep convection. This second application of the modeling framework makes use of measurements from the Cloud, Aerosol, and Complex Terrain Interactions (CACTI) field campaign, held in Argentina from October 2018–April 2019.

ARM continues to deploy mobile facilities as approved through the user proposal process. In FY 2022, the first and second ARM mobile facilities will be deployed in the continental United States. The first facility is deployed near Houston, Texas, and will focus on the interaction of aerosols and deep convection. The second facility is deployed in the Rocky Mountains, near Crested Butte, Colorado, and will focus on the interaction of atmospheric processes and mountain hydrology.

The AAF is undergoing a period of change, as the G-1 aircraft, which served ARM from 2010–2018, has been retired and the process of implementing a Bombardier Challenger 850 regional jet as the new ARM research aircraft is underway. The Challenger 850 is currently undergoing a modification project that includes the addition of mounting points for scientific instruments and an extensive reworking of the aircraft interior to provide power, communications, mounting systems for research equipment, and workspace for researchers.

PNNL leads the development of UAS capabilities within ARM. PNNL manages and operates a very capable mid-size UAS, the ArcticShark, that can carry payloads of up to 100 pounds as high as 18,000 feet for periods of up to eight hours. The ArcticShark underwent modifications and testing in FY 2021 and was cleared to return to flight. The AAF team is currently undergoing a series of training exercises in preparation for research flights focused on aerosols at the ARM Southern Great Plains observatory.

PNNL is responsible for the overall technical direction of ARM's scientific infrastructure through leadership of a collaboration among nine DOE laboratories. PNNL has lead responsibility for a variety of facility components, including the management and operation of the AAF and related operations, technical leadership for various instruments and data product development processes, and communications. This capability is funded by BER.

Health: The Challenger 850 modification contract is in place and underway. In FY 2021, the FAA identified the Challenger 850 modification project as significant. The significant modification determination triggered possible new design requirements, a resubmission of the project plan, and an extended review by the FAA. The AirARM team is currently working through these issues with the modification contractor team. Having passed a series of flight tests, the AAF team is now preparing for the first science flights with the ArcticShark to be conducted at the ARM Southern Great Plains site in FY 2022. Earlier this year, the AAF team partnered with Mississippi State University to test the ArcticShark's instrument payload on the Mississippi State University Tigershark platform in a series of successful flights over the Southern Great Plains site. The radar engineering team continues to seek high bay space and field test sites to support radar maintenance between deployments. The team has identified an interim solution for high bay space. The portfolio is strong and staffing is in good shape, with the addition in FY 2022 of a new lead for radar data analysis.

Science and Technology Strategy for the Future/Major Initiatives

Scientific Vision

PNNL advances the frontiers of knowledge, taking on some of the world's greatest S&T challenges. Distinctive strengths in chemistry, Earth sciences, biology, and data science are central to our scientific discovery mission (Figure 2). PNNL's research drives innovation that advances sustainable energy through decarbonization and energy storage and enhances national security through nuclear materials and threat analysis.

Our strategy is described by the six Major Initiatives presented in this section of the Laboratory Plan. Each of these Major Initiatives describes our intent to leverage our distinctive strengths to address a major science or technology challenge. These challenges are of importance to one or more of PNNL's primary missions of scientific discovery, sustainable energy, and national security. Of note this year is the strong alignment of our strategy with national decarbonization objectives.

PNNL's first Major Initiative, **Catalysis for Renewable Carbon and Hydrogen**, leverages PNNL's long-standing strength in chemistry. This Major Initiative will advance our understanding of catalysis, chemical pathways, and materials synthesis in ways that will enable decarbonization of hard-to-electrify aspects of our energy systems. While this effort is focused on scientific advances, we will also strive for benefit in areas such as transportation fuels focusing on sustainable aviation fuel, clean hydrogen production, quantum information systems, energy storage technology, and microelectronics.

Our **Predicting the Evolution of the Multiscale Earth System** Major Initiative will advance the science necessary to improve the range and confidence of future Earth system models. This requires that we improve our ability to resolve the complex details of how elements of the Earth system interact across an immense range of scales. Our research will inform efforts to enhance the resilience of human and natural systems and enable more confident evaluation of the consequences of decarbonization decisions.

Our **Understanding, Predicting, and Controlling the Phenome** Major Initiative will deliver an understanding of how the phenome of a microbe or microbial community is defined by its genome and its environment. Our approach derives functional information from examining the relationships between proteins, metabolites, their associated genes, and the environment. Our success will allow us to design biological systems that provide new avenues to decarbonization, and improve the bioeconomy, biosecurity, and human health.

PNNL's final science Major Initiative, **Machine Reasoning for Scientific Discovery**, strives to provide a scalable machine reasoning capability that will accelerate scientific discovery. Our approach will require the integration of data acquisition, domain models, reasoning systems, and advanced hardware to transform system performance. While our focus will be on advancing the necessary scientific foundations, we intend to apply this capability to advance discovery for important problems in chemistry, Earth science, and life science.

The Major Initiative centered on PNNL's sustainable energy mission is **Grid Control and Energy Storage.** This Major Initiative will address two challenges of critical importance for decarbonizing the energy system. First, PNNL will design and demonstrate advanced grid sensing and control technology that will enable dramatically higher levels of electrification and carbon-free generation. Second, PNNL will develop and deploy grid-scale energy storage technology as required for a future grid that is flexible and resilient.

PNNL's final Major Initiative focused on our national security mission is **Accelerating Development and Qualification of Nuclear Materials Processing.** We intend to revitalize the national ability to produce nuclear materials by leveraging strengths in material science, process monitoring, and materials characterization. Our goal is to deliver a science-based understanding of nuclear materials processing systems that enables confident model predictions. Not only will such understanding accelerate development and qualification timelines, but it will enable more rapid incorporation of emerging innovation to the benefit of national security and nuclear energy.

Infrastructure

Overview of Site Facilities and Infrastructure

PNNL is based in southeastern Washington State, in the city of Richland, with buildings on the Laboratory's main campus and in the 300 Area of the Hanford Site. PNNL also conducts operations in Sequim, Washington, and satellite locations in Seattle, Washington; Portland, Oregon; and College Park, Maryland.

PNNL's strategy for providing mission-ready F&I planning is underpinned by four goals and guidelines detailed in our PNNL-Richland Campus Master Plan and PNNL-Sequim Campus Master Plan.

- Maintain a ready-to-serve, mission-ready campus
- Increase federal ownership of the campuses and facilities, and reduce dependance on third-party leasing
- Leverage local support for utility infrastructure and services, fire, police, and emergency response capability
- Invest in F&I to increase resiliency and maintain current low deferred maintenance.

Mission-Ready, Federally Owned Campuses. The existing F&I are foundational to enabling the research mission at PNNL. PNNL's integrated approach to maintaining and renewing the existing assets across campus takes a wholistic approach informed by ICM, operations, research, and planning organizations. PNNL's integrated planning approach is designed to forecast, plan, and execute a variety of projects identified below that complement the seven planning objectives above.

- Repurpose Guesthouse ($2M – IGPP, project initiated in FY 2021)
- BIL Boilers Replacement ($640K – SLI-GPP, project initiated in FY 2021)
- 3425 Secondary Vestibule Installation ($700K – IGPP-Other, project initiated in FY 2021)
- Remodel LSL2 Labs 404-424 to Support Exit of Off-site Lease ($6.2M – IGPP, project initiated in FY 2021)
- BSF-CSF Cooling Tower ($550K – IGPP, planned to be initiated in FY 2022)
- LSL2 Lab Materials Research Modification ($560K – IGPP, planned to be initiated in FY 2022)
- PDLE High Bay Modification ($800K – IGPP, planned to be initiated in FY 2022)
- Seattle ESF Modification ($1.2M – IGPP-Other, planned to be initiated in FY 2022)
- PSL Chemistry and Lighting Research Modification ($2M – IGPP, planned to be initiated in FY 2022)
- Campus Experience ($2M – IGPP, planned to initiate in FY 2022)
- Repurpose BIL ($4.3M – IGPP, planned to initiate in FY 2022)
- Battelle Auditorium (AUD)-PSL Steam to Hydronics Conversion ($7.7M – SLI-GPP, planned to initiate in FY 2022)
- LSW High Ceiling Laboratory Conversion ($5.7M – IGPP, planned to be initiated in FY 2022)
- CSF Lab 1812 Conversion ($650K – IGPP-Other, project planned to initiate in FY 2023)
- 3420 Heat Exchange Installation ($600K – IGPP, planned to be initiated in FY 2023)
- SEF Landscape Modification ($1.7M – IGPP-Other, project planned to initiate in FY 2023)
- Trace Inorganic Analysis Complex Strategy 331 Lab 152N ($2M – IGPP, project planned to initiate in FY 2023)
- 3020EMSL Boiler #3 Replacement ($650K – IGPP-Other, project planned to initiate in FY 2024)
- 318 Steam to Hydronics Conversion ($2.2M – IGPP-Other, project planned to initiate in FY 2024)
- LSL2 Steam to Hydronics Conversion ($8M – SLI-GPP, planned to initiate in FY 2024)
- 3212 Lab Conversion ($2M – IGPP, project planned to initiate in FY 2026).

Federally Owned Campuses and Lease Strategy. PNNL has implemented a two-part approach to achieving the goal of establishing federally owned campuses. The first part of this goal is to transition all existing contractor-owned real property to federal ownership while the second is to minimize reliance on third-party leases by relocating staff from leased facilities to government-owned facilities while terminating leases where appropriate.

DOE is in the final stages of acquiring all contractor-owned facilities, the capstone of a five-year agreement between DOE and Battelle Memorial Institute to transfer ownership of this real property. The final transition of this phase in Richland and Sequim will be completed in FY 2022. With this achievement, PNNL will look ahead to the next goal of transferring the remainder of the contractor-owned land to DOE by 2035. Ultimately, this will complete the federalization of PNNL.

PNNL is also aggressively reducing its dependance on leased facilities. The PNNL-Richland campus and adjacent areas include 17 leases totaling ~863,000 gsf. The following outlines PNNL's immediate and long-term plans for thirteen leased facilities improving utilization of government-owned facilities. Once executed, this plan will result in a reduction in annual lease liabilities of $26.8M. Table 5 provides PNNL's leasing strategy and Appendix 4 provides planned lease actions for PNNL leases greater than 10,000 gsf.

Leverage Local Utilities and Services. Water, sewer, and electrical utilities for the PNNL-Richland campus are provided by the city of Richland and are well maintained. Additionally, natural gas is provided by Cascade Natural Gas and is well maintained. In coordination with the city of Richland, PNNL recently assumed operational control of the Hanford 300 Area water and sewer systems and will take over the natural gas system operations during FY 2022. The city of Richland has an agreement with each individual contractor in the Hanford 300 Area to support electrical service. In FY 2023, PNNL will transition all emergency services support to the city of Richland. The city of Richland constructed a new city fire station adjacent to PNNL's core campus to serve this need.

At the PNNL-Sequim campus, current sewer and water needs are serviced by septic sewer and potable well water. These services will be transitioned to local municipalities over the next two years. The City of Sequim provides emergency services to the PNNL-Sequim campus.

Resiliency and Low Deferred Maintenance. PNNL's campuses and facilities have been well maintained and boast an average building age of 28.7 years, with a very low deferred maintenance backlog, resulting in an overall condition index of 94. In planning future investments, PNNL is guided by an understanding of the needs of our Major Initiatives (see Section 4.0) and by cues from our ICM review of the health of our core capabilities (see Section 3.0 and Appendix 1 for discussion of process and results). Any areas of concern identified through our ICM are evaluated for the most efficient solution in the context of mission alignment and optimized functionality, reliability, utilization, and operating costs.

In addition to the above, PNNL also uses the following benchmarks:

- Maintain a laboratory asset condition index of ≥95
- Maintain a maintenance investment index ≥2 percent.

PNNL is planning for overall maintenance and repair funding in excess of 2 percent of PNNL's RPV through 2033. In 2021, we exceeded the maintenance and repair benchmark of 2 percent of the RPV; however, the condition index of government-owned facilities dipped below the benchmark of 95. Recognizing this, PNNL has committed to increase the overhead planned major maintenance investment profile and developed a planned major maintenance strategy to increase the condition index back above the benchmark.

PNNL assesses every real property asset annually to identify deferred maintenance items that are then calibrated across the PNNL campus to establish a deferred maintenance priority. The calibration is a risk-based decision process giving priority to deferred maintenance items that have the highest mission impact regardless of ownership (EM or SC). Factors considered include safety, security, importance of a building or system, likelihood of failure, cost of repair, and the ability to operate in an impaired or failed state. Those deferred maintenance items with the highest priority are funded sooner in PNNL's planning strategy. The existing campus strategy has addressed projects that resolve all existing deferred maintenance ($24.4M) by 2033 in additional to proactively planning for high-risk repair needs and efficiencies before they progress into deferred maintenance.

Campus Strategy

Within the context of the vision and goals discussed above, PNNL's 10-year campus strategy is driven by alignment with S&T emerging mission and infrastructure needs. In support of this, PNNL has committed to an increased level of indirect F&I funding starting in FY 2023. Figure 5 illustrates PNNL's plan to sequence the internally funded and DOE-funded projects required to maintain, replace, and modernize F&I, per the nearly $1.2B recapitalization plan. The rolling 10-year campus strategy is evaluated and updated annually through a disciplined process and, as the campus strategy evolves, PNNL will adjust the plan as needed to support our mission. Successful implementation of the complex and interdependent components of our 10-year campus strategy will require a large-scale project integration effort that includes stakeholders, project staff, and DOE.

Objective 1: Execute Line Item Projects

Energy Sciences Center (ESC) ($93M Line Item – DOE-SC Science Laboratories Infrastructure [SLI]): This line item project will enhance basic and applied research programs that are pursuing novel catalyst design and molecular-level control of chemical transformations. The ESC delivered a ~139,000 gsf facility consisting of 52 laboratory modules, 200 workstations, and collaboration space. This project received beneficial occupancy in January 2022. CD-4 approval is anticipated in the fourth quarter of FY 2022.

Grid Storage Launchpad (GSL) ($77M Line Item – DOE-OE): This line item project will deliver the mission to accelerate the development of next-generation, low-cost, long-duration grid storage technologies; provide independent validation of new technologies under grid operating conditions; and foster greater collaboration across DOE and the entire R&D community. The GSL will deliver an ~85,000 gsf facility of a laboratory, workstations, and collaboration space. PNNL has received CD-2/3 approval at $77M total project cost; it will enable independent testing and validation of next-generation, grid-scale energy storage technologies under realistic grid operating conditions.

M_2P Capability ($80–$120M Line Item – BER): CD-0 mission need for the M_2P capability has been approved, and BER has asked PNNL to support activities leading up to CD-1. The project estimates readiness for CD-1 in late FY 2022. The objective of the project is to address the gap in the ability to interrogate and characterize microbes and microbial communities at a pace that matches the rapid developments in high-throughput genome sequencing, synthesis, engineering, and systems modeling. The mission need statement identifies a cost range of $80–120M.

Pacific Ultra Rare Event Lab (PURE) (TBD – TBD): QIS is an area of explosive growth worldwide, encompassing a broad spectrum of technologies that use features of quantum mechanics—entanglement, uncertainty, and superposition—for practical benefit above and beyond the possibilities of classical technologies. Building on our synthesis science capabilities, we are developing new quantum materials for computers and sensors, and quantum sensing for access to "new" physics beyond the standard model of particle physics. All current QIS infrastructure at PNNL is on the surface; however, we have demonstrated that interactions of radiation with QIS devices severely degrades their performance. Therefore, any research into the effects of radiation on QIS devices will need to be underground. The

Shallow Underground Laboratory (SUL) at PNNL is a world-class capability in low-level radiation measurements, and the dilution refrigerator currently being installed in the SUL positions PNNL uniquely to continue investigating the effects of radiation on QIS devices. We expect to need several more dilution refrigerators, with no room for growth, due to the ongoing demand for this space by the original missions driving the SUL, such as nuclear forensics and nuclear explosion monitoring, a need which is also expanding. There is also a need for connecting with clean, indoor surface labs. Our grand vision for underground QIS would be to host a noisy intermediate-scale quantum computing user facility for the United States in expanded SUL facilities in the 2030s, which would allow solving quantum chemistry problems on quantum computers.

Manufacturing Acceleration Center (MAC) (TBD – TBD): PNNL is envisioning the development of a Manufacturing Acceleration Center that will provide a platform for reducing life cycle energy and resource consumption in the development and demonstration of scalable new manufacturing pathways for materials and fuels that will provide significant competitive advantage to the U.S. manufacturing sector. The Manufacturing Acceleration Center could include high bay space to house growing lab capabilities in advanced manufacturing technologies, such as solid phase processing, composites and polymers systems, and low-carbon fuels, with adjacent support lab, office, and collaboration space. This facility would strengthen PNNL's ability to support the core capabilities of Applied Materials Science and Engineering, Chemical Engineering, and Biological and Bioprocess Engineering.

Objective 2: Reduce or Eliminate PNNL Carbon Emissions (NZERO)

PNNL's Lab-wide initiative to achieve NZERO at our campuses, developed in consultation with DOE, includes a variety of infrastructure investments and the integration of innovative technologies into existing infrastructure and operations (see Figure 6). Through aggressive, near-term investments and deployment of associated operational strategies, initial planning efforts indicate PNNL's emissions can be reduced up to 50 percent within a five-year period and fully achieve our goal of NZERO emissions within eight years. Complimentary to the reduction of emissions, resiliency will be enhanced by reducing the amount of energy required to operate PNNL and leveraging the use of distributed energy sources and microgrids. Most substantially, near-term actions to reduce emissions include, but are not limited to, the following:

- Install several district energy systems to broadly improve overall operating efficiencies of PNNL facilities heating and cooling
- Electrify building heating sources and on-campus transportation to eliminate carbon-based fuel
- Upgrade F&I (e.g., heating, ventilation, and air conditioning [HVAC]; heat recovery; and lighting).

PNNL is developing the planning documents required to initiate the first two projects in support of this objective (see below), which can be executed as early as FY 2023 or once project funding has been established. PNNL has also developed a detailed implementation plan with a prioritized list of projects based on the impact to reducing carbon emissions.

- 3400, 3410, 3420, 3425, and 3430 District Energy System Installation ($19.5M – TBD, schedule TBD)
- Life Science Laboratory 2 (LSL)2, Research Operations Building (ROB), the Math Building (MATH), and Battelle Auditorium (AUD) District Energy System Installation ($19.75M – TBD, schedule TBD)

Objective 3: Develop National Security Research Complex

Critical energy infrastructure in the United States and the DOE facilities that conduct research, development, and analysis to defend it are under constant attack by adversaries seeking to disrupt operations and acquire U.S. knowledge and innovation. Safeguarding the security and resilience of U.S. infrastructure and of the classified environments and data used to prevent, detect, analyze, and respond to threats against it requires transformative new capabilities to address a growing landscape of technical surveillance dangers.

To mitigate the risk, a new infrastructure protection capability is needed to harness the integrated power of advanced computing, data analytics, AI/ML, and radiofrequency technologies, including advanced wireless communications modalities such as 5G and beyond. PNNL is proposing to construct a National Security Research Complex (NSRC) consisting of up to eight federally owned, secure research facilities that would include the following:

- Multidisciplinary teaming at the intersection of science and security fields
- A physical environment that bridges research and production missions
- Experimental testbeds, including flexible laboratory spaces that can be rapidly reconfigured to adapt to emerging threats.

This activity would support the Nuclear Engineering, Systems Engineering and Integration, Decision Science and Analysis, Cyber and Information Sciences, Systems Engineering and Integration, and Advanced Computer Science, Visualization, and Data core capabilities.

The NSRC will be funded through a program adder providing direct benefit to multiple sponsors simultaneously while not impacting other DOE sponsors. The first five proposed secure facilities are being planned over the next 10-year planning horizon, with sight on up to three additional facilities beyond that planning window to support future mission needs while allowing current missions to relocate out of leased facilities.

- Advanced Secure Communications ($24.7M – IGPP-Other, planned to initiate in FY 2023)
- Secure Physical Sciences ($23.3M – IGPP-Other, planned to initiate in FY 2024)
- Secure Computational and Data Sciences ($21.4M – IGPP-Other, planned to initiate in FY 2025)
- Material Science and Laboratory Analysis ($22M – IGPP-Other, planned to initiate in FY 2027)
- NSRC Building #5 ($23.6M – IGPP-Other, planned to initiate in FY 2028)
- Mission-Driven Secure New Buildings 6 through 8: PNNL is currently evaluating the mission drivers to construct additional secure facilities to support a variety of PNNL research missions.

Objective 4: Extend the Life and Nuclear Mission Capabilities for 325 Radiochemical Processing Laboratory (325RPL) Facility

The most important nuclear challenges facing the United States include the domestic production of nuclear material; safely storing, managing, and dispositioning radioactive waste; developing signatures that can be used to determine whether a facility is conducting proliferation activities; and forensics of nuclear and other radioactive material to determine the origin and history of materials. Multidisciplinary R&D will be required in each of these areas to overcome the challenges. Research in these critical areas requires nuclear facilities. Nuclear facilities across the complex are mostly subscribed, and over half are more than 40 years old. While the overall asset condition of 325RPL is Adequate, the condition index of the facility is at 89, identifying the need for significant investments to bring the facility up to the PNNL standard of 95.

The NNSA-SC memorandum of agreement to extend the life cycle of the 325RPL facility is crucial for long-term support of these critical research challenges. 325RPL was designed and constructed in 1953, is in the 300 Area of the Hanford Site, and remains DOE-EM owned. It is one of only two remaining DOE-SC operated Hazard Category II non-reactor nuclear facilities. Life cycle extension for 325RPL is required to address the aging infrastructure and space configurations to continue to meet mission needs and operate safely; modification to the 325RPL would include the following projects:

- 325RPL Exterior Replacement ($10M – GPP-NNSA, planned to initiate in FY 2022)
- 325RPL Electrical Upgrade ($6M – GPP-NNSA, planned to initiate in FY 2023)
- 325RPL Steam to Hydronics Conversion ($10M – GPP-NNSA, planned to initiate in FY 2023)
- 325RPL 100 Hallway Office to Lab Conversion ($17.6M – GPP-NNSA, planned to initiate in FY 2023)
- 325RPL HVAC Upgrade ($13M – GPP-NNSA, planned to initiate in FY 2024)
- 325RPL 500 Hallway Lab Renovation ($16M – GPP-NNSA, planned to initiate in FY 2025)
- 325RPL 400 Hallway Lab Renovation ($16M – GPP-NNSA, planned to initiate in FY 2027)
- 325RPL Hot Cell Renovation ($20M – GPP-NNSA, planned to initiate in FY 2027)
- 325RPL 300 Lab Hallway Renovation ($16M – GPP-NNSA, planned to initiate in FY 2028).

In addition to the NNSA investments identified above, PNNL has planned an additional investment of $31.1M in 325RPL over the next 10 years. This investment will be inclusive of projects designated to address construction of a new office building, and modifications, upgrades, and repairs to the Shielded Analytics Laboratory, High-Level Radiochemical Facility, manipulator, and hot cells.

These improvements would support the Nuclear Engineering, Chemical Engineering, and Nuclear and Radiochemistry core capabilities.

Objective 5: Extend the Life of 300 Area Radiological Facility Capabilities and Utilities

PNNL occupies multiple buildings in the 300 Area of the Hanford Site that support important missions, including 325RPL; the Life Sciences Laboratory (331 Facility), which conducts work in characterizing and monitoring aquatic and terrestrial ecosystems as well as geophysical methods for monitoring field-scale and regional phenomena; and the Radiological Calibrations Laboratory (318 Facility), which provides testing and calibration of a large variety of radiological instrumentation, dosimetry, and radiation effects research. Key infrastructure and building systems that are managed by PNNL are reaching the end of their useful life and need replacement. PNNL has agreement (through Pacific Northwest Site Office [PNSO]) with DOE-EM to occupy these Hanford 300 Area facilities through 2046; the continued reliability of the systems in these facilities and in the 300 Area is paramount to their safe operation.

These 300 Area facilities support multiple core capabilities, including Biological Systems Science, Nuclear and Radiochemistry, Nuclear Engineering, Chemical Engineering, Environmental Subsurface Science, and Chemical and Molecular Sciences.

Modifications to the 300 Area would include the following:

- 318 Hot Water Piping Upgrades ($8.5M – IGPP, planned to initiate in FY 2023)
  300 Area Waterline Building Distribution Replacement ($2M – IGPP, planned to initiate in FY 2023)
- 300 Area Stevens Drive Waterline Upgrade ($2M – IGPP, planned to initiate in FY 2023)
- 300 Area Office ($7.3M – IGPP, planned to initiate in FY 2023)
- 318 HVAC Upgrade ($10M – IGPP, planned to initiate in FY 2024)
- 331 HVAC Upgrade ($5M – IGPP, planned to initiate in FY 2024)

- 331 Research Support Office ($8.1M – IGPP, planned to initiate in FY 2024)
- 331 Hot Water Piping Upgrade ($3.5M – IGPP, planned to initiate in FY 2025)
- 300 Area Research Test Bed Establishment ($1.2M – IGPP, planned to initiate in FY 2026).

Objective 6: Align PNNL-Sequim Campus Strategy with Current and Future Research Needs.

As DOE's only marine science laboratory, PNNL conducts R&D in support of coastal and ocean-based technologies and is focused on positioning the capabilities with evolving sponsor needs. Growth within marine renewable energy has led to investments from federal, state, and university sponsors for projects (e.g., tidal ladders, solar array, cabled research array, energy storage) that depend on the capabilities and access available at the PNNL-Sequim campus. This includes the procurement and operation of DOE's first diesel electric hybrid vessel.

Additional facilities and capabilities needed to accommodate existing and future research were identified during a research needs workshop led by the research directorates. F&I improvements have been prioritized into the following areas:

- High ceiling and large equipment engineering space/labs
- Prototyping and electronics lab space
- Sequim Bay waterfront access to support the deployment of vessels and other autonomous vessels/sensors
- Updates and expansion to wet-lab space and other seawater dependent research.

Current research, along with planned F&I improvements, has driven internal investments that are being made to position the campus to accomplish the goals of the emerging strategy. Current F&I projects that are included in the current PNNL-Sequim campus strategy include the following:

- MSL5 Room 506 Isolated Radiological Work Area Conversion ($770K – IGPP, planned to complete in FY 2022)
- PNNL-Sequim Campus Water-Sewer Conversion ($4.8M – IGPP, planned to initiate in FY 2022)
- PNNL-Sequim Water Distribution Upgrade ($3M – IGPP, planned to initiate in FY 2023)
- PNNL-Sequim Campus Storage ($3.6M – IGPP, planned to initiate in FY 2023)
- PNNL-Sequim Campus Uplands Access Road ($1M – IGPP, planned to initiate in FY 2025)
- MSL7 Office Relocation ($800K – IGPP, planned to initiate in FY 2026)
- PNNL-Sequim Campus Shoreline Access Upgrade ($4M – IGPP, planned to initiate in FY 2030)
- PNNL-Sequim Campus Large Instrument High Bay ($11.2M – GPP-TBD)
- PNNL-Sequim Campus Research Accessible Shoreline Upgrade ($3.2M – GPP-TBD)
- PNNL-Sequim Campus Technology Development and Biology Building ($10M – GPP-TBD)

Objective 7: Deliver Mission-Ready Facilities and Infrastructure

EMSL backfill and capability expansion: Four separate projects are planned between FY 2023 and FY 2025 for a total of $22M to backfill space vacated in EMSL when the capability relocations into the ESC have been completed. The plan includes repurposing approximately 13,000 square feet to accomplish four objectives: grow science areas of strategic importance to EMSL, incorporate new capabilities that benefit EMSL, unpack/relocate current laboratories to promote safe and efficient research, and create core lab spaces to consolidate equipment and capabilities that crosscut EMSL's Integrated Research Platforms.

- 3020EMSL HPC Infrastructure Upgrade ($6.5M – GPP, planned to initiate in FY 2022)
- 3020EMSL Laboratories Remodel to Grow Ion Mobility, Isotope Tracing, Automation, and Analytical Capabilities ($5M – GPP, planned to initiate in FY 2022)

- 3020EMSL Laboratories Remodel to Develop Maker Space and Core Capabilities ($5M – GPP, planned to initiate in FY 2023)
- 3020EMSL Laboratory's to Enable Renovate Unpack Priority Capabilities ($7M – GPP, planned to initiate in FY 2024).

Install infrastructure to support future site development: PNNL has proposed a $33M investment through multiple infrastructure projects to develop the north end of the PNNL-Richland campus that is currently undeveloped. These projects will provide full-scale infrastructure that is required to efficiently manage campus development and PNNL's NZERO goals. Through a series of projects (see below), PNNL plans to deliver water, power, sewer, road, and a district energy system to provide the long-term infrastructure required to support the PNNL-Richland campus meeting the future mission demands.

- PNNL-Richland North Infrastructure ($17M – IGPP, planned to initiate in FY 2022)
- PNNL-Richland North Central Infrastructure ($6.2M – IGPP, planned to initiate in FY 2024)
- PNNL-Richland George Washington Way Extension Relocation ($5M – IGPP, planned to initiate in FY 2026)
- PNNL-Richland North Arterial Roads ($5M – IGPP, planned to initiate in FY 2029)

PNNL campus development: PNNL has proposed a $246M investment over the next 10 years to construct 14 office, laboratory, warehouse, and shop buildings. Informed by PNNL's data-driven capability gap analysis, these 14 facilities will be required to meet the future mission demand. The capability gap was adjusted to account for the implementation of Hybrid Workplace strategies, which include hoteling, shared-dedicated, and virtual work assignments for staff. In addition to construction of new facilities, PNNL is proposing the repurpose of existing space from a support function into newly renovated research space to better align research capabilities across the PNNL-Richland campus and support the exit of third-party leases.

- Richland Storage Warehouse ($6.2M – IGPP, planned to initiate in FY 2022)
- General-Purpose Lab ($15M – IGPP, planned to initiate in FY 2024)
- PNNL-Richland North Office ($15M – IGPP, planned to initiate in FY 2025)
- Engineering Lab-Office ($19M – IGPP, planned to initiate in FY 2025)
- PNNL-Richland South Office ($19M – IGPP, planned to initiate in FY 2026)
- Systems Engineering Lab-Office ($19M – IGPP, planned to initiate in FY 2026)
- Applied Material Science Lab-Office ($19M – IGPP, planned to initiate in FY 2027)
- Mission-Driven New Buildings: PNNL is continuously evaluating the mission drivers to construct additional facilities to support a variety of PNNL core capability missions. In the FY 2028 to FY 2033 timeframe PNNL has approximately $135M of investments planned to meet these mission demands.

Site Sustainability Plan Summary

Fundamental to the S&T outcomes that PNNL delivers every day is a commitment to sustainability—a serious responsibility. Sustainability at PNNL encompasses environmental stewardship in our operations, as well as how the Laboratory demonstrates social responsibility and advances economic prosperity—all in a manner that delivers lasting benefit to our sponsors, community, and the nation.

From innovative best practices in sustainable operations to environmentally focused scientific breakthroughs, PNNL is committed to making the world a better place to live for many generations to come. In FY 2021, despite the unprecedented disruptions and challenges of the ongoing COVID-19 pandemic, staff at PNNL have remained productive. Key accomplishments and initiatives in advancing PNNL sustainability are highlighted below.

Transitioning to Net-Zero Emissions and Resilient Operations

PNNL's strategy to reduce the use of fossil fuel is focused on the "four Rs"—replacing our current greenhouse gas sources with low-impact sources; reducing energy use in our buildings and fleet vehicles; enhancing our resilience to utility disruption by adding clean, on-site distributed energy resources where they are most needed; and leveraging our research capabilities to learn by testing methods under realistic operating conditions. Additional information is available in the Implementation Plan for Net-Zero Emissions and Energy-Resilient Operations (NZERO) pilot at PNNL.

As one of four national laboratories participating in a DOE NZERO pilot, PNNL is embarking on an initiative to achieve NZERO emissions and resilient operations by 2030. The NZERO initiative will enable PNNL to be among the first federal facilities to achieve NZERO emissions by optimizing our resources and operations to achieve 24/7 carbon-free energy and mitigate the impacts of utility disruptions. Along the way, PNNL will use the PNNL campuses as a living laboratory—testing new technologies and approaches and using the knowledge we gain to shape a model for others.

Some of PNNL's key interim targets for meeting the NZERO goals are to reduce emissions by 50 percent within three years; reduce emissions by 75 percent and achieve NZERO emissions at the Sequim, Washington, campus by 2027; and achieve NZERO emissions and 24/7 carbon-free energy across PNNL by 2030.

Reducing Energy Use

In FY 2021, PNNL's energy intensity for "Goal Subject" buildings was 177.4 kBtu/gsf, a net increase of approximately 6.4 percent compared to the FY 2015 baseline and a 6.7 percent increase versus last year. For "Excluded" buildings, energy intensity was 357.4 kBtu/gsf, a 5.7 percent decrease compared to the FY 2015 baseline and a 0.3 percent increase versus last year.

Some of the increase in energy use can be explained by local weather. In FY 2021, a 30 percent increase in cooling degree days was observed as compared to FY 2020. This is due to record setting weather conditions in Richland, Washington, during the summer season, which set both a new all-time record for highest daily temperature of 118°F and a record for the number of days (35) in which temperatures exceeded 100°F. The sweltering temperatures greatly impacted energy consumption. Not only was load and use high, but heat rejection equipment has a reduced efficiency at these elevated temperatures. For reference, PNNL's typical design temperature for the summer is 101°F. Heating degree days were roughly the same. Also, PNNL is transitioning from COVID-19 curtailed operation to limited operation; facility energy usage is steadily increased as compared to last year.

Reducing Water Use Intensity

By the end of FY 2021, PNNL's potable water use intensity had increased by approximately 20 percent compared to FY 2020, primarily due to record high setting weather conditions in Richland, Washington, as described previously. Additionally, PNNL noticed a marked reduction of water usage in FY 2020 compared to FY 2019, due to a reduction in the number of people on campus because of COVID-19 workplace restrictions. As restrictions have eased to enable limited campus operation, the additional people on campus are contributing to an increase in water usage. PNNL continues to perform line flushing (especially in the 300 Area) to control chlorine levels in the water distribution systems.

The current water use intensity, 29.8 gal/gsf, is 57.5 percent less than the FY 2007 baseline water use intensity of 70.1 gal/gsf.

Sustainable Building

Currently, PNNL has 11 (or 517,841 gsf) of 24 (or 1,065,666 gsf) applicable buildings compliant with the Guiding Principles issued by the Council of Environmental Quality. This is 46 percent by building count, or 49 percent by total square footage.

At PNNL, all new construction, major renovations, and alterations of buildings greater than 10,000 gsf will comply with the Guiding Principles. This commitment is institutionalized by incorporating the Guiding Principles, including the energy reduction requirements per the ASHRAE Standard 90.1, into PNNL's engineering design standards and the general specification for new constructions and major renovations projects.

Currently, there are two buildings under construction. The ESC building is expected to complete commissioning in FY 2022. This will be the first new facility at PNNL to use the 2016 Guiding Principles as a path toward sustainable building status. The GSL building is designed to consolidate and enhance the grid energy storage research capability and will meet the 2020 GP requirements.

PNNL is on Track to be 50001 Ready

In FY 2020, PNNL signed an agreement to support the DOE 50001 Ready Cohort initiative. This 50001 Ready Energy Management System, when implemented fully, will improve PNNL's ability to continually identify, monitor, track, and improve energy conservation measures. PNNL received the 50001 Ready recognition from DOE in December 2021.

Elevating Energy/Water Resilience through Technical Resilience Navigator

DOE's Federal Energy Management Program Technical Resilience Navigator (TRN) tool provides a systematic approach to examining resilience needs and goals, assessing on-site energy and water systems, evaluating risk, identifying resilience gaps, and developing and prioritizing solutions to resolve those gaps.

In FY 2020, PNNL was selected by the Federal Energy Management Program to pilot its TRN tool to determine the effectiveness of the methodologies and provide lessons learned and improvement opportunities. PNNL plans to utilize the results from the TRN pilot to develop its Vulnerability Assessment and Resiliency Plan. The PNNL TRN project won the 2021 DOE Sustainability award for Innovative Approach to Sustainability category.

PRINCETON PLASMA PHYSICS LABORATORY

Lab-at-a-Glance

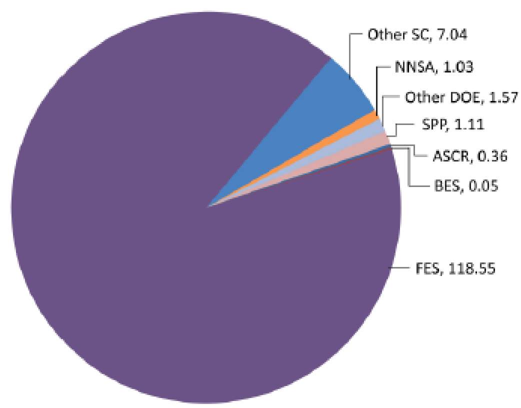
Location: Princeton, NJ
Type: Single-program Laboratory
Contractor: Princeton University
Site Office: Princeton Site Office
Website: www.pppl.gov

- **FY 2021 Lab Operating Costs:** $129.71 million
- **FY 2021 DOE/NNSA Costs:** $128.6 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $1.11 million
- **FY 2021 SPP as % of Total Lab Operating Costs:** 0.8%

Physical Assets:
- 90.7 acres and 32 buildings
- 798,000 GSF in buildings
- Replacement Plant Value: $957.9 M

Human Capital:
- 608 Full Time Equivalent Employees
- 10 Joint Faculty
- 39 Postdoctoral Researchers
- 46 Graduate Students
- 88 Undergraduate Students
- 358 Facility Users
- 21 Visiting Scientists

FY 2021 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 with 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 and sustainable manufacturing for technologies of tomorrow; and (3) to further the development of the scientific understanding of the plasma universe from laboratory to astrophysical scales.

PPPL's missions are supported by five core capabilities:

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

The Laboratory's highest priority is the completion of the National Spherical Tokamak Experiment, a world-leading user facility. Simultaneously, PPPL is partnering in the international fusion project, ITER, to enable U.S.

participation in this critical experiment. PPPL also aspires to be the design partner with industry for the accelerated realization and construction of future fusion Pilot Plants.

The Laboratory is evolving and broadening its scientific and engineering expertise in targeted emerging technologies to enhance the nation's economic health, competitiveness and environment. Indeed, PPPL aims to drive the next wave of scientific innovation in plasma nanofabrication and sustainable manufacturing technologies to maintain U.S. leadership in critical industries. Princeton University and PPPL are educating and inspiring a diverse cadre of world-class scientists, engineers, technicians, and operations staff to serve the Laboratory and the national interest .

Core Capabilities

PPPL has made history as a world-leading experimental and theoretical plasma physics and fusion facility, with depth and breadth of research that is unparalleled in the U.S. or the world. This status 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.

The Princeton Plasma Physics Laboratory (PPPL) has five DOE-designated core capabilities, two emerging core capabilities, one new, and one proposed new capability that enable the vital role of the Laboratory in executing DOE's missions, as well as in aiding the development of science initiatives that are responsive to national needs:

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) *[Emerging]*
7. Condensed Matter Physics and Materials Science *[Emerging]*
8. Chemical and Molecular Science *[New]*
9. Applied Materials Science and Engineering *[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 many *technologies of tomorrow*. These technologies require a multidisciplinary set of capabilities that PPPL is committed to strengthening and growing.

PPPL's unique capabilities in diagnosing and understanding plasmas will support the next generation of industrial plasma processing. Through the activities outlined below, PPPL is increasing efforts to strengthen and/or diversify into research areas embodied in these additional core capabilities mentioned above.

Plasma and Fusion Energy Sciences

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 is also preparing advanced X-ray diagnostics for the JT-60SA tokamak (Japan).

PPPL's researchers contribute computational plasma physics and theory expertise to the development of whole device modeling suites for plasma experiments, to the utilization of exaflop computers in the DOE Exascale Computing Project, and to Scientific Discovery through Advanced Computing (SciDAC) Centers. Initiatives in plasma-material interactions, such as nanomaterial synthesis, plasma processing, and plasma-surface modification.

Noteworthy updates illustrating increased integration of physics and engineering codes include:

- New tools capable of simulating flows and heat transfer were used to model plasma-facing components (PFCs) with complex cooling structures associated with the design and optimization of ITER diagnostic modules
- The fluid dynamics model was expanded to include a magnetohydrodynamics capability, allowing analysis of the flows of conducting liquids in magnetic fields, such as tritium-breeding blankets. The capability to model transitions through all four phases of matter was tested in simulations of complex fusion devices.

Systems Engineering and Integration

PPPL is well positioned to lead the systems engineering and integration of new fusion facilities to incorporate innovative designs for reduction of capital costs and risk mitigation. Systems engineering and integration principles are ingrained in PPPL's daily work processes across the engineering staff from design to field integration, with due consideration for technical risk and failure modes throughout the engineering lifecycle. This process helps develop more efficient systems with implementation cost as part of the design and establishes better lines of communication within the workforce.

PPPL is establishing a virtual prototyping environment that incorporates modeling and simulation, to support all aspects of systems engineering by enabling, prediction, analysis, optimization and capturing complex emergent behaviors. PPPL's systems and design engineering expertise allows the Lab to assume a leadership role in designing and establishing a virtual prototyping environment. These capabilities will be essential in the planning, design and integration of research and development activities leading to the conceptual design and development of a fusion power plant.

Large-Scale User Facilities/Advanced Instrumentationn

PPPL's large facilities and extensive capabilities for plasma production, confinement, control, and measurement systems make it an ideal site for research development and collaborations. PPPL specializes in technologies to safely heat, fuel, control, and exhaust plasmas at temperatures as high as 550 M°K, with a broad application and uses beyond NSTX-U.

Technologies that are being developed as prototypes for future devices include flexible neutral beam injection and ion cyclotron range of frequency (ICRF) waves that can be used for both heating and current drive.

Gas injection at supersonic speeds will be tested as a means to efficiently fuel the deep core. Real-time plasma control methodologies are being developed that will allow for control of the plasma, and tailoring of plasma profiles, to maintain stable, high-performance plasmas for their entire lifetime. An impurity powder dropper (IPD) and an impurity granule injector have shown success on domestic and international facilities, and these will be employed to improve wall conditions, mitigate heat flux and control edge instabilities. Liquid lithium component prototypes will be tested as a basis for more expansive liquid lithium divertor concepts 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.

Mechanical Design and Engineering

PPPL has implemented a collaborative and holistic design approach, using systems engineering techniques coupled with enhanced computational capability, to ensure that requirements are identified as early as possible, and that designs are verified through their evolution from concept to final design review. Engineering processes and procedures have been updated to align with the PPPL quality program. The Laboratory's Quality Assurance Program Description has clearly defined roles for engineering in design verification, validation and implementation.

Virtual engineering will be an important and expanding capability for the design of the next generation of fusion experiments, and the Engineering Department is establishing a strong presence in this area. Integrated simulation and workflows for optimized design, with the optimization integrating physics and engineering considerations, are being developed. The designs of the MUSE stellarator and, to an even greater extent, the ARPA-E supported permanent magnet stellarator (PM4Stell), will both drive and benefit from these capabilities. Initial use of integrated simulation capability for other programs such as ITER diagnostics to establish workflows as part of system design will be available. These capabilities will benefit from enhanced computing power that allows application of nonlinear features in finite element analysis and incorporation of multiphysics code capabilities. These capabilities will make PPPL engineering a leader in many areas, including:

- Completion of the NSTX-U Recovery and support of operations, including the development and use of "digital twins,"
- Collaboration with other institutions in design and manufacture, such as on COMPASS-U, ITER, WEST, and JT-60SA,
- Leading in collaborative efforts to design and build a fusion pilot plant,
- Developing liquid metal plasma-facing components and new HTS magnet designs,
- Supporting PPPL's expanded research into semiconductors and nanotechnology

Power Systems and Electrical Engineering

PPPL offers both the physical infrastructure and the technical capabilities for meeting the extraordinary power system demands intrinsic to fusion energy research machines.

As part of the Metuchen-Trenton-Burlington (MTB) project, PPPL's utility provider, PSE&G, has replaced its 138kV lines with 230kV. A new 230/138kV (550 MVA) autotransformer has been installed and placed into operation near the PSE&G Plainsboro Substation and is currently feeding the Laboratory's 138 kV line to the main switchyard. This transformer has been selected in conjunction with the Laboratory, to support the future experimental load requirements. The capacity of the main switchyard transformers is sufficient to support the NSTX-U power load and auxiliary experimental system loads for the planned 10-year run of NSTX-U.

Anticipated, future developments to support this capability include:

- expansion of power conversion engineering staff to enhance systems engineering capabilities, integrate fusion design activities, facilitate advances in fusion technology, and reduce the development risk in future designs through virtual, modern engineering practices; and
- expansion of radio frequency (RF) engineering staff to continue enabling research in low-temperature plasma (LTP) material interaction for industrial applications.

Emerging, New, and Proposed Core Capabilities

PPPL's unique capabilities in diagnosing and understanding plasmas will support the next generation of industrial plasma processing. PPPL is increasing efforts to progress and/or diversify into research areas embodied in four core capabilities:

- Computational Science (Emerging)
- Condensed Matter Physics and Materials Science (Emerging)
- Chemical and Molecular Science (New)
- Applied Materials Science and Engineering (Proposed New)

In recent decades, one of the two goals of the Fusion Energy Sciences program in the United States has been to build the knowledge needed to develop a fusion energy source. This knowledge is generated by the careful design and study of experiments and simulations. Interpretation of what scientists observe in fusion experiments requires computation, and thus the knowledge the scientific community has about fusion as an energy source, is literally encoded and expressed in whole-device models of fusion systems. In this very real sense, fusion energy science is **computational science**. Recognizing the centrality of computation to the Laboratory, FES, and wider DOE missions, a new Computational Sciences Department (CSD) was established. This department focuses on seven distinct areas: software technology, high performance computing, data science and learning, algorithms and applied mathematics, multiscale integrated modeling, experiments and validation, and visualization and data. The Laboratory aims to extend its capabilities and expertise in nanofabrication science, especially in the context of low-temperature plasma science. Nanofabrication science in this context necessarily involves **condensed matter physics and materials science** since the purpose of nanofabrication technology is to modify materials that will be used in solid state electronic or quantum devices. In order to lead the new initiatives in nanofabrication for advanced electronics and Quantum Information Science, PPPL hired a new Associate Laboratory Director for Low-Temperature Plasma-Surface Interactions (LTPSI), who is collaborating closely with existing PPPL staff with LTP expertise, as well as with industry and several Princeton University departments (Princeton Institute of Materials, Chemical and Biological Engineering (CBE), Electrical Engineering, and Physics).

PPPL is also proposing a new, closely-related core capability in **chemical and molecular science** associated with understanding and control of plasma chemistry. This core capability is related to PPPL's new efforts in developing plasma nanofabrication science and technology for materials that will be used in solid state electronic and quantum devices.

In addition, PPPL is proposing a new, closely-related core capability in **applied materials science and engineering**. PPPL's planned diversification into studying low-temperature plasma applications to problems in advanced, next-generation semiconductor and QIS device manufacturing involve theoretical, experimental and computational studies of plasma-materials interactions. PPPL's intention to diversify into sustainability science through electromanufacturing, including the use of plasmas and/or electricity to disrupt fossil-fuel-driven industries such as chemical, steel, mining, and recycling, will leverage experimental and computational strengths at PPPL and Princeton University in plasma, electrochemical, and materials science and engineering. As this initiative grows, it will contribute both to basic science in areas where phenomena are not well understood, as well as applied science and engineering that will bring discoveries to deployment.

The Laboratory expects to establish these four core capabilities over the next five years.

Science and Technology Strategy for the Future/Major Initiatives

The Biden-Harris administration has stated two clear national priorities that drive much of PPPL's strategy. The first is the imperative to address climate change as spelled out by the Executive Order[5] by establishing *".... a carbon pollution-free electricity sector by 2035 and net-zero emissions economy-wide by no later than 2050."* Second is a commitment to enhance national economic competitiveness in technologies of tomorrow particularly (but not exclusively) in the microelectronics/semiconductor sector. Indeed, the White House recently stated, *"President Biden prioritized domestic semiconductor manufacturing and research and development (R&D) shortly after taking office."*[6] PPPL has unique capabilities that are needed to address key research aspects of these two priorities and our strategy, missions, and program align with these needs. This necessitates the targeted expansion of our activities outlined in this plan.

PPPL is seeking to accelerate and tailor its three missions to deliver on these national priorities by:

1. **Developing the scientific knowledge and advanced engineering to enable fusion to power the U.S. and the world.** Energy analysts acknowledge the need to develop fusion as a new "firm energy" source to realize the Administration's climate change goal.7 The administration is therefore *"developing a bold decadal vision to accelerate fusion"*1 and DOE is launching an initiative to implement and accelerate fusion delivery coordinated by a Lead Fusion Coordinator reporting to the Under-Secretary for Science and Innovation. As this new structure evolves, PPPL will direct its considerable fusion science and technology capabilities to support the initiative. 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. The Laboratory is increasingly collaborating and partnering with private fusion companies and foundations to move fusion science and technology toward a Pilot Plant and market viability.
2. **Advancing the science of nanoscale fabrication and sustainable manufacturing for technologies of tomorrow**. Nanoscale fabrication for microelectronics and eventually sub-nanoscale fabrication for quantum systems is central to the U.S.'s future economic security and competitiveness, and industry needs have facilitated many new partnership opportunities for the Laboratory. To meet the Administration's climate goals, PPPL's low-temperature plasma science expertise, coupled with electrochemical/plasma processing expertise at Princeton, offers a unique opportunity to build out a new program in "sustainable manufacturing". Industry partnerships and expanded research opportunities are facilitating the growth of an attractive, diverse, multi-purpose R&D portfolio.
3. **Furthering the development of the scientific understanding of the plasma universe, from laboratory to astrophysical scales**. A new collaborative experiment (FLARE) will enable new studies of magnetic reconnection, and exascale simulations of ultra-relativistic plasmas will be used to study the physics at the heart of multi-messenger astronomy. This mission brings PPPL into close and productive collaboration with Princeton's Astrophysics Department and leverages and grows DOE capabilities in exascale algorithms and computing. PPPL will also advance understanding of high-energy density plasma science of importance to astrophysical systems, fusion energy, and national security.

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.

Infrastructure

Overview of Site Facilities and Infrastructure

The 90.7-acre Princeton Plasma Physics Laboratory is situated on Princeton University's 1,750-acre Forrestal Campus located in Plainsboro Township, New Jersey. This land, punctuated by dense woods, brooks, and nearby streams, has been leased to the DOE for operation of the Laboratory. The Laboratory is surrounded by several hundred acres of undeveloped land, including protected wetlands, and is conveniently proximate to both Philadelphia and New York City.

The Laboratory has a workforce and user population of approximately 750 and utilizes 763k gross square feet (GSF) of the Princeton University Forrestal Campus, 32 government-owned buildings. There are currently no leased buildings or facilities. PPPL updated its land lease agreement with the DOE on April 1, 2019, extending the lease through 2056. There were no other real estate transactions during FY 2021 and there are no current plans for transactions in FY 2022. Primary 138 kilovolt (kV) power is provided by the local electric utility company. Ensuring the reliability and capacity of these utilities and systems is essential to mission readiness, as well as execution of PPPL's expanded vision.

All of PPPL's buildings and trailers are currently categorized as "Operating". All of PPPL's Other Structures and Facilities (OSF) are also categorized as "Operating" with the exception of one OSF asset, MG Free Cooling Ext. Pipe (Property ID # 7132030301, 400 linear feet).

Infrastructure Data Summary

Total Building Assets	**32**
Total Other Structured Facilities (OSF)	27
Total Deferred Maintenance 2019 ($)	**$76.9M**

As discussed in earlier sections, PPPL is embarking on significant mission expansion and requires the infrastructure that enables this strategy of multi-purpose science initiatives, public/private projects, and the associated population growth. Condition assessments have identified 62% of PPPL's buildings to be Substandard and Inadequate. PPPL relies on the completion of major Science Laboratories Infrastructure (SLI) projects to provide the new and improved spaces necessary to safely support current research and operations. Nearly $12 million of the current General Plant Projects (GPP) portfolio is in construction, with another $7 million in design. The Laboratory has received CD-1 approval of more than $200 million in SLI Projects. CD-1 milestones for both the Princeton Plasma Innovation Center (PPIC) Building and the Critical Infrastructure Recovery & Renewal (CIRR) projects were approved in the second quarter of FY 2021, and the CD-1/2/3 DOE Independent Project Review for the Tritium System Demolition and Disposal (TSDD) project was also conducted successfully. The PPIC project will provide much needed modern state-of-the-art adaptable laboratory and collaboration space that will support the expanding scientific program. CIRR will enhance PPPL's resiliency, significantly improve efficiency with renewed utility infrastructure, and provide increased data capabilities to leverage artificial intelligence for operations. The only gross square foot reductions under consideration at this time are associated with the SLI construction of the PPIC. PPIC will demolish two existing, "inadequate" buildings (Theory Building and a portion of the Administration Building), and the CIRR project will replace significant original infrastructure systems such as Electrical, HVAC, Chilled Water Generation, Underground Utilities, and IT. These systems, while not buildings, carry Deferred Maintenance (DM). Recovery and repair of these systems will reduce DM and dramatically improve the various systems' availability, reliability, and capability.

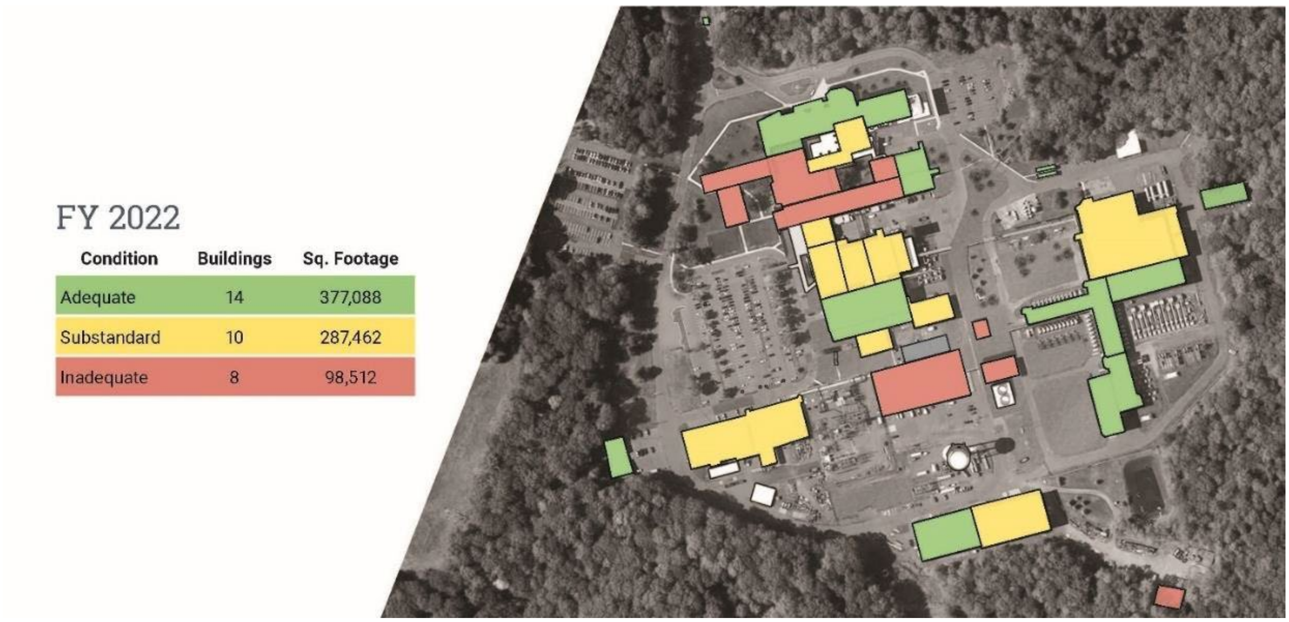


Figure: Building Condition

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 undertaken a thorough evaluation of the space needs anticipated post-COVID to support the needs of the modern workforce. This evaluation has determined that no buildings will be underutilized, 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. Some of these changes are slated for improvements via the CIRR project, as mentioned above, and others are represented in PPPL's infrastructure investment projections.

Campus Strategy

PPPL plays a key role in the delivery of strategic goals outlined by FES, as well as general governmental goals for Science and Technology leadership in the development of technologies of the future. As the leading national laboratory for future fusion concepts, PPPL is actively working with universities and industry partners to further develop an expert understanding of plasma and its applications to new technologies, which are central to U.S. economic health, security, and competitiveness. Many industries, such as the microelectronics industry, utilize plasmas to synthesize and shape the materials in their products. These industries are actively proposing and initiating new partnership programs with PPPL researchers, which further underscores the need for additional investment in flexible, robust, and reliable infrastructure that will foster ground-breaking research occurring both on-site and remotely.

To support the future vision, that include new, expanded opportunities across science disciplines, PPPL's campus must evolve to enable this vision. The campus strategy goes beyond the goal of providing reliable, efficient systems in new and planned facilities, and aims to position PPPL infrastructure as a strategic asset that fully enables the research experience. As PPPL continues to grow its expertise and staff in support of mission-driven plasma research, user facility expansion, and increasing opportunities for national and international collaboration, it becomes even more critical that the campus grows strategically to meet those needs to provide safe, modern, adaptable, efficient facilities and infrastructure. PPPL strives to integrate sustainability into its site development, with core principles considered in these forward-looking plans that include consideration of resilience and sustainability concepts such as decarbonization and Net Zero initiatives for new construction and major renovations. Lessons learned from the Global Pandemic and current repopulation of staff shall also be incorporated into project design.

The FY 2022 Maintenance and Repair (M&R) budget has been allocated flat to the FY 2020 funding levels, and still well below the recommended 2% of replacement plant value (RPV). While PPPL continues to replace and modernize existing legacy infrastructure with GPP and SLI investments, further funding is needed. When PPIC and CIRR are completed, these projects will have replaced old, inefficient buildings (one 40+ years old and one 62+ years old); provided a new modern state-of-the-art, resilient and flexible research building with nominal maintenance needs and high operating efficiencies, sustainable technologies; and replaced/modernized ~$80M in building systems and general plant infrastructure. These building systems and associated general plant infrastructure are well beyond their useful life and were not designed to accommodate the current and future needs for modern research. The Tritium System Demolition and Disposal (TSDD) project, fully funded in FY 2022, will recover thousands of square feet of usable space and free-up the FuRTH test cell, making this national asset available for public/private partnerships as discussed in previous sections. Once proposed projects commence, the lab will phase and coordinate the execution of projects with lab operations to minimize disruptions.

While DM is rising, the effects of the SLI infrastructure replacement projects (PPIC and CIRR) will result in reductions to DM once these projects are constructed. The GPP pipeline of projects is critical to sustaining, modernizing, and maintaining PPPL existing infrastructure. The campus strategy is currently at a pivotal point in which new science diversification plans have been defined.

Infrastructure – Core Capability Gap Analysis

The Campus Master Plan for the Princeton Plasma Physics Lab (PPPL) was initiated in Q4-2021 and developed as a parallel effort with the 2022 Campus Plan and Science Initiatives. The primary goal of the master plan is to address specific capability gaps that have been identified by site leadership and provide a holistic framework for the development of the site over the next decade. This effort will set the stage for a more integrated and cohesive transformation of the campus into a modern state-of-the-art research institution.

The Campus Master Plan effort engaged PPPL core management, key staff/stakeholders and site leadership. The campus master planning effort progressed through a structured workplan and was informed by a variety of assessments and studies. Additionally, the team conducted a series of programming interviews with staff and key stakeholders to review their current and future program needs. Discussions also included ideas for improving the day-to-day user experience, availability and variety of collaboration and amenity spaces, and opportunities for landscape recreation.

PPPL looks forward to the completion of current projects – the PPIC, CIRR, and TSDD – to provide needed and currently unavailable scientific capability, to co-locate scientific staff populations, and to resolve functionality and reliability issues; however, further planning and assessment is ongoing with regard to specific infrastructure capabilities that will support growth in research and development and a more nimble state of readiness for future Laboratory opportunities within the DOE, as well as advanced industries. Most of PPPL's spaces were designed and built in the late 1950s and lack the physical capabilities and infrastructure to support modern research and anticipated research advancement. These spaces do not have sufficient floor area, structural characteristics, modern laboratory services or volume to support the development of new fusion concepts or diagnostics for at-scale large fusion experiments.

Existing lab spaces are fully occupied or oversubscribed and do not support needs for joint collaborations using large-scale data sets. Adjacent office spaces that enable researchers to benefit from collaboration with subject matter experts in computational science, machine learning, artificial intelligence, exascale computing, data management, data acquisition, simulation, imaging, visualization, and modeling also are not currently available. Further, the present space is inadequate for the current ventures in microelectronics, nanofabrication research, and associated diagnostics, all of which require low vibration space and electromagnetic shielding. Existing space is cost-prohibitive to reconfigure and does not contain the environmental controls needed for smaller-scale diagnostic development. While opportunities are being pursued with Princeton University relative to microelectronics, nanofabrication, and quantum information sciences (QIS), the Laboratory must aggressively renew the existing campus to provide the needed research space to attract and retain the best and brightest researchers.

The Campus Plan outlines the necessary facilities, infrastructure, and utilities to serve as the platform for mission success. Delays in funding or key approvals to campus upgrades, such as PPIC, will prevent mission diversification more than year-for-year as opportunities stretch and then disappear.

The Princeton Plasma Innovation Center (PPIC)

PPPL's immediate program needs include modern laboratories, collaboration space, and office space to accommodate growth in research and engineering staff, as well as visiting researchers. PPIC will not offer new spaces in time for existing and near-term, emerging research, but will accommodate these user groups, as well as additional students and external partners at the time of its anticipated opening in FY 2027. The future program at PPPL will require an integrated portfolio of staged facilities. In addition to present renovations for the L-Wing underway to accommodate near-term quantum diamond research, PPPL seeks to renovate and modernize a portion of the CAS building to provide space and utilities for the next steps in quantum, microelectronics, and sustainability science. The capstone will be PPIC; note that all three areas will be needed when the program is fully developed.

PPIC's modern laboratory spaces and clean rooms are vital for continued work in nanofabrication research, and necessary to advance technologies of tomorrow through collaboration with external, private partners, who expect and need these modern, state-of-the-art resources and spaces. These spaces satisfy needs for:

- R&D on microelectronics and quantum device fabrication processes;
- Environmental controls and modular clean room(s);
- Modeling activities; and
- Materials and surface analysis equipment.

The building specifications will be particularly important to the development of the emerging core capability of Condensed Matter Physics and Materials Science and to advancement in low-temperature plasma 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 have tight temperature and humidity control, be adaptable to suit evolving research needs and have a structure that supports demanding vibration parameters. Scientific staff also will continue to depend on the availability of Princeton University laboratories and partners to support research that cannot currently be conducted on site until PPIC is available.

Critical Infrastructure Recovery & Renewal (CIRR)

The CIRR project will replace significant original infrastructure systems to improve PPPL's mission readiness and position the Laboratory for long-term growth. The systems targeted for improvements and upgrades include:

- Electrical distribution system and standby power;
- HVAC Systems;
- Chilled water generation;
- Underground utilities;
- Communications distribution network.

This execution of the CIRR project is critical to strengthening the existing infrastructure that supports ongoing research. Scientific productivity is dependent on a capable, available and reliable support infrastructure. Meeting this mission need will improve operational efficiencies, minimize the potential for future disruptions, and lay the foundation for programmatic growth. Incorporating modern, efficient equipment and systems will both increase PPPL's sustainability and decrease the current deferred maintenance. It will also enable PPPL researchers to contribute their unique computational capabilities in support of industry needs.

PPPL's New Liquid Metals Development Laboratory

In preparation for NSTX-U, active research in prototyping liquid metal plasma-facing components (PFCs) is taking place with Galinstan in smaller-scale devices. However, to support NSTX-U's major future program in flowing liquid metals, a space to safely explore the use of lithium in quantities as great as 50 pounds will be needed. A conceptual physics design of NSTX-U in-vessel liquid metal systems was initiated in FY 2021. Future integrated physics and engineering design will drive NSTX-U liquid metal system requirements, and this, in turn, will inform the design and eventual construction of the liquid metals laboratory.

With the completion of defined program needs, a proposed new structure meeting International Building Code (IBC) and National Fire Prevention Association (NFPA, 5000, 484, and 45) standards which include features such as an argon clean agent fire suppression system and stainless-steel plating under experimental equipment may be needed. PPPL is actively investigating options to meet these needs via partnership and collaborations with other laboratories as well as considering on-site new construction options.

Renovations in Support of the Microelectronics and Sustainability Initiatives

PPPL is pursuing the development of new low-temperature plasma applications in advanced nanofabrication for microelectronics, quantum information science (QIS), and sustainability science. Renovated laboratory space in the Component Assembly and Storage (CAS) Building and L-Wing will create a modern Low-Temperature Plasma Laboratory, that will support this new, unique, and multidisciplinary research initiative focused on developing the scientific understanding necessary to develop the next generation of microelectronics, quantum devices, and sustainability efforts.

The renovation of L-wing lab spaces will house diamond co-doping reactors, microwave plasma-enhanced chemical vapor deposition (CVD) crucial to understanding and control of plasma-surface interactions at the atomic scale using *in-situ* plasma diagnostics. The renovation of the L-wing labs is targeted for completion in early FY 2023.

The Low-Temperature Plasma Laboratory will support the quantum diamond CVD program, associated projects, and the Lab's sustainability efforts in a contiguous space capable of housing several support areas integral to experimental activity. The design and program for the new building is in progress, with a targeted occupancy of mid-FY 2024.

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 2027, the completion of the RCC and CVHub do not come in time to meet the needs for near-term domestic and international collaboration. To address this gap, the VizWall Modernization for Visualization and Conferencing project is being proposed. 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.

PPPL's Fusion Research and Technology Hub (FuRTH)

PPPL's vital, growing external partnerships – research programs sponsored by private industry and/or a number of foundations – are not supported by PPPL's current campus layout or available infrastructure. These partnerships must be fostered to continue supporting efforts for national competitiveness in meaningful collaboration toward the development of technologies of the future. FuRTH is envisioned to support formal public/private partnerships to further enable advancements of fusion technologies. The Fusion Research and Technology Hub (FuRTH) would consist of the existing TFTR test cell, surrounding work area, and a new collaboration office building on D-Site to support science, engineering and operations collaborators.

The test cell space, created through completion of the Tritium System Demolition and Disposal (TSDD) Project, makes available a shielded, concrete space measuring 148' x 115' x 54.' This high-value infrastructure will support PPPL's initiatives to grow and diversify its R&D portfolio. Removal of the neutral beam boxes in the Test Cell, as well as the Tritium process systems in the basement below, will provide valuable experimental space for PPPL's industrial partners, especially local fusion start-ups. The TSDD project is now underway with expected completion in FY 2023.

The TSDD Project is currently in the process of removing the PPPL Tritium Systems. In early March, the Torus Cleanup System molecular sieve dryer beds were removed and disposed of as waste which represented a 96% reduction in the site inventory of tritium. This action is expected to lead to the reduction from Haz Cat 3 for the remainder of the project.

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.

The FuRTH office building is proposed to be constructed adjacent to the Test Cell to enhance laboratory operational efficiency and diversify PPPL's research portfolio. Its proximity to the active experimental areas will offer flexible, transient office space and proper security controls to accommodate on-site private industry research partners. This new building will provide two stories of working spaces to accommodate:

- Researchers and technicians employed by these collaborating companies;
- PPPL researchers and operations staff supporting this research;
- Additional PPPL staff necessary for supporting growth of research programs; and
- Provide much needed, and timely, swing space as staff is displaced to construct PPIC.

Facility for Laboratory Reconnection Experiments (FLARE)

Magnetic reconnection – the topological rearrangement of magnetic fields – underlies many explosive plasma phenomena at all scales in the visible universe. PPPL, with funding from DOE and Princeton University, is working to complete the upgrades to the Facility for Laboratory Reconnection Experiments (FLARE) for operation at PPPL. FLARE will provide the first laboratory access to reconnection involving multiple X-lines, the regime of the most astrophysical interest. To date, the FLARE facility relocation and upgrade is about 75% complete. PPPL aims to begin FLARE operation in early 2023, with participation from external users enabled by DOE's MagNetUS program.

General Infrastructure Supporting Research

Many elements of the PPPL infrastructure need upgrading, renewal, or replacement to enable the current and future mission. Frequent failures, including electrical subsystems, chilled water, and potable water have had direct impact on PPPL's ability to conduct research and meet DOE objectives. For example, a chilled water failure in February 2021 impacted the LTX-beta run capability, and a potable water failure in June 2021 resulted in Lab evacuation until temporary repairs were in place. While emergency repairs are completed, PPPL continues to implement its planned infrastructure improvements.

Over 40 years old, the D-Site infrastructure is deteriorating and lacking in the environment to support ever increasing levels of scientific research needs. In April 2021, roof replacement for four buildings on D-Site was completed. The project incorporated a vastly increased level of insulation and 100,000 SF of new roofing, associated removal of abandoned HVAC equipment, new fall protection, and fixed ladders and stairs. The total project cost was $4.3M. Construction started for the replacement of all series 100 HVAC systems and instrumentation, which includes the conversion from pneumatic to digital (DDC) system controls. The total project cost is projected to be $9.3M. Also, in 2021, designs were completed for enhancements to building safety components, and the replacement of the D-Site building envelope to replace deteriorating building exterior panels and replace them with a high efficiency, highly insulated, functional, and aesthetically pleasing building exteriors. These projects will significantly reduce energy consumption and improve the environment to better support the activities and personnel working in this complex.

Site Sustainability Plan Summary

Princeton Plasma Physics Laboratory (PPPL) strives to be a sustainability leader within the Department of Energy (DOE), while simultaneously acknowledging the challenges of executing sustainable projects for laboratories. Sustainability, in the context of integration of sustainable technologies and concepts into projects identified in the Campus Master Plan, suggests both an aspirational and realistic approach to achieve the maximum benefits using current technologies and allowing for the potential to integrate new solutions over time. The DOE sustainability goals are fully integrated into PPPL's ISO14001-certified Environmental Management System (EMS) as EMS objectives and targets. PPPL has begun developing a climate vulnerability assessment and resilience plan (VARP) under the DOE's sustainability reporting program. This plan will identify critical site assets, assess their vulnerability to climate impacts, and outline a portfolio of potential resilience strategies. We expect that this plan will inform development of the campus plan in future years.

PPPL's FY 2020 Scope 1 and 2 greenhouse gas (GHG) emissions were 78.1% below the FY 2008 baseline. This is primarily due to reduced fugitive sulfur hexafluoride (SF6) emissions from experimental power systems and reduced energy usage from the curtailment of onsite staffing in response to the COVID-19 pandemic. Scope 3 GHG emissions were 38.8% below the FY 2008 baseline primarily due to pandemic limits on travel, lower site electricity usage and associated transmission and distribution (T&D) losses, and reduced employee commuting resulting from curtailed onsite operations.

PPPL maintains a robust waste diversion program that achieved a combined recycling rate of 69% for municipal solid waste (58%) and construction waste (72.1%). 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) in FY 2021. PPPL continues efforts to facilitate the purchase of environmentally-preferable products through Lab-wide subcontracts and by enhancing sustainable acquisition guidance and resources available to employees. On-site renewable energy and high-performance building improvements continue to be emphasized in the Laboratory's Campus Plan.

The new PPIC building will be constructed with implementation of High Performance and Sustainable Building provisions in the design of the facility. PPPL continues to implement infrastructure projects and operational improvements to reduce its energy and water intensity. PPPL's total energy consumption for goal subject and excluded assets increased in FY 2021 compared to FY 2020 by approximately 3.9%, due to an increase in onsite work activity under PPPL's phased COVID-19 resumption plan. PPPL's potable water intensity (Gal/GSF) for goal subject and excluded assets decreased approximately 28% in FY 2021 compared to FY 2010. When comparing FY 2021 potable water intensity to the FY 2007 baseline, PPPL's water intensity decreased 41%, exceeding the 40% reduction goal.

PPPL ensures efficient management of its vehicle fleet through its annual vehicle and 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.

recent parking study has identified potential locations for longer-term deployment of EV charging stations and investigations to initiate some early installations are ongoing, with broader deployment being considered as part of the Critical Infrastructure Recovery and Renewal (CIRR) Project. The parking study also identified opportunities to reduce the heat island effect and stormwater quantity and improve quality. PPPL continues to explore opportunities to enhance its environmentally sustainable practices as it advances and diversifies research initiatives in fusion energy science, basic sciences, and advanced technology.

As seen in the chart below, the decrease in electric usage is linked to HEMSF-NSTX-U, which was last operational in 2016. NSTX-U's projected electric usage will increase concurrent with planned operations. The electric usage of the Princeton Plasma Laboratory Computing Center (PPLCC) is expected to double over the next 3-4 years due to the anticipated expansion in research computing.

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 2021 Lab Operating Costs:** $497.2 million
- **FY 2021 DOE/NNSA Costs:** $471.0 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $24.6 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 5.3%
- **FY 2021 DHS Costs:** $1.6 million

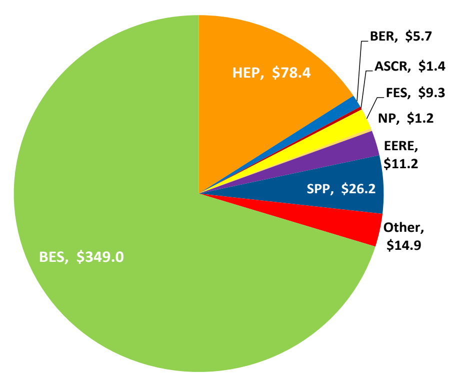
Physical Assets:

- 426 acres and 172 buildings
- 2.35M GSF in buildings
- Replacement Plant Value: $3.3 B
- No Excess Facilities
- 0 GSF in Leased Facilities

Human Capital:

- 1,685 Full Time Equivalent Employees (FTEs)
- 20 Joint Faculty
- 235 Postdoctoral Researchers
- 276 Graduate Student
- 37 Undergraduate Students
- 2,062 Facility Users
- 12 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Facility users as reported to DOE by the user facilities LCLS, SSRL, FACET-II, cryo-EM, and NLCTA

Mission and Overview

SLAC National Accelerator Laboratory is a vibrant multi-program laboratory that pushes the frontiers of human knowledge and drives discoveries that benefit humankind. We invent tools that make those discoveries possible and share them with scientists all over the world. Our research helps solve real-world problems and advances the interests of the nation. To date, four Nobel Prizes have been awarded for research done at SLAC.

SLAC sits on 426 acres of Stanford University land in the heart of Silicon Valley and is managed by the university for the U.S. Department of Energy (DOE). This unique partnership and support advances the work of the laboratory, providing infrastructure, capabilities, and expertise that amplify our impact across shared areas of focus, including sustainability research and industries of the future. SLAC runs five joint research centers with Stanford, and together we educate and develop the U.S. scientific workforce in key technological areas.

SLAC is the world-leading laboratory in X-ray and ultrafast science owing to our six decades of expertise developing critical accelerator concepts and technologies and to our two user facility light sources: the Stanford Synchrotron Radiation Lightsource (SSRL) and the Linac Coherent Light Source (LCLS).

LCLS is the world's first hard X-ray free-electron laser (XFEL) and a revolutionary tool for chemistry, materials science, biology, atomic physics, plasma physics, and matter in extreme conditions. SLAC is commissioning the upgrade to LCLS, LCLS-II, and developing a second upgrade, LCLS-II-HE. Each will provide a major jump in capability and ensure the U.S. maintains its leadership for years to come.

SLAC started 60 years ago as a place to discover fundamental particles and forces. Today, we deploy our scientific talent and technology from mile-deep caverns to an orbiting satellite in the search for dark matter, dark energy, and the fundamental nature of the neutrino. SLAC manages the construction and will manage the data center of the world's largest digital camera, which will produce panoramic images of the complete southern sky once installed at the Vera C. Rubin Observatory in Chile.

SLAC hosts, supports, and collaborates with more than 4,000 U.S. and international researchers – including many students – at SSRL, LCLS, the Facility for Advanced Accelerator Experimental Tests (FACET), and the Stanford-SLAC and National Institutes of Health (NIH)-funded cryogenic electron microscopy (cryo-EM) facilities.

SLAC's location in Silicon Valley and our connections with DOE, Stanford, and other leading research centers speed our progress. Through continued diversification of our research programs, SLAC aims to strengthen our impact, specifically exploring applications of our user facilities and core capabilities that support the broader DOE mission, the mission of other federal agencies, and expansion of our collaboration with industry.

Core Capabilities

The SLAC National Accelerator Laboratory's (SLAC's) mission is founded on unique user facilities, research capabilities, and scientific expertise, and the laboratory provides science and technology stewardship to the following seven U.S. Department of Energy (DOE) core capabilities:

1. Large-scale User Facilities / Advanced Instrumentation
2. Accelerator Science and Technology
3. Advanced Scientific Computing, Visualization, and Data
4. Chemical and Molecular Science
5. Condensed Matter Physics and Materials Science
6. Particle Physics
7. 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.

Linac Coherent Light Source (LCLS). LCLS creates X-ray pulses a billion times brighter than those generated by synchrotrons. The LCLS takes X-ray snapshots of atoms and molecules at work, revealing fundamental processes in materials, technology, and living organisms. Movies from these snapshots allow scientists to study chemical reactions, phase changes in materials, and proteins at room temperature. Each of the nine experimental stations is equipped with a suite of specialized diagnostics tailored to the broad user communities that access LCLS. Approximately 40% of beamtime is devoted to the chemical sciences (principally atomic and molecular science and catalytic chemistry), 40% to materials science (principally quantum materials, disordered materials, and materials in extreme conditions), 15% to biosciences (principally high-resolution structural biology and enzymology), and 5% to new methods development. Nearly 1,000 users access LCLS each year, with typically 30% new users and an over-subscription rate of 4-5x.

The LCLS facility incorporates the Megaelectronvolt Ultrafast Electron Diffraction (MeV-UED) instrument, which has a 100 femtosecond (fs) time resolution, making it the most advanced Ultrafast Electron Diffraction (UED) facility in the world. With the additions of a terahertz (THz) to mid-infrared pump source and a three-fold increase in repetition rate, the UED facility continues to expand our ultrafast science capabilities.

Stanford Synchrotron Radiation Lightsource (SSRL). SSRL is a synchrotron-based X-ray source equipped to generate extremely bright X-rays with high reliability and low emittance. At SSRL, researchers can study our world at the atomic and molecular levels, leading to major advances in energy production, environmental remediation, nanotechnology, new materials, biology, and medicine. With its 25 X-ray beamlines with 33 experimental stations, SSRL provides unique educational experiences and serves as a vital training ground for future generations of scientists and engineers. Our accelerator research and development (R&D) program aims to improve the performance and reliability of the accelerator complex to meet the needs of academic, national laboratory, and industrial users. The addition of undulator beamlines will form new bridges to LCLS.

Cryo-Electron Microscopy (EM)/Electron Tomography (ET). SLAC operates one of the world's leading centers for cryo-EM research and technology development. Its seven state-of-the-art instruments can, at near-atomic resolution, image single particles and create 3D images through cryotomography. The Stanford-SLAC cryo-EM facility, accessible to SLAC and Stanford researchers and external collaborators, operates four instruments with the remaining three available at the Stanford-SLAC Cryo-EM Center (S^2C^2). The recently funded Stanford-SLAC CryoET Specimen Preparation Center (SCSC) will add to the growth in available technologies. Coupling these new capabilities with SSRL and LCLS end station programs will allow researchers to use a multipronged approach, over a range of time and length scales, to investigate the structure and function of biological materials. The current focus is on addressing and meeting COVID-19 research needs.

Facility for Advanced Accelerator Experimental Tests (FACET-II). See "Accelerator Science and Technology" core capability below.

Particle Physics facilities and instruments. See "Particle Physics" core capability below.

Advanced instrumentation. SLAC is an international leader in the development of advanced instrumentation and computational tools to serve the needs of our facilities and scientific mission areas supported by a suite of cutting-edge technical competencies and expertise in detectors, electronics, data management systems, lasers and X-ray optics, THz/high-power radio frequency (RF) technologies, sample preparation methods, and sample delivery environments. An integrated co-design framework allows us to optimize instrumentation from the source to the data acquisition system and address the needs of massive-scale data analytics. SLAC is expanding high-power RF capabilities in the emerging THz frequency regime, providing new flexible pump sources for high-repetition-rate ultrafast X-ray sciences. Our development of a novel femtosecond (fs) laser system has demonstrated the highest average power in the world for this type of laser system. The Nano-X laboratory aims at advancing nano-optics for shaping X-rays in space and time at LCLS and DOE synchrotron facilities. Our renowned detector R&D group is conducting a program on ultrahigh-rate detectors to enable ultrafast (megahertz) science. The program promotes an integrated co-design framework leveraging multidisciplinary expertise across the laboratory to address the challenges of detectors' high-rate operation and data production. This framework allows teams to form within agile structures, and pair scientists, detector developers, and computer scientists to optimize and accelerate the development cycle and meet the scientific timeline of the experiments at our facilities.

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), LDRD investments, and Strategic Partnership Projects (SPP) from National Institutes of Health (NIH). SLAC's efforts support the DOE-SC mission and core capabilities in scientific discovery and innovation. Data Analytics at the Exascale for Free-Electron Lasers project (ExaFEL) is supported by the Exascale Computing Project, 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

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), LDRD investments, and Strategic Partnership Projects (SPP) from National Institutes of Health (NIH). SLAC's efforts support the DOE-SC mission and core capabilities in scientific discovery and innovation. Data Analytics at the Exascale for Free-Electron Lasers project (ExaFEL) is supported by the Exascale Computing Project, 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.

Free-electron laser R&D. The current LCLS instrument upgrades will increase the free-electron laser (FEL) pulse repetition rate, enabling one instrument to operate in a highly stable continuous wave (CW) mode and deliver uniformly spaced bunches. Our Research and Development (R&D) program aims to completely control the spectral and temporal properties of the X-ray beam, critical for the full discovery potential of LCLS and upgrades. Our program has successfully and continually streamed new tools and technologies to our scientific users. Recently, the X-ray laser-enhanced attosecond pulse (XLEAP) generation program has demonstrated high power sub-femtosecond (fs) pulses in the soft X-ray regime, and a SLAC LDRD funded project has demonstrated the optics feasibility and alignment precision of an FEL scale cavity.

MeV-Ultrafast Electron Diffraction. Our MeV-UED R&D program has led to a new paradigm in ultrafast electron scattering, producing a broad array of scientific opportunities in materials science and chemical dynamics. To enable Grand Challenge science and broaden the scientific reach of UED, the program is developing a new generation of ultrafast high-brightness electron beam and detector capabilities. These developments will broaden our scientific reach into the realms of bioscience and liquid-phase dynamics with improved time resolution, direct electron detection capabilities, and kilohertz (kHz) pump-probe acquisition rates.

High-brightness electron beam generation. SLAC recently launched a comprehensive R&D program on high-brightness beam generation. A high-brightness electron beam at the undulator is a key component for generating coherent hard X-rays and is also critical for future experiments in UED/ultrafast electron microscopy (UEM) and plasma wakefield acceleration (PWFA). The R&D program includes detailed start-to-end simulations to solve problems that degrade beam emittance and is developing superconducting radio frequency (SRF) electron sources and plasma-based sources critical for the success of future X-ray experiments, UED/UEM, and particle colliders.

Facility for Advanced Accelerator Experimental Tests (FACET-II). FACET-II will allow SLAC to maintain leadership in the development of beam-driven PWFA. The 10 gigaelectronvolt (GeV) electron beams from the new FACET-II photoinjector are ideally suited to studying high-gradient acceleration of beams with state-of-the-art quality. The unprecedented peak-currents achievable will enable research into high-intensity gamma ray bursts from plasma instabilities and ultralow emittance beam generation from plasma-based injectors. Plans are under development to add high-energy high-intensity positron beams, a capability that will be unique in the world and an essential tool for identifying techniques for high-gradient acceleration of positrons required for plasma-accelerator-based linear collider designs.

Advanced RF accelerator technology. New RF accelerator technology developments are enhancing the capabilities of existing DOE accelerator facilities, along with new initiatives from electron, hadron, and radionuclide medicine to X-ray, gamma ray, and deuteron sources for national security to materials processing. Our DOE-HEP stewardship programs have developed extremely high-efficiency high-intensity linear accelerator (linac) and deflector designs for electron and ion beams. The integration of new superconducting thin-film deposition tools will allow us to design innovative RF linac topologies. To support the mission of revitalizing the domestic industrial accelerator technology base, we are evaluating the facility improvements needed to integrate this capability and secure our global leadership position in accelerator science, technology, and engineering.

Educating the next generation of accelerator physics leaders. The renowned SLAC-Stanford accelerator education program benefits from the science and engineering challenges we tackle and our unique set of accelerators and test facilities, where graduate students and postdocs can acquire hands-on experience needed to further their careers. This program has produced more than 60 PhDs in accelerator physics, including multiple awards for the American Physical Society thesis award in beam physics.

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.

Advanced Computer Science, Visualization, and Data

In 2022, the SLAC Shared Science Data Facility (S3DF) will start supporting all data-heavy computing workflows from LCLS, UED, cryo-EM, and Rubin pre-ops. The initial installation will provide 2 petaflops in CPUs, 5 petaflops for accelerated computing, and 30 petabytes (PB) of storage, including 3 PB of flash-based burst buffers. A new data reduction pipeline (DRP), integrated with S3DF and capable of extracting key features of the data generated by the LCLS upgrades, is also being deployed. To this end, several optical fibers have been installed between the experimental areas and the SRCF, the data center hosting the DRP and S3DF.

SLAC has several ongoing world-leading efforts around advanced data systems: on-the-fly data reduction and monitoring for multiple TB/s throughputs; workflow automation, including interfacing to the Superfacility API for offloading data processing at DOE High End Computing (DOE-HEC) centers; artificial intelligence and machine learning (AI/ML) training and inference workflows; integration of user-developed algorithms within the data pipeline; edge computing and edge-ML, including processing for multi-megapixel detectors operating in the tens of kHz range; ability to redirect data analysis to multiple supercomputers depending on availability; ability to scale data analysis frameworks to the exascale regime; and integration and development of modern libraries (e.g., Legion) and advanced features for existing tools (e.g., HDF5).

The major contributors to the SLAC advanced data systems efforts are from DOE-SC, primarily DOE-BES and DOE-HEP, with DOE-FES and DOE-BER also providing critical funding. All SLAC data systems capabilities are closely driven by the need to handle experimental and observational data generated by DOE facilities and missions, including the SLAC X-ray FEL (XFEL), cryo-EM, UED, and several astrophysics programs. None of these undertakings would be successful without an advanced infrastructure able to acquire, reduce, process, and manage the massive data throughput generated by these experiments.

Funding for this core capability comes from DOE-HEP, DOE-BES, DOE Advanced Scientific Computing Research (DOE-ASCR) and local SLAC/Stanford investments.

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 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, we have 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. We also 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) and contribute their expertise.

Ultrafast chemical science. The movements of atomic nuclei and electrons that drive chemical reactions take place on attosecond to picosecond timescales, 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 Photon Ultrafast Laser Science and Engineering (PULSE) Institute. The scope, depth, and experimental capabilities of our 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. 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, along with our world-class materials synthesis, characterization, and theory activities.

Our 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. SLAC scientists partner with Stanford through the Precourt Institute for Energy and through the development of the new School for Sustainability, which fosters outreach activities for energy science education and training, thus helping to develop the next generation of talent.

Our scientists develop and use X-ray beamlines at our facilities to implement SLAC's ultrafast materials science strategy. We exploit our world-leading light sources and UED facility to pursue important scientific lines of inquiry identified in recent Basic Research Needs (DOE-BRN) workshops and roundtable reports. This work has 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 LCLS-II, a golden age of scattering and spectroscopy is emerging, bringing unprecedented opportunities for understanding, designing, and manipulating materials at angstrom to micrometer (µm) 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 in teasing out how their physics evolves in response to external factors. This exploration not only is of fundamental scientific interest, but also is essential for designing new materials with properties tailored for a wide range of technological applications 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 DOE-Energy Efficiency and Renewable Energy (DOE-EERE) and LDRD investments. It serves the DOE-SC mission in scientific discovery and innovation).

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 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? In pursuit of these 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 are also using these capabilities to build the Large Synoptic Survey Telescope (LSST) camera for the Vera C. Rubin Observatory, located in Chile, South America. We continually find ways to apply these tools and develop new ones for expanding the frontiers of discovery.

Advanced quantum devices. Our quantum program has several thrusts that will be enabled by the Detector Microfabrication Facility (DMF) we are currently constructing with Stanford support. This new capability for the DOE complex will allow us to produce superconducting devices on a large scale. Our thrust in "quantum sensor supremacy" involves developing more sensitive quantum sensors to carry out previously impossible probes of fundamental physics. Quantum simulations explore fundamental physics, such as black hole pairs. Quantum transduction allows sensing and simulation at a broader range of length scales and with more degrees of freedom. These abilities are critical for the high energy physics programs in quantum information science (QIS), Dark Matter New Initiatives (DMNI), and studies of the Cosmic Microwave Background (CMB) radiation, as well as for enabling technology for future research in fundamental physics. We will also broadly impact society in areas such as biomedical imaging, drug discovery, and new materials development.

Large-scale microfabrication of superconducting devices. With our expertise in designing and building arrays of superconducting devices and readout systems, we are playing a major role in building the Cosmic Microwave Background Stage 4 (CMB-S4) project. In addition, the DMF will provide science grade wafers, a core element of the project. These technical contributions combined with earlier work in the Background Imaging of Cosmic Extragalactic Polarization (BICEP) CMB program will allow us to use CMB-S4 data to contribute to studies of cosmic inflation, neutrino masses, gravitational lensing, and the evolution of galaxy clusters.

ATLAS detector systems. The A Toroidal LHC Apparatus (ATLAS) experiment at the Large Hadron Collider (LHC) 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 and the U.S. pixel staves, as well as studies of pile-up and jet reconstruction. We also have a major role in the construction of the most important detector subsystem. We contribute infrastructure and expertise in several key areas, including 3D and complementary metal oxide semiconductor (CMOS) pixels, strip detectors, and high-speed data transmission and readout.

Time projection chambers for neutrino research and dark matter. SLAC's two major neutrino programs – the Enriched Xenon Observatory (EXO) search for neutrinoless double beta decay (NDBD) and the Deep Underground Neutrino Experiment (DUNE) to study neutrino oscillations – are powered by our expertise in liquid noble time projection chambers (TPCs), associated high-speed readout and purification systems, and ML analysis reconstruction techniques. SLAC and Stanford led the development of EXO-200, which made important contributions to NDBD limits and first observed the two-neutrino process. That success positions us for a leading role in the next NDBD program, where one of the leading candidate technologies is the next Enriched Xenon Observatory (nEXO), a multi-ton scale-up of EXO-200. For DUNE, we have a leading role in developing the project's near detector. Our Liquid Noble Test Facility (LNTF) will help build and test prototypes for this concept and play a critical role in the final design process of the near detector. The LNTF and our experience in building the LUX-ZEPLIN (LZ) liquid xenon (LXe) TPC provide a critical core capability to lead a generation-3 (G3) dark matter experiment.

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 minimizes power consumption, increases reliability, and reduces the overall costs for the final application. These chips can also be used 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.

Funding for this core capability comes from DOE-HEP and DOE Nuclear Physics (DOE-NP), as well as SPP from the National Science Foundation (NSF) and NASA, and LDRD investments. SLAC's efforts serve the DOE-SC mission in scientific discovery and innovation.

Plasma and Fusion Energy Science

The SLAC program in plasma and fusion energy sciences exploits the laboratory's unique combination of high-power lasers and LCLS, which has launched a new era of precision in high energy density (HED) science by probing ultrafast changes of matter in extreme conditions (MEC). Fusion science research drives new technology developments in 100 hertz (Hz) repetition rate and high-power petawatt-class lasers and develops the physics of energetic phenomena and radiation sources that are 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 (WDM) states with an accuracy that makes critical experimental testing of physics models possible. This testing is important for the design of full-scale fusion experiments. They also provide understanding of structural, transport, and radiation physics properties of fusion plasmas. These programs were recently expanded through new capabilities at LCLS that include probing of electrical conductivities of MEC.

Theory and simulation. Another major research area is the development of methods to use high-power, short-pulse lasers to accelerate particles in plasmas. Our experimental efforts are coupled to a theory program that can provide resolution at 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 our predictions have led to the demonstration of the first-order Fermi acceleration process that can lead to very high particle energies relevant to explaining the origin of cosmic rays. Through the HED program, we have created a new theory group, are expanding our footprint in the simulation of HED phenomena, and are exploring new scientific frontiers that our HED facilities – in particular the upgrade of the LCLS MEC instrument – are making accessible. We expect to make major advances by using novel ML tools to model experiments at realistic scales of time and space**.**

High-resolution diagnostics and technology. We have demonstrated ultrafast pump-probe experiments on WDM, 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 unique to ultrafast studies of dense plasmas.

HED facilities. Following the approval by DOE-SC of the MEC upgrade at Critical Decision 1 (CD-1), we have optimized the layout of laser drivers and diagnostic and target capabilities to maintain our world leadership role in this area. This upgrade includes a new separate underground hall and access tunnel to provide the required space and radiation shielding for petawatt (PW)- and kilojoule (kJ)-class laser drivers that have been endorsed by the 2020 Brightest Light Initiative and the 2020 Division of Plasma Physics Community Planning Process reports and are responsive to the recent National Academies report in this area.

Funding for this core capability comes from DOE-FES and LDRD investments and serves the DOE-SC mission in scientific discovery and innovation.

Science and Technology Strategy for the Future / Strategic Initiatives

SLAC contributes to meeting the nation's critical scientific and technological challenges through our diverse research programs, world-leading user facilities, strong relationship with Stanford, and Silicon Valley connections. The six ongoing strategic initiatives that focus our efforts and help us attract the world's best scientists and engineers are:

- **Lead the world in X-ray and ultrafast science** by solving the most difficult problems in chemistry, materials science, biology, and plasma physics using the ultrashort, ultrabright pulses of coherent X-rays produced by LCLS, the forthcoming LCLS-II, and future 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 our probing of 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
- **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 Office of Science mission
- **Build new capabilities for transformative quantum information science technologies** by leveraging QIS developments to address major DOE Office of Science research challenges, and by using SLAC's core competencies to further advance the frontiers of QIS
- **Drive biological, chemical, and materials science for sustainability** by leveraging our world-class facilities and unique partnerships to produce transformative research spanning from basic to applied science

Our vision, strategic initiatives, and core capabilities set the foundation for the laboratory's continued growth, ensuring the advancement of scientific discovery across the spectrum of Grand Challenges identified by the DOE, the nation, and the world.

Infrastructure

Overview of Site Facilities and Infrastructure

SLAC sits on 426 acres of land leased from Stanford. In 1962, DOE and Stanford signed an initial land lease agreement, which was renewed in 2010 and expires in 2043. The university has been extremely supportive of the laboratory's science and infrastructure development, directly contributing $150 million in building improvements over the past two decades. The strong partnership between Stanford and DOE facilitates SLAC's execution of seven DOE-SC core capabilities.

SLAC's total real property inventory consists of 364 assets, including 172 buildings, 166 other structures and facilities (OSFs), and 26 trailers. The most common land use of these properties is "mixed-use," composed of offices, laboratories, research facilities, and support structures. Approximately one-fourth of the square footage is dedicated to underground tunnels and unique experimental facilities – the largest and most important of which are the 2-mile-long Klystron Gallery and corresponding accelerator housing.

The utility infrastructure that serves as the backbone of SLAC's facilities and science mission includes electrical power, chilled and hot water, domestic water, fire protection systems, low-conductivity water (LCW), storm water, sanitary sewer, natural gas, telecommunications, and compressed air.

The average age of SLAC-operated facilities and utilities infrastructure is 39 years, with 37% of assets built more than 50 years ago. Since approximately 2004, Stanford has built seven facilities at SLAC. In that same timeframe, DOE has funded a combination of new construction and renovation projects for our facilities, resulting in seven High Performance Sustainable Buildings (HPSBs). This construction brings down the average age of all real property, but our utilities, especially around the original areas of the laboratory and along the linear accelerator complex, are still in dire need of renewal.

As we plan for mission need in the upcoming decade, it is vital to remain cognizant of our infrastructure's current state. We continue to assess the current conditions of our real property and build strategies to revitalize our laboratory. Investments support resiliency and redundancy of our utilities, provide flexible and collaborative spaces for a new era of science working environments, and modernize and expand existing facilities to support our growth and create high impact science today and into the future.

Campus Strategy

We manage our campus proactively – each investment is strategically aligned with our vision to be a world-leading laboratory. As illustrated in Figure 2 below, SLAC's ten-year investments in facilities and capital infrastructure are all planned to be executed in concert with major growth in science programs. In addition, this section includes both required and supplementary summary tables, as well as a discussion of current and future priorities supporting the laboratory's initiatives.

Unprecedented challenges in recent years have proven SLAC's preparedness and validated our commitment to plan infrastructure needs to include risk mitigation of various types. Climate change-driven wildfires in the local area threaten the reliable delivery of power to the laboratory. A global pandemic forced all to rethink and restructure onsite and remote labor forces. Economic changes and supply chain hardships have impacted the delivery of projects. Amidst all this change and uncertainty, SLAC, DOE, and Stanford demonstrated adaptability, flexibility, and an ability to maintain mission readiness for current and future science.

The pandemic dramatically changed employee work environments but also provided opportunities. SLAC developed guiding principles for our approach to onsite, hybrid, and remote work. Work agreements with staff define the near-term planning and staff commitment to these modes of work that create a unique opportunity to reduce commute related carbon emissions. Based on these work agreements, the laboratory's workforce is currently 45% on site, 30% hybrid, and 15% remote, and 10% are still being determined. Benefits of this included added flexibility on the use of space and an estimated decrease in commuting of more than 2,000 trips per week, reducing 1,500 metric tons of annual greenhouse gas (GHG) emissions.

Onsite activities will take advantage of more flexible use of infrastructure, including laboratories, instruments, and tools, available on an as-needed basis. Our "Future of Work" initiative will implement this type of responsive infrastructure in one of our largest administrative office facilities, Building 41. The "Building 41 Pilot" will use bookable touchdown spaces, workspace hoteling, contemporary furniture design, and updated technologies – all aimed at supporting a spectrum of work scenarios.

Our campus strategy is to ensure that our physical infrastructure is reliable, efficient, and effective. The SLAC Long-Range Vision Plan (2015) provided a blueprint for physical infrastructure that continues to guide our support of DOE's science mission over the long term. Our next update to this plan will require a significant paradigm shift that incorporates our Future of Work initiative. The strategy for achieving this vision includes a near-term focus to address current capability gaps and deteriorating utility infrastructure, thus enabling future science over the next 15-20 years. We will leverage both direct and indirect infrastructure investments to close gaps and maintain mission-ready facilities today and into the future.

SLAC's infrastructure investment strategy focuses on optimizing the use of current assets, expanding and/or modernizing facilities to provide flexible and adaptive spaces, and synchronizing stewardship of operations and maintenance (O&M) in support of current and future science missions. Our three campus strategy goals are:

1. Renew utility systems – create a resilient, flexible campus through a combination of indirect investment and line-item construction programs,
2. Transform the workplace environment – create flexible working environments through renovation and new construction that will foster cross-disciplinary collaboration and accommodate changes in workplace culture, and
3. Modernize SLAC's existing facilities – reimagine and repurpose our spaces by maintaining a prudent investment program, aligning with our mission strategies, and applying DOE's sustainability goals.

The figure below provides a location map of SLAC's 10-year planned programmatic and institutional investments and includes Stanford projects. Each project is listed under the campus strategy goal it meets, illustrating how various investments are leveraged for a unified infrastructure vision. Over the years, DOE programmatic and Science Laboratory Infrastructure (SLI) support has been instrumental in transforming the laboratory's physical character through new infrastructure systems benefiting scientific programs and continued fit-out of laboratory spaces. General Plant Projects (GPP)-SLI support has been essential in addressing severely degraded, aging critical electrical and cooling water systems. In addition, SLAC continues to increase the institutional infrastructure budget to fund small- and mid-scale projects such as roof renovations, underground leak repairs, replacement of underground cooling water piping and electrical infrastructure, and modernization of the cooling tower.

The investments described in the following sections demonstrate how our campus strategy optimizes systems for life cycle, systems management, O&M, and the integration of sustainability into each project.

Campus Strategy Goal 1: Revitalize and Modernize Utility Infrastructure

Utility resiliency and reliability are essential for meeting the requirements of user facilities, scientific instruments, laboratories, and experimental equipment. With construction of next-generation systems, high-energy accelerators, process plants, and state-of-the-art equipment, world-class science requires tight tolerances and high reliability. It is critical that we transform our aging infrastructure by modernizing systems to meet the demands of the science we support. Furthermore, modernization of infrastructure will help to mitigate emerging threats and operational risks and reduce carbon emissions through increased efficiency.

It is important to highlight that new high-energy science will result in significant increases in electrical consumption. Our energy demand is expected to double by 2027 in comparison to 2021, putting our electrical usage comparable to that of the mid-2000s. This reality requires us to create other opportunities to help offset the scientific electrical consumption. Increasing the utilization of carbon-free electricity to reduce electricity-based emissions is being pursued through the Western Area Power Administration (WAPA), on behalf of SLAC's participation in the electrical consortium. Demonstration of this commitment is underway with a long-term renewable energy power purchase agreement (PPA) that is being finalized. We anticipate that this agreement will provide 50,000 megawatt hours per year (MWh/year) of carbon-free electricity to SLAC within the next three years. A follow-up proposal for a larger solar power purchase project is also being investigated through WAPA.

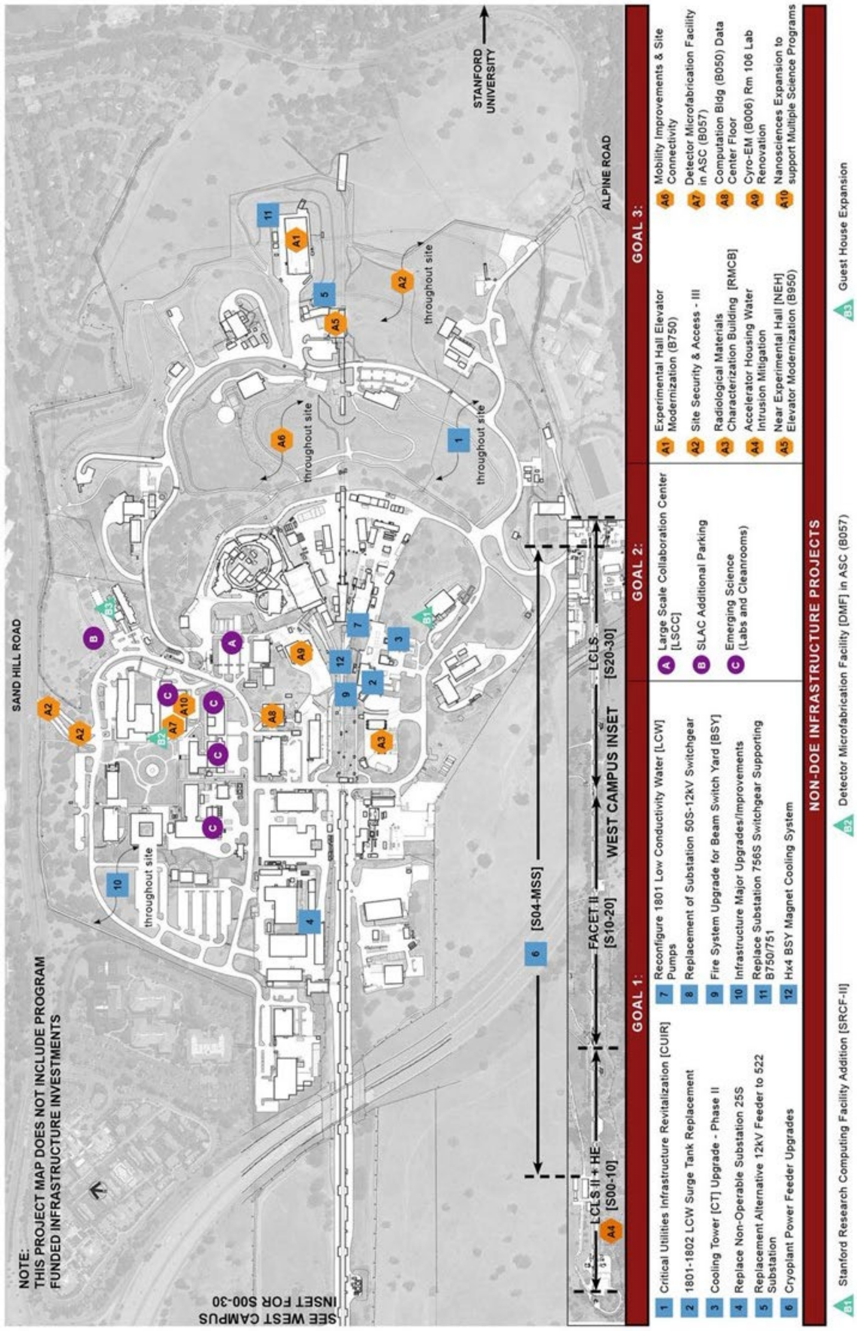


Figure: SLAC's 10-Year Planned Facility and Infrastructure Investments

Electrical Power

Our highest reliability risks continue to be in our legacy electrical infrastructure. Significant progress has been made over the last decade to upgrade major components. Since 2010, we have invested $67 million of direct and indirect investments in our electrical system and have implemented a robust maintenance plan. However, large segments of the original electrical infrastructure still require modernization. Ensuring reliable and resilient power requires a plan designed to manage the incoming power source, replace major systems, and address critical challenges for scientific operations.

In partnership with our utility provider, Pacific Gas and Electric Company (PG&E), we are installing devices to protect and ensure delivery on the DOE-owned 5.4-mile 230-kilovolt (kV) transmission line. Key to that delivery is vegetation management along the DOE power line easement corridor to protect from tree and fire hazards. SLAC successfully implements an annual vegetation management plan to target areas for removal and trimming based on aerial and ground surveys. This activity is a critical climate change vulnerability that is being proactively mitigated. SLAC has also awarded a System Impact Study to PG&E to evaluate and provide recommendations on increasing power on the alternate incoming power source. This study is expected to be completed this year and will inform the laboratory's resiliency and business continuity plans.

In 2021, SLAC completed a 12 kV feeder cable replacement project for the LCLS region of the Klystron Gallery, accelerator housing, and Cryoplant to provide redundant feeders to these areas. Approximately 40,000 linear feet of aging cabling were removed and replaced to protect electrical capability and eliminate hazards. In 2022-2023, we are executing a project to replace a nonoperable substation (Substation 25S) to provide reliable power distribution to six critical support buildings.

Major maintenance and repair activities are focused on our master substation, user facility substations, and power distribution cables to mitigate resiliency risks to the various programs we support. We have implemented a distribution relay replacement program with the goal of giving us full visibility on system status and moving toward full Supervisory Control and Data Acquisition (SCADA) with data analytics capabilities in the future. Important to the efforts described above is the development of Electrical Requirements documents by our Facilities and Operations (F&O) systems stewards to identify priorities for future system upgrades.

Cooling Water

Our next highest operational reliability priority is the revitalization of cooling water systems. Both Science Laboratory Infrastructure General Plan Project (SLI-GPP) and SLAC indirect investments have been leveraged in recent years, with major accomplishments completed in 2021 and others soon to be completed. These projects will benefit critical cooling loads in the linac's beam switch yard (BSY), which delivers "beam" to various science programs downstream: SSRL, LCLS experimental halls, and research end stations and yards.

Modernization of Cooling Tower 1701 (a SLI-GPP project) is nearly complete, providing a more reliable and efficient cooling system to support the needs of the linac, SSRL, and the eastern end of the SLAC campus. Additionally, this upgrade provides much more efficient pumps and fans that reduce energy consumption and water losses from overspray. These features are estimated to save over 500,000 gallons of water and 1.1 MWh of electricity annually. A follow-on Phase II project will also modernize redundant, backup cooling capacity currently supplied by a portion of the original legacy cooling tower infrastructure. The Heat Exchanger 2 installation is substantially complete and will provide critical cooling for the linac beam dumps. We recently completed an upgrade to heat exchanger control valves, allowing finer control to support operations to user facilities at SSRL and LCLS, as well as to programs at the end stations for DOE-HEP.

Additional projects underway include replacing obsolete pumps at the LCW pad that supports SSRL and the linac BSY. The modern replacements will provide a reliable and efficient system for years to come. Another project involves upgrading the system that provides magnet cooling water for the linac BSY. In addition to cooling water and LCW, the second of the two air compressors that provide site-wide compressed air necessary for many scientific control systems and building systems will be replaced this year, providing a complete modernization of this system.

Underground Utilities – Sanitary Sewer & Storm, Domestic Water, and Telecommunications

Capability gaps contributing to operational risks also include the state of the following underground utility systems: sanitary sewer and lift stations, storm drainage, domestic water and fire protection, natural gas, and telecommunications. Much of this infrastructure is degraded and past its normal service life, and in some cases, this has already reduced system capability. In 2022, we are targeting two critical sanitary sewer lift stations in the research yard. One has already failed, and the other is at high risk of failure. These have been funded through institutional indirect investments and are being replaced by the end of the calendar year.

In the case of telecommunications, adding capability is difficult because current pathways are full. Assessments will commence to determine how computing and critical fiber optics communications networks will be modernized to support both current requirements and the additional capacity requirements that will be realized once new science projects, such as LCLS-II, LCLS-II-HE, MEC-U, and the Rubin U.S. Data Facility, are operational. Modernization of this infrastructure will also improve SLAC's cybersecurity posture and response readiness.

Critical Utilities Infrastructure Revitalization Project

CUIR is a SLI line item (LI) infrastructure investment project developed to modernize utilities infrastructure to provide reliable and sustainable operations, enabling SLAC to remain mission ready for users, researchers, and staff scientists to deliver world-class science and enhance the impact of DOE's scientific programs. CUIR contains key aspects that directly address the DOE sustainability goals for SLAC as well as support progress toward a sustainable laboratory. CUIR received CD-0 approval from the Energy Systems Acquisition Advisory Board (ESAAB) in May 2019 and CD-1 ESAAB in January 2022 with a Total Estimated Cost (TEC) range of $160 million to $307 million. The project is tailored into three subprojects to address laboratory requirements and priorities, take advantage of operational downtimes to perform construction activities, and sequence construction activities to mitigate mission impacts. The subprojects are planned to be executed in phases to ensure adequate resources are available for successful planning, coordination, and implementation.

- **Subproject 1 – Critical Electrical Work (FY 2022 to FY 2028).** Critical Electrical Work (Subproject 1) is focused on improving reliability and redundancy along the linac to support LCLS-II-HE, FACET-II, LCLS, and the Cryoplant. The critical electrical work includes modernization of the SLAC master substation by replacing and upsizing the existing vintage 12.47 kV transformers and switchgear, paired with modernized Supervisory Control and Data Acquisition (SCADA) to further enhance energy metering and energy dashboard functions. Moreover, construction of new electrical 12.47 kV circuits pathway along the Klystron Gallery and a new substation (K-5B) will reduce energy inefficiency losses and increase power distribution capacity to the linear accelerator for LCLS-II-HE. Subproject 1 increases the flexibility in SLAC's power system and opens more windows and paths to energy utilization. The modernized electrical equipment and controls directly support DOE's energy tracking and operational efficiency goals and will reduce energy use and GHG generation. Subproject 1 will also improve power resiliency at SLAC by providing standby power for the Cryoplant to ensure continuous operation in the event of an unplanned power outage.
- **Subproject 2 – Linac Utilities and Equipment (FY 2024 to FY 2029).** Linac Utilities and Equipment (Subproject 2) is focused on modernization and increased reliability of the civil and mechanical systems along the linac. Subproject 2 includes replacement of the aged and deteriorated water main pipeline to provide domestic water and fire protection, leaking sanitary sewer and deteriorated pumps to reduce the risk of hazardous leaks and shutdown of waste management facilities, stormwater drain piping to reduce the risk of flooding and undermining, and the addition of water piping to improve resiliency. Subproject 2 also includes replacement of pumps, heat exchangers, valves, and aged piping in the klystron, waveguide, and accelerator LCW process water systems. Upgrades to SLAC's sanitary sewer systems will better protect the environment by reducing the number of spills. Furthermore, upgrades to our storm drainage system will reduce sediment entering the pipes and impacting SLAC's storm water quality.
- **Subproject 3 – Sitewide Utilities (FY 2027 to FY 2030).** Sitewide Utilities (Subproject 3) includes additional sitewide upgrades, with a focus on mechanical systems and implementation of sensors, controls, meters, and data analytics on infrastructure utilities. The newly installed sensors and data analytics system will allow more efficient control of cooling towers and LCW mechanical systems, where

water use efficiency, power consumption, and early leakage/abnormal temperature fluctuations in the system will be recorded, analyzed, and optimized. Subproject 3 directly supports the DOE utility metering goal and increases the potential for identifying inefficiencies to enable GHG reduction.

The CUIR project is anticipated to reduce approximately 30% ($25 million) of SLAC's deferred maintenance (DM) backlog. Upon completion of CUIR, our utility system will be modernized with additional sensors, controls, and meters to enable data analytics and achieve higher operational reliability, optimize usage, attain faster diagnostics, and fine-tune analysis. Completion of CUIR is essential for the continued success of DOE's science programs.

Campus Strategy Goal 2: Flexible and Adaptive Spaces for Groups to Work Collaboratively

SLAC's campus vision and strategy advances our core competencies, as well as emphasizes collaboration. Reviewing operational lessons learned from the COVID-19 pandemic on how we interact onsite highlighted the importance of creating new opportunities for collaboration in our facilities, such as:

- Incorporating flexible and adaptive spaces to mix on- and off-site colleagues,
- Creating/Implementing new designs to focus on optimizing the use of both interior and exterior meeting spaces,
- Patterning of pedestrian traffic intersections, and
- Enhancing cross-research planning to foster organic collaboration.

The concept for touchdown and temporary workspaces has already proven successful in the Arrillaga Science Center (ASC), which hosts a range of laboratory and office support spaces that create opportunities for collaboration among the hosted programs and collaborators. We are developing centralized focal areas for collaboration around the Quad, which serves as a natural outdoor meeting place for formal events and informal exchanges.

Large Scale Collaboration Center

The LSCC (CD-1 Q1 FY 2020, cost range is $58.4 million to $92.4 million, TEC $64 million) represents a new model and vision to provide collaborative spaces for developing new science. While the ASC already delivers multi-mission laboratory and office spaces, the LSCC will provide an advanced research and visualization facility for massive-scale data analysis between disparate user groups. The facility is designed to allow deep collaboration among programs, such as LCLS-II and LCLS-II-HE (DOE-BES, NIH), and large data streams from the Vera C. Rubin Observatory (DOE-HEP, NSF), FACET-II (DOE-HEP), SSRL (DOE-BES, DOE-BER), cryo-EM (DOE-BER, DOE-BES, NIH), and associated DOE-ASCR activities. Further, SLAC's beamline and accelerator staff and data analytics scientists will gain access to advanced tools and simulation codes linked to our HPC and across the DOE complex.

Science drivers for the LSCC are as follows:

- Major science facility upgrades noted above in 2020-2025 will result in substantial increases in data rate.
- Science innovations will require advances in data analytics.
- LSCC will act as a focal point for harnessing this data to tackle the Grand Challenges in science.
- Strong flow of ideas among large-scale programs at SLAC will encourage co-development between the sciences.

The LSCC is being designed to explicitly enable data scientists and data analytics staff to gain real-time, massive-scale data analytics in our X-ray and ultrafast science programs, physics of the universe, HED science, and bioimaging sciences. Early examples of a cross-functional approach have already produced remarkable results in the interpretation of complex images in a wide variety of situations through the application of data analytics methodologies.

Cross-fertilization of science and data ideas is envisioned across all DOE-sponsored programs at SLAC, augmented by the further development of many active Bay Area laboratory partnerships and Silicon Valley industry collaborations.

The LSCC will also help support growth at SLAC and will have the capacity to co-locate over 100 personnel from major programs. SLAC's population has been growing at an average rate of 4% per year over the past five years. While the new remote and hybrid work styles will accommodate much of this, the anticipated population growth by the time the LSCC is completed could be as many as 400 additional people.

Campus Strategy Goal 3: Modernize, Consolidate, and Repurpose Existing Facilities

Our new building designs will promote collaboration, synergy, flexibility, and sustainability; projects that modernize existing buildings must also meet these goals. Office space consolidation may provide increased opportunity for repurposing or excessing obsolete facilities. As we modernize our assets, we must incorporate adequate workspaces, information technology (IT), sustainability, and security infrastructure to secure DOE's resources of people, science, facilities, and equipment.

Initiatives to address climate risk vulnerabilities and carbon emission reductions are rooted in our modernization strategy. We are currently executing an ongoing effort to upgrade aged lighting in multiple facilities. We are focusing on science-supporting high bay buildings that utilize rows of 1,000 W lamps that were designed in the 1960s and are powered around the clock. Completed high bay upgrades (costing over $500,000) have annually reduced electricity consumption by 800 MWh and avoided 180 metric tons of carbon emissions.

Over the last decade, SLAC direct and indirect funding were invested in the modernization of our most critical infrastructure. The next phase of building modernization focuses on the major renovation of some of our most critical aging buildings that, despite best efforts and regular maintenance, have become "substandard" in their ability to provide the capabilities and configurations required by current and future science initiatives.

Site-wide Building Enclosures

The Site-wide Building Enclosures is an SLI-GPP request to upgrade and modernize 1960s- and 1970s-era buildings across the site that support mission-critical science and support functions. These facilities have long supported laboratories, specialized shops, and office spaces but are now affecting operations because major building enclosure components are beyond their useful life. Building envelopes, including roofs, doors, windows, and exterior enclosure materials, are severely degraded. Several facilities have been identified that are strategically located for optimal use; however, the facilities in their existing configurations do not support current science requirements. This project will improve overall workforce productivity in these buildings by repairing persistent water leaks and renovating facility systems to restore functionality.

Site Security and Access Improvements III

The Site Security and Access Improvements III project represents the final phase of a decadal long security modernization project and will complete the protection of DOE assets and enhance science collaboration across the laboratory. The project has been planned in two phases. The first will replace the main entrance gatehouse with a modern security dispatch center. The second phase will reconfigure SLAC's main entrance and exit at Sand Hill Road by reconfiguring the roads in a meandering pattern for a speed reduction effect, improving the walking paths, adding turnstiles, and adding bike lanes, all with the intent to improve both safety for security officers and efficiency in verifying access badges. The project will also install radiation portal monitors at SLAC's main entry and Alpine Road exit gates to reduce the risk of accidental offsite transport of activated materials. Additional security gate improvements will reduce the size of the accelerator gated access area, where the area around Positron-Electron Project Ring Road will be converted into a general access area for improved use.

Our campus strategy is driven by science needs and requirements, as well as funding sources. Projects are executed to ensure mission readiness of our facilities, and the process and project execution schedules are designed to remain fluid to meet changing needs.

Non-DOE Infrastructure Projects Supporting our Campus Strategy and Strategic Initiatives

As demonstrated by previous contributions, Stanford remains committed to SLAC and continues to drive the development of a “best-in-class” laboratory in support of the DOE mission. We continue to leverage this partnership to grow the laboratory with key support facilities benefiting DOE science programs, staff, and the user community. Such facilities already exist at SLAC with the ASC, SRCF, the Stanford Guest House, and the Arrillaga Recreation Center gym. Stanford now intends to expand these facilities by looking for opportunities to fit-out or complete construction of interior spaces without an assigned use and that remain in the ASC, double the capacity at the SRCF via the SRCF-II project, and possibly double the number of rooms at the Stanford Guesthouse to support the growing visiting user community at SLAC.

Detector Microfabrication Facility

Stanford and DOE have partnered for the construction of the DMF in the ASC, which will support our strategic initiatives in frontier programs in physics and QIS. This superconducting device foundry will consist of 5,500 square feet of Class-100 cleanroom space with tooling optimized for qubits, detectors, and advanced quantum devices. The DMF will leverage capabilities at SLAC in materials science and characterization to encourage the development of new materials and fabrication processes for quantum devices, deliver state-of-the-art quantum information technologies, and enable fundamental scientific discoveries. SLAC will install the required tools for this cleanroom after completion of the fit-out construction with initial occupancy planned for the summer of 2022 and transition to operations in 2023.

Stanford Research Computing Facility Expansion

Currently under construction, SRCF-II represents a Stanford commitment of approximately $40 million to add approximately 18,000 square feet, doubling both the footprint and peak power (from 3 MW to 6 MW) of the existing SRCF data center. Both SRCF and SRCF-II will support the SLAC-Stanford science research community by hosting HPC infrastructure in an advanced data center facility. SLAC will have access to half of the power capacity increase. This expansion is needed to support the Rubin U.S. Data Facility, enable real-time data extraction from LCLS-II and LCLS-II-HE, and provide support for science programs across SLAC and Stanford. The expanded facility will be flexible for varying HPC equipment loads within individual rack rows and be energy efficient with lower operational costs compared to traditional data centers. SRCF-II will provide an effective and efficient data center solution for DOE’s science mission computing needs.

Asset Management

SLAC's asset management program includes efforts supporting real property data accuracy, process improvements for condition assessment, and follow-on action preparation to ensure our facilities are mission ready. Activities include critical property management tasks, such as validating mission needs, budgeting for capital improvements, and determining facility life cycle. Decisions involve data gathering efforts enforced through DOE's Condition Assessment requirements and Facilities Information Management System (FIMS) Data Validations, and we have started the process for climate vulnerability and resilience planning assessments. Described below are SLAC's most recent DM trends, maintenance investment index (MII), overall asset condition(s) reflected in the condition index (CI), and replacement plant value (RPV). These ongoing efforts are key factors in the overall life cycle tracking of assets and provide the basis to achieve optimal facilities stewardship for SLAC's broader campus strategy and long-range vision.

Continued Data Accuracy and Process Improvement for Real Property Life Cycle Planning

In the last year, we have leveraged newly established relationships made possible by hiring actions and expanding Facilities Management and Planning (FMP) within F&O. These helped us pursue process and program enhancements that have enabled broader integration of teams across SLAC in the areas of planning, coordination with science and technical subject matter experts, operational support, project execution, and quality assurance. These process and program enhancements include cross-walking real property inventory data elements into our computerized maintenance management system (CMMS) and structuring our CMMS to streamline our annual actual maintenance (AAM) data collection and categorization. The FMP and technical teams continue to identify current impediments and assess current and future space utilization. Asset usage codes are assessed by planning and performing Condition and Functionality assessments, energy audits, and re-commissioning for energy efficiency, particularly for our mission-critical user facilities and utility infrastructure. This holistic approach better positions the infrastructure investment planning arm of F&O to determine the level of effort required to rectify deficiencies in the field, whether it is at the O&M Shops level for maintenance, a capital investment requiring SLAC indirect investments, or programming for a DOE GPP or SLI request.

Mission readiness applies not only to facilities, but also to our laboratory's general land use and the necessary removal of obsolete facilities to make land available for new mission requirements. FMP has heightened as a priority the need to act on standby facilities as one of our facility life cycle challenges. With a newly appointed excess facilities program manager (EFPM), strategically situated within FMP, we are updating our procedures for excessing facilities via the DOE-Asset Management (MA-50) process. We have also updated the existing Excess Facilities Program document to ensure it reflects current reporting requirements and coordination with the Site Office and MA-50. The EFPM will identify opportunities to dispose of old trailers and other obsolete structures that once supported science programs and have long since ended. These efforts will result in the removal of unnecessary real property from the site and reduce costs associated with surveillance, maintenance, repairs, and DM associated with these facilities. This will also help us right-size the real property footprint to meet our current mission need and make land available for future mission needs.

Maintenance and Repair

To update our RPV, our FIMS administrator utilizes standardized DOE RPV models with modifications to consider the uniqueness of our facilities. Consequently, our reported RPV increased from $3.1 billion in FY 2020 to $3.3 billion in FY 2021. This increase results from recalculating RPV models for our OSFs and utility infrastructure backbone. We will continue to review updates annually and gain DOE concurrence on the methodology, models, and factors used to adjust RPV to ensure that the indices derived are accurate.

DOE has historically assumed a "rule of thumb" maintenance target of 2-4% for the MII. MII is defined as the percentage ratio of AAM in relation to RPV as follows: MII=AAM/RPV. For FY 2021, our reported AAM was $25.5 million and RPV was $3.3 billion, which results in a low MII (0.77% across all property types). However, DOE MA-50 now recognizes that this target is typically assumed in commercial industry but may not represent the type of industrial infrastructure within the DOE complex. At SLAC, high-value/low-maintenance infrastructure items in the accelerator housing and experimental tunnels do not reflect the maintenance criterion of a 2% MII for conventional infrastructure.

MII values were calculated separately for operational assets by property type: building, trailers, and two categories of OSFs (utilities and other). The results are summarized in the table below. Also provided is the CI for each asset type, represented as the ratio of repair needs (RN) to RPV. While MII is low, the overall CI is relatively good when considered in relation to the average asset age. It is important to note that SLAC prioritizes mission-critical assets in its resource allocation strategy. Currently, 13% (49) of our properties are categorized with an operational status of standby, are not considered mission critical, and typically have a very low AAM, which results in a lower MII in general for our site. Overall continued investment in prioritized maintenance activities increased by 25% from FY 2020 to FY 2021.

The FY 2021 data illustrates our largest maintenance investment continues to be assets with the lowest CI, namely our aging utility systems. Most of the laboratory's utility infrastructure is old and inefficient, which increases overall maintenance and anticipated emergent repair costs. Our request for SLI-LI CUIR closes infrastructure capability gaps in mission-critical civil, mechanical, and electrical utilities. Generally, OSFs carry the lowest MII, as can be expected from high-value, low-maintenance facilities such as support structures that include retaining walls around the site, roads, and walkways. Although SLAC does not invest at the typical industry standard for buildings (MII of 2%), these assets are managed to keep them in relatively good condition, as demonstrated by the average CI of 92%.

Maintenance Investment Index and Average Condition Index
by Property Type for Operational Facilities

		Buildings		OSFs				Trailers	
				Utilities		Other			
AAM	**MII**	$13,159,379	0.53%	$11,860,005	1.73%	$329,217	0.27%	$103,953	0.95%
RPV		$2,486,705,979		$685,753,253		123,006,056		$10,927,438	
Average CI (percentage)		92%		75%		95%		83%	
Source: FIMS Year-End Data FY 2021									

Deferred Maintenance Trends

In 2017, SLAC re-baselined its DM from $26 to $80 million by applying 2016 DOE-SC Infrastructure – Mission Readiness Working Group guidance. In continuation of this effort, starting in 2020 and continuing into 2021, staff from ten DOE-SC and Office of Nuclear Energy (DOE-NE) laboratories collaborated to create a guidance document with the intent of enabling the laboratories to develop site-specific internal procedures that will foster consistent reporting across all DOE sites of values for RN, DM, and modernization of real property assets, such as buildings, trailers, and OSFs. SLAC utility stewards, who are subject matter experts responsible for assessing systems, used this methodology to validate their respective deficiencies.

As an integral part of SLAC's campus strategy, reducing DM is a weighting factor that drives the development of projects that range from significant SLI-LI construction efforts to Institutional General Plant minor repair projects. The Mission Readiness team has enhanced the Work Induction process and the Project Implementation Manual to close communication gaps among stakeholders and streamline these important procedures. Additionally, they have applied project mapping in the Condition Assessment Information System (CAIS) to accurately capture and track RN and DM associated with planned and active projects. This rigorous approach to determine the existing conditions of our utilities contributed to an increase in DM after a steady decrease between 2018 and 2019, as evidenced by a DM cost of $83 million for FY 2021.

It is important to note that the DM value is subject to many variables in any given year. Each year, deficiencies are removed as minor and major projects are completed. SLAC has been proactively reducing the DM backlog with laboratory indirect investments in infrastructure projects including electrical feeder and substation replacements, mechanical pumps, compressors, and sanitary sewer lift station replacements. Cumulatively, these will retire as much as $8 million when completed by end of FY 2022. The combination of our planned maintenance activities, corrective repairs, infrastructure investments, and proposed SLI projects will result in an anticipated 86% decrease of our current DM.

Site Sustainability Plan Summary

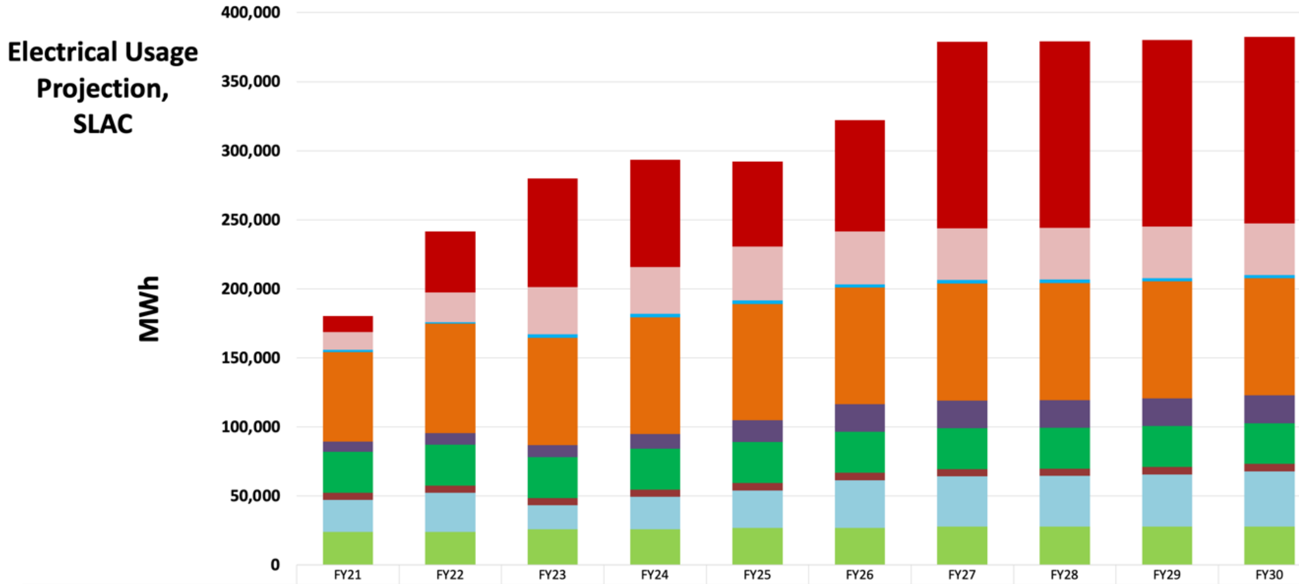
Our sustainability strategy is to optimize infrastructure system efficiency to reduce utility and resource consumption, optimize operations, and minimize carbon emissions. Sustainability is a cornerstone of the campus strategy goals to revitalize and modernize our laboratory's infrastructure. The examples below highlight some of the impactful actions taken to implement this plan:

- We engaged with energy consultants to verify performance of the revitalized heating, ventilation, and air conditioning (HVAC) and lighting systems at the Electronics Building Annex (Building 34) to close the gap toward certifying as a HPSB. SLAC also installed hands-free water conserving plumbing fixtures when updating restrooms, showers, and breakrooms. The cumulative upgrades over the last three years enhanced the workspace for the Accelerator Directorate Electronics Engineering Division while reducing building energy by 35%, saving $11,000 annually.
- We modernized Cooling Tower 1701 by incorporating variable cooling water pumps and fans, thus reducing pump energy consumption and overspray water losses. These features are estimated to save over 500,000 gallons of water and 1.1 MWh of electricity annually, equating to $70,000 annual savings.
- We have, over the last several years, proactively addressed climate risk vulnerabilities through wildfire mitigation with vegetation management along the five-mile-long SLAC 230 kV electrical transmission line. SLAC has initiated a climate risk vulnerability assessment, in line with recent DOE guidance, to identify additional risks and possible mitigations.
- We have reduced harmful emissions through a revised and more efficient shuttle service (Marguerite SLAC-Line) between the key science facilities at SLAC and the Engineering Quad at Stanford. The shuttle service revisions were based on feedback from a user survey that resulted in rerouting and revising the stops to achieve door-to-door service in 15 minutes, which is faster than self-driving, parking, and walking. The 100% electric shuttle buses replaced the former gasoline burning vehicles, which eliminates an estimated 3.2 metric tons in GHG tailpipe emissions annually.

Even with the improved efficiencies from the executed and planned state-of-the art energy and water infrastructure at SLAC, the nature of high-energy science will result in significant increases in electrical consumption as indicated in the figure below.

SLAC's sustainability and carbon emission management plans include the following efforts:

- We will invest more than $2 million over the next two years to support targeted energy conservation projects, operational maintenance reducing projects, and site-wide sustainability programs. To further progress toward near net-zero energy, water, and waste buildings, we plan to modernize buildings that support science programs through the proposed SLI-GPP funded projects. In addition, we will replace aged mechanical and electrical systems with modern high-performance counterparts to further enhance efficiency and resolve DM items.
- SLAC will also incorporate, in support of CUIR, advanced sensors and SCADA. These actions will support data analytics to enhance automation and optimize utility consumption in electrical, gas, water, and sewer systems.
- We will finalize efforts that are underway in partnership with our electrical consortium and the power utility WAPA on a long-term renewable energy PPA. SLAC is estimated to receive 50,000 MWh of solar carbon-free electricity, thus avoiding 11,000 metric tons of GHG emissions annually. This will effectively support the power needs for all of SLAC's office and laboratory buildings, except for high-energy science facilities.
- SLAC will create a strategy for increasing the purchase of carbon-pollution-free electricity to successfully execute the DOE guidance toward national emission reduction.



	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30
HEMSF LCLS-II	11,700	44,200	78,700	77,700	61,770	80,610	135,000	135,000	135,000	135,000
HEMSF FACET I/II	12,600	21,480	34,100	34,100	38,880	38,100	37,400	37,400	37,400	37,400
HEMSF HEP Test Fac.	1,600	820	2,400	2,400	2,400	2,400	2,400	2,400	2,400	2,400
HEMSF LCLS Accel	64,800	79,300	77,700	84,600	84,400	84,500	84,700	84,700	84,700	84,700
HEMSF LCLS Exp Fac.	7,700	8,580	8,800	10,500	15,760	20,000	20,130	20,130	20,130	20,130
HEMSF SPEAR3	29,600	29,600	29,600	29,600	29,600	29,600	29,600	29,600	29,600	29,600
HEMSF SSRL	5,100	5,170	5,250	5,270	5,300	5,300	5,300	5,300	5,300	5,300
Multi-prgm Support (Not Incl Goal Subj Bld.)	23,160	28,300	17,300	23,400	27,100	34,500	36,200	36,500	37,700	39,900
Goal Subject Bldg.	24,000	24,000	26,000	26,000	27,000	27,000	28,000	28,000	28,000	28,000

Figure: SLAC Electricity Usage Projection

THOMAS JEFFERSON NATIONAL ACCELERATOR FACILITY

Lab-at-a-Glance

Location: Newport News, VA
Type: Single-program Laboratory
Contractor: Jefferson Science Associates, LLC
Site Office: Thomas Jefferson Site Office
Website: www.jlab.org

- **FY 2021 Lab Operating Costs:** $173.6 million
- **FY 2021 DOE/NNSA Costs:** $171.1 million
- **FY 2021 SPP (Non-DOE/Non-DHS) Costs:** $2.5 million
- **FY 2021 SPP as % Total Lab Operating Costs:** 1.4%
- **FY 2021 DHS Costs:** $0 million

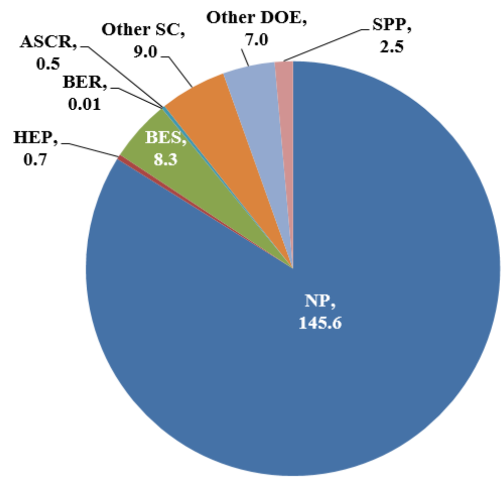
Physical Assets:

- 169 acres and 69 buildings
- 882,900 GSF in buildings
- Replacement Plant Value: $1,244 M
- 0 GSF in Excess Facilities
- 66,627 GSF in Leased Facilities

Human Capital:

- 758 Full Time Equivalent Employees (FTEs)
- 25 Joint Faculty
- 34 Postdoctoral Researchers
- 55 Graduate Student
- 26 Undergraduate Students
- 1,694 Facility Users
- 1,559 Visiting Scientists

FY 2021 Costs by Funding Source ($M)



Mission and Overview

Thomas Jefferson National Accelerator Facility (TJNAF) is a world-leading research institution for exploring the nature of matter, providing unprecedented insight into the details of the particles and forces that build our visible universe inside the nucleus of the atom. TJNAF was established in 1984 in Newport News, Virginia, and is operated by Jefferson Science Associates, LLC (JSA), for the Department of Energy's (DOE) Office of Science (SC).

Research at TJNAF reveals the fine details of the constituents of matter, from the familiar protons, neutrons, and electrons in the atom, to the lesser-known quarks and gluons inside the atom's nucleus.

Enabling these studies is TJNAF's world leadership in the development and deployment of large-scale superconducting radiofrequency (SRF) technology. SRF technology powers TJNAF's flagship facility, the Continuous Electron Beam Accelerator Facility (CEBAF). The technical and research successes accomplished with CEBAF as a unique SRF particle accelerator have made possible a wide array of applications, from ever more powerful free-electron lasers for research to detectors that enable life-saving advances in nuclear medicine.

TJNAF strives to attract and retain a diverse and talented workforce to both support its scientific mission and to maintain its core capabilities and expertise in Nuclear Physics; Large-Scale User Facilities/Advanced Instrumentation; Accelerator Science and Technology; and Advanced Computer Science, Visualization, and Data. TJNAF is exploring ways to capitalize on its expertise in the computational sciences to provide large-scale high-performance computing services to an array of research fields for accelerating and maximizing scientific insight in the future.

TJNAF actively partners with industry to advance critical technologies to benefit the nation. The lab also invests in the next-generation Science, Technology, Engineering, and Mathematics (STEM) workforce, training one-third of U.S. PhDs in nuclear physics annually. TJNAF's outreach programs positively impact thousands of students and teachers while helping them build critical knowledge and skills for a brighter future.

Core Capabilities

Nuclear Physics

TJNAF is a unique world-leading user facility for discovery studies of the structure of nuclear and hadronic matter using continuous beams of high-energy, polarized electrons. The nuclear physics program at TJNAF spans a broad range of topics in modern nuclear physics. 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. 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.

Excellent synergy exists between the TJNAF experimental, theoretical, and computing programs. The Joint Physics Analysis Center (JPAC) develops theoretical and phenomenological understanding of production and decays of hadron resonances, which helps bridge the analyses and interpretation of experimental data from TJNAF with the results of LQCD calculations. The Jefferson Lab Angular Momentum (JAM) collaboration pulls expertise in QCD theory, phenomenology, and HPC to develop new and better tools to help extract the 3D tomography of hadrons from TJNAF data. TJNAF was the first to make use of GPUs for HPC based on heterogeneous architectures (for LQCD calculations) and continues this innovative approach to present needs, including wide embracement of AI/ML in Nuclear Physics techniques.

TJNAF actively partners with BNL to provide important expertise and capability to ensure successful implementation of the EIC, including taking responsibility of scope that benefits from TJNAF's long-time intellectual investment in the EIC, TJNAF's core expertise, and its wide international user community.

Large-Scale User Facilities/Advanced Instrumentation

The CEBAF electron beam can be simultaneously delivered to the experimental halls at different energies. With the completion of the 12 GeV Upgrade, the beam energy can be up to 12 GeV, converted to 9 GeV photons for experimental Hall D, and up to 11 GeV to Halls A, B, and C. Each experimental hall is instrumented with specialized experimental equipment designed to exploit the CEBAF beam. The detector and data acquisition capabilities at TJNAF, when coupled with the high-energy electron beams, provide the highest luminosity (10^{39}/eN/cm^2/s) capability in the world. The TJNAF staff designs, constructs, and operates the complete set of equipment to enable this world-class experimental nuclear physics program, in close collaboration with a large domestic and international user community of more than 1,700 users annually.

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 to the 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.

Accelerator Science and Technology

SRF Accelerators. The SRF accelerator system consists of multiple integrated technologies with expertise spread throughout multiple disciplines and departments. TJNAF maintains collaboration and communication among all associated sub-systems essential to maintaining and enhancing SRF capabilities. System integration essential to an effective SRF system includes cavity fabrication and processing, cryomodules, low-level RF controls, high-power RF, cryogenics, software and hardware controls, and monitoring systems. Ensuring that each of these sub-systems maintains state-of-the-art capabilities is critical to maintaining a world-leading program in SRF accelerator system capabilities. To accomplish the mission, the SRF Institute must maintain a comprehensive set of expertise and facilities to support SRF technologies at TJNAF and be ready to respond to current and future needs of the TJNAF, the DOE complex, and other partners. TJNAF's SRF facilities occupy approximately 60,000 SF of contiguous space all under one roof, which includes 30,000+ SF of new work centers, 25,000 SF of renovated high bay assembly and test work centers, and approximately 5,000 SF for parts inventory and storage. A unique feature of the SRF facility is the ~8600 SF chemroom/cleanroom suite. This state-of-the-art facility is fully engaged to support cryomodule construction and refurbishment needs of CEBAF, LCLS-II HE, SNS PPU, and planning for the EIC project SRF production; strongly contribute to critical fundamental SRF R&D and prepare for future projects such as PERLE, ILC, or FCC-ee.

The ability to use the TJNAF LERF as an accelerator R&D test bed for ERLs and techniques required to establish cooling of proton/ion beams, or other future initiatives, provides a mutually beneficial cross-fertilization between the TJNAF LERF and Nuclear Physics. The LERF vault has recently been configured to enable higher throughput of cryomodule testing for LCLS-II HE.

Cryogenics. Over the last 30 years, TJNAF has developed a unique capability in large-scale cryogenic system design and operation that is a critical resource for the U.S. national laboratory complex, including the design of construction projects requiring large-scale cryogenics at SLAC (LCLS-II), Michigan State University (Facility for Rare Isotope Beams), Oak Ridge National Lab (SNS), TJNAF (12 GeV Upgrade), and NASA (James Webb Space Telescope testing), as well as improving the cryogenic efficiency of existing systems (BNL). In the process, several 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. TJNAF provides commissioning support to SLAC and routine operational support to ORNL.

Advanced Computer Science, Visualization, and Data

Through our support of the 12 GeV Nuclear Physics program, we have developed software and methodologies that are more broadly applicable. TJNAF has deployed in production AI/ML-based data quality monitoring and automated AI/ML calibration methods for drift chambers. These abilities are accelerating the pace of analysis. We have developed a second-generation multi-threaded framework (JANA2). We have developed a Geant4 toolkit for EIC simulation studies (eAST) for detector optimization that includes ease of leveraging new and rapidly evolving computing architectures.

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 HPC 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.

TJNAF is leading in the transition from the traditional NP and HEP event-by-event readout model to a streaming model where all detector channels are continuously read in parallel. TJNAF is developing software and hardware to support streaming data acquisition for CEBAF experiments and as a collaborator in the EIC Streaming Readout Consortium. The Environment for Realtime Streaming Acquisition and Processing (ERSAP) is an application environment for Streaming Readout Data Acquisition and online data processing. ERSAP provides a distributed streaming data-oriented framework with support for multiple programming languages.

TJNAF is developing core competency and capacity in targeted areas in AI/ML as defined in the Basic Research Needs for Scientific Machine Learning, focusing on integrating uncertainty quantification into deep machine learning models. This work provides better decision support and is in use at the SNS. TJNAF works on various aspects of design and control algorithm and contributed significantly to the scalable reinforcement learning framework, the Easily eXtendable Architecture for Reinforcement Learning. TJNAF data scientists are leading Reinforcement Learning efforts and applications to optimize dynamic workflows and compute power consumption.

Science and Technology Strategy for the Future/Major Initiatives

The TJNAF science strategy for the future involves pursuit of four major initiatives (Table 4.1) that advance key objectives in the field of Nuclear Physics and also enable TJNAF to more broadly contribute to the programs of the Office of Science. These initiatives allow TJNAF to diversify its scientific mission by building upon our foundation in nuclear physics to pursue new research directions and facility capabilities, particularly in advanced computing.

Table 4.1: TJNAF Major Initiatives

Strategic Areas	**5-7 year goals**
Nuclear Physics at CEBAF	• Ensure that TJNAF pursues complementary discovery science in the EIC era. • Realize CEBAF reliability at 12 GeV and develop concepts for future upgrades.
Electron-Ion Collider	• Demonstrate leadership in the EIC scientific program and deliver on TJNAF Project Partnership responsibilities.
Accelerator Science and Technology	• Fully develop and staff cryogenic, SRF, and accelerator research capabilities that enable TJNAF to deliver new accelerator projects at TJNAF and across the DOE complex.
Computational Science and Technology	• Be the first in class High-Performance Data Facility with associated research programs in Data and Computational Science.

The four major initiatives form a compelling and coherent vision for the Jefferson Lab of the future. Centered on our strong heritage in Nuclear Physics, and motivated by grand challenges within the field such as the quest to image the nucleon, our strategy brings together fundamental nuclear physics, computational science and the underlying accelerator technology to drive discovery in nuclear science, design and build the facilities of the future, and power new methods and facilities to integrate experiment, theory, and computation, enabling a new paradigm of scientific discovery.

The first major initiative is Nuclear Physics at CEBAF. The currently planned program of experiments will require the better part of the next decade to execute. Here, CEBAF will continue to provide unique capabilities to advance our understanding of hadronic matter at high luminosity far beyond what will be available at the future EIC. The planned CEBAF experimental program is launching a new era in three-dimensional imaging of the nucleon to facilitate solutions to long-standing anomalies in nuclear medium modifications, and to provide benchmarks for Quantum Chromodynamic calculations. Furthermore, advances in nuclear theory, particularly first principles calculations in LQCD, provide essential support for future developments at CEBAF and EIC.

TJNAF has established itself as a major partner in the development, construction, and scientific utilization of the new EIC Project, the second major initiative. This effort is both synergistic and complementary to the Nuclear Physics program at CEBAF, and exploits TJNAF's world-leading expertise in utilizing electron scattering in experimental nuclear physics as well as accelerator science and technology. The theory program at TJNAF is well equipped to provide leadership in guiding and interpreting eventual EIC experimental results.

The third major initiative is Accelerator Science and Technology. TJNAF will continue to be a world-leading center for SRF technology research and production, both for fundamental scientific research and for applications to industry, medicine, and national security. In order to reach its full potential, TJNAF will fully develop and staff the SRF, cryogenic, and accelerator research capabilities, thus enabling the lab to deliver on new accelerator projects across the DOE complex. Examples of additional elements of this initiative include machine learning for accelerator operations, development of a polarized positron source, and advanced photocathode development.

TJNAF will continue to advance the role of computation in Nuclear Physics while expanding our horizon beyond Nuclear Physics to other disciplines and research areas. TJNAF has developed a vision for an advanced computational facility – the High-Performance Data Facility -- to accelerate scientific discovery across DOE Office of Science programs by providing large-scale high-performance computing that brings parity between simulated, experimental, and observational data to accelerate and maximize scientific insight. This facility will provide services to Office of Science programs that enable interdisciplinary teams of scientists to attack fundamental problems in science and engineering that require nimble shared access to large data sets, often aggregated from multiple sources.

Infrastructure

Overview of Site Facilities and Infrastructure

TJNAF is located on a 169-acre DOE-owned federal reservation within the City of Newport News in southeast Virginia. Adjacent to the federal reservation is the Virginia Associated Research Campus (VARC), a five-acre parcel owned by the Commonwealth of Virginia and leased by SURA, which sub-leases five acres to DOE for TJNAF use. Also adjacent is an 11-acre parcel owned by Newport News that contains the Applied Research Center (ARC) where JSA leases additional office and lab space. SURA owns 37 acres adjacent to TJNAF where it operates a 42-room Residence Facility at no cost to DOE.

TJNAF consists of 69 DOE-owned buildings comprising 882,990 SF of office, shop, technical, and storage space. JSA leases additional office and lab space in the VARC (37,643 SF) and ARC (11,435 SF). JSA also leases two off-site storage warehouses (17,549 SF). Distribution of space by type is summarized in Table 6.1. There are currently no excess facilities and none are expected within the next 10 years. In addition to real property assets, 42 personal property shipping containers represent 12,920 SF of added storage.

TJNAF provides office and workspace for approximately 760 JSA contractor, JSA, and federal government employees plus 1,600 transient users and visiting scientists. Facility space is well utilized with a current asset utilization index of 99.6%. The condition of TJNAF facilities is generally good as summarized in the table below.

Type of Use	Total Usable Square Feet, Owned and Leased
Technical and Laboratory	258,768 (39%)
High Bay	150,198 (23%)
Office	101,420 (16%)
Storage	92,847 (14%)
Common	54,579 (8%)
TOTAL	657,812 (100%)

Table: Distribution of Usable Space by Type of Use

Condition		Mission-Unique Facilities		Non-Mission-Unique Facilities		Other Structures and Facilities	
		Number	SF	Number	SF	Number	SF
Rating	Adequate	36	339,976	30	353,596	36	N/A
	Substandard	0	0	7	249,069	3	N/A
	Inadequate	0	0	1	6,638	0	N/A
	TOTAL	36	339,976	38	609,303	39	N/A
Utilization	Underutilized	0	0	0	0	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/kilowatt-hour (kWh) and water from Newport News at an average rate of $3.69/HCF (HCF=hundred cubic feet) and disposes of wastewater through the HRSD at an average rate of $8.77/HCF. Utility service meets mission requirements although occasional, unplanned commercial-power outages periodically disrupt accelerator operation.

The TJNAF Land Use Plan is maintained on the TJNAF website and summarized in Enclosure 1. In addition to DOE-owned land, the SURA-owned land, as well as Newport News-owned land reserved for TJNAF interests, preserves expansion opportunities critical to the lab's strategic plan. The Land Use Plan also accommodates a future High-Performance Data Facility strategically placed on the campus.

The SLI-funded CEBAF Renovation and Expansion (CRE) project received CD-1 in March 2020. The project includes the acquisition of the ARC, renovation of CEBAF Center, and a 22K SF building expansion—which will eliminate the VARC lease. The ARC acquisition process is anticipated to be concluded in FY22. An extension of the current 11,435 SF lease is in place until the acquisition is complete. No real estate actions were performed in FY21 and the only additional real estate action planned for FY22 is a 15-20,000 SF off-site warehouse lease, which is required until the completion of the TJII project.

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 a continued focus on CEBAF infrastructure reliability. Accelerator reliability is the product of the joint availability of all component systems (cavities, magnets, controls, infrastructure, and so forth). To meet the CEBAF 85% availability goal, the Accelerator Division has allocated to facilities infrastructure an availability requirement of >98.5%, which translates to <81 hours of total downtime over a 32-week experimental period. To accomplish this, Facilities Maintenance and Operations completed 5,100 preventative maintenance tasks and 1,717 corrective tasks in FY 2021.

The impact of electrical transients to the operation of high-power electronic equipment remains the greatest cause of impact to accelerator operations and the area of major concentration. JSA continues to work with Dominion Energy to improve power quality including preventive maintenance of the substations feeding the lab (22, 33, and 40 million watts (MVA)), removing trees near transmission lines, inspecting overhead lines, coordinating utility preventive maintenance tasks with accelerator downtimes, proactively monitoring line voltage variations within tariff limits, and meeting regularly to review power reliability. In FY21 upgrades were also performed to provide remote ground fault relay operation capabilities and replacement of automatic voltage regulators

To support increased accelerator operations during the warm summer months, a project was identified to increase the cooling capacity of the linac service buildings. The scope of the project increases chilled water capacity, improves air flow, reduces infiltration of unconditioned air, and increases air conditioning. The first two phases of the project were completed in FY21 and the final phase is anticipated to be completed by FY25.

Replacement of accelerator fire detection and suppression systems was completed in FY20. This project replaced end-of-service-life components including all fire suppression, detection, and monitoring systems. A nitrogen-filled dry pipe system replaced the existing air-filled system, which will slow corrosion, improve the life of the system, and decrease maintenance costs. Replacement of fire detection systems in the experimental halls was completed in FY21.

Presented in Table 6.3 is the correlation between S&T mission requirements, required infrastructure capability, current shortfall in this capability, and optimum solution, which then becomes the basis for the infrastructure plan detailed in Enclosure 2, here. This campus strategy reflects a high priority on CEBAF reliability while also giving consideration for infrastructure upgrades needed to support a future High-Performance Data Facility and incorporating US Administration expectations for sustainability, resilience, decarbonization, and net zero initiatives.

Core Capability (SC-X)	Infrastructure Requirement	Current Shortfall	Optimum Solution and Need Date
Accelerator Science and Technology (SC01)	Provide liquid helium to the Test Lab to enable the development, production, and testing of SRF components and cryomodules, both for use by TJNAF in CEBAF and projects for other labs.	The Cryogenics Test Facility (CTF) has experienced heavy utilization due to the CEBAF upgrade and BES multi-lab partnership projects. Approximately $5M of system components have reached end-of-life and others require upgrading to maintain	Complete the **CTF Upgrade.** Funding was provided in FY20 under the SLI-GPP program.

		adequate capacity for projected workload.	
	Provide sufficient high bay, storage, and office space needed to design, produce and test SRF components and systems.	10,000 SF of high bay space in the Test Lab is unavailable for SRF needs due to occupation by Physics' large-scale assembly and testing activities. SRF office space needs in the Test Lab exceed available capacity. 10,000 SF of technical storage is leased in warehouse space remote from TJNAF. This introduces additional labor and time requirements to control and access this high-value material.	The **TJII** project will construct a new 45,000 SF Test Lab High Bay Annex for Physics' large-scale assembly and testing activities, thus making existing Test Lab high bay space available for SRF. Physics' engineering office space will be relocated to a modernized EEL to ensure adequate space is available for SRF in the Technology and Engineering Development Facility. A new 15-20,000 SF warehouse will relieve the demand for remote, off-site leased storage. Need date is immediate.
	LERF for dedicated cryomodule testing for DOE Projects, and R&D on electron guns and future accelerator concepts	Mechanical systems are at end-of-service-life and electrical systems are at or past capacity. Finishes are well worn and need to be renewed.	The **LERF Renovation** will ensure the facility can meet its planned operational use. Need date is FY25.

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 grams/second (g/s) of LHe at >96% reliability.	Two plants, CHL1 and 2, must operate to meet the 2K cooling requirements, but CHL1 is unable to meet the up-time requirements due to an aging cold box.	Complete the **CHL1 2K Cold Box Replacement**. This Project was initiated in FY17 as an SLI-GPP project, and is now nearly complete.
	210 tons of cooling capacity are required in each of the two linac service buildings to support CEBAF operations.	Existing cooling system is 36% undersized for current loads. Shortfall is 75 tons in each linac.	The **LINAC Additional Cooling** project increases chilled water capacity, improves air flow, reduces infiltration of unconditioned air, and increases air conditioning. The first two phases are complete and the final phase is needed by FY25.
	45,000 SF of environmentally controlled high bay and technical space to support SRF production, cryogenics fabrication, and equipment assembly and staging for four experimental halls operating at 34 weeks/year.	High bay space in the EEL, Test Lab, and TED buildings is heavily overutilized. Overcrowding increases the safety risk to staff and visiting scientists. Off-site space is currently being leased to meet the demand.	The **TJII** project will construct a new 45,000 SF Test Lab High Bay Annex for Physics' large-scale assembly and testing activities. Need date is immediate.
Nuclear Physics (SC20)	End station refrigeration capable of supplying Halls A, B, and C with 4000W of 4K cooling and 40 g/s of LHe at >85% reliability.	Current End Station Refrigerator serving Halls A, B, and C only has 1500W of 4K cooling and 11 g/s of LHe, has been operating nearly continuously for 20 years and is near end-of-life.	Complete installation of the SSC Cold Box to activate the **End Station Refrigerator 2 (ESR2)**. This will close the capability gap and provide a long-term solution to meet the experiment plan. Need date is immediate. Project is underway as an FY20 GPP-funded project.

	Up to 210,000 SF of office and collaborative space that meets DOE high-performance, sustainable building standards to house staff, students, and visiting users.	CEBAF Center (127,000 SF) is overutilized and substandard due to aging mechanical systems that require immediate replacement. An additional 45,000 SF of office space is leased in adjacent buildings at disadvantageous rates.	The **CRE,** including acquisition of the ARC, renovates the CEBAF Center and provides an additional 144,000 SF of space. The project consolidates staff and vacates leased space. Need date is immediate. Initial project funding was received in FY20.
	The EEL provides 54,800 SF of technical and lab space for Physics, Engineering, and Facilities staff and is integral to our campus plan.	EEL has end-of-life mechanical systems and numerous code deficiencies. Office and technical space is insufficient, poorly distributed, and not integrated with the campus.	The **TJII** project fully renovates and modernizes the EEL facility to meet mission needs. Need date is immediate.
Support Facilities and Infrastructure (SC25)	Provide 100,000 SF of outside storage to accommodate large experimental assemblies, support structures, and equipment for future experiments and operations.	Current laydown space is scattered in multiple locations around site. Stored material in some of these sites is visible from off-site and creates an eyesore. Some 70,000 SF of existing laydown area will be lost due to future building construction.	The **Laydown Yard Expansion** roughly doubles an existing, centrally located storage area which is not visible from off-site. Consolidation will improve material management and provide an opportunity to eliminate unneeded material. Need date is FY25.
	To meet DOE sustainability goals for 2025, TJNAF must reduce potable water consumption by 36% relative to 2007 baseline.	Must reduce potable water consumption from current intensity of 63.5 gal/GSF to 41 gal/GSF.	The **Cooling Tower Water Reuse** project develops a 50M gal/year alternate water source for use in cooling towers by directing and treating water from off-site retention ponds. Need date is FY25.

	Relocate Facilities Maintenance and Operations functions.	Functions are located in two substandard buildings (13 and 19) located in the administrative core of the campus. Critical spares are inefficiently scattered across the campus.	**The TJII** project provides a fully integrated solution and relocates these functions to a new Integrated Maintenance and Logistics Center (IMLC) located in the lab's service corridor. Need date is immediate.
	Relocate logistics functions.	TJNAF logistics functions are primarily located within high bay space within the EEL building, which is already oversubscribed and needed to support research and technical operations.	The **TJII** project provides a fully integrated solution and relocates these functions to a new IMLC located in the lab's service corridor. Need date is immediate.
	Suitable access roads, parking, and pedestrian walkways to facilitate collaboration and meet safety and regulatory requirements.	Continued expansion of the TJNAF campus as outlined in this plan along with development of property immediately surrounding TJNAF requires expansion and alteration of campus access and parking to support vehicle loads, and maintain compliance with safety and regulatory requirements.	The site-wide Roads, Parking, and Sidewalks Improvement project rebuilds existing roads and resolves impacts created by both on-site and adjacent off-site construction. Need date is FY29 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 no longer be available after FY30.	The **Central Utility Plant (CUP) Upgrade** project includes replacing the existing chillers with new chillers to be installed in the CUP. Need date is FY24.
	Suitable potable water distribution to reliably meet need for 120M gal/year use.	Portions of the water system exceed 50 years and have experienced severe corrosion. The site lacks a full water loop with isolation valves to allow for normal	The **Potable Water Utility Upgrades** project replaces aging sections of piping and provides for completion of the site water distribution loop with adequate isolation valves for system

		maintenance without severely affecting operations.	operations and maintenance. Need date is FY29.
	Relocate service entrance road to the TJNAF campus.	TJNAF service vehicle traffic flow and Facilities Maintenance and Operations functions do not support future growth of administrative, research, and technology portions of the TJNAF campus.	The **TJII project will construct a new service entrance road** to directly connect the TJNAF campus to a major public road, which will facilitate the future relocation of the facility maintenance and logistics functions. Need date is FY26 or sooner if practical.
	Meet renewable energy goals established by DOE.	TJNAF currently relies on the purchase of renewable energy credits to meet DOE sustainability goals, which require that renewable electric energy account for not less than 7.5% of a total agency electric consumption.	The **Renewable Energy Integration** project provides a 3-4 MW photovoltaic and battery storage system on-site, which will assist to meet renewable energy goals and provide a resilient microgrid for the campus. Need date is FY30.
	Meet potable water intensity reduction goals established by DOE.	Potable water intensity is expected to dramatically increase beginning in FY26 due to campus growth and data center cooling demands.	The **Cooling Tower Water Reuse Expansion** project provides an additional 50M gal/year alternate water source for use in cooling towers. Need date is FY31.
Advanced Computer Science, Visualization, and Data (SC02) and Computer Science (SC10)	162,000 SF of data center space and administrative space for 100+ staff to grow core capabilities in computational science.	CEBAF Center data center (6,000 SF) is at capacity, and insufficient administrative space exists in CEBAF Center	Construct Phase 1 of a new High-Performance Data Facility with sufficient administrative space for 100-165 staff.

		to support the growth of the CST.	

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 $280M over a decade. We assume that the Commonwealth of Virginia will provide funding for Phase 1 of the data center. In addition to providing essential capabilities for mission performance, these investments will eliminate $5M of deferred maintenance.

The primary focus of our Facilities Operations and Maintenance program is to increase the mean time between failure of facility systems through accelerated replacement of end-of-life systems and adding redundancy for critical systems to eliminate downtime from single-point failures. Similarly, when failures occur, TJNAF will reduce the mean time to repair by making sure sufficient stock of critical spares is on hand to immediately restore operation, rather than accept lengthy downtimes to source replacements.

The most recent TJNAF Condition Index is 0.98. However, this could drop over time if Facilities Operations and Maintenance funding continues to be limited to 1.25% of replacement value. Modernization projects and construction of new facilities through SLI and GPP funding have enabled TJNAF to maintain a modest deferred maintenance value ($7.5M in FY21). Over the next decade, no significant increase in deferred maintenance is expected as JSA implements the capital spending plan.

Site Sustainability Plan Summary

TJNAF remains strongly committed to achieving targets established in the DOE Strategic Sustainability Performance Plan. In FY21, significant accomplishments were made in areas such as renewable energy, waste management, electronics stewardship, and sustainable acquisition. Notably, TJNAF was recognized by DOE for its commitment to environmental excellence in procurement, a distinction that earned the lab a GreenBuy Superior Award for having achieved five consecutive Gold level awards. Only three sustainability interim targets were not met in FY21: potable water use intensity, electricity use intensity, and sustainable buildings (by building count).

Given the energy and water requirements for CEBAF operations as well as projected energy and water loads for a future HPDF on campus, achievement of potable water use intensity and electricity use intensity reduction goals represent a significant challenge. However, considerable progress is being made in both of these critical areas.

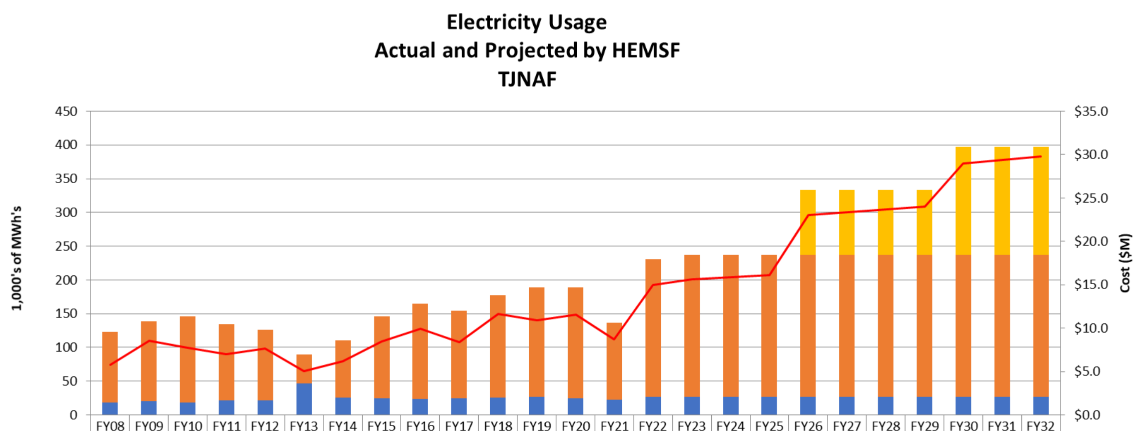
Several facilities currently utilize clean, renewable geothermal heat pump systems that produce and consume thermal energy. Photovoltaic (PV) systems are currently being considered for several facilities, and energy conservation measures, such as replacement of fluorescent and high intensity discharge (HID) lighting with light emitting diode (LED) fixtures, are completed each year. Additionally, a large PV array capable of producing 3-4 MW is being considered, which could completely offset administrative campus energy loads. On-site renewable efforts are supplemented annually by the purchase of renewable energy credits (RECs) as needed. Increasing the number of RECs purchased annually is a part of TJNAF’s strategy to meet carbon pollution-free electricity and emissions reduction goals set in Executive Order 14057.

Similar progress is being made in potable water reduction efforts. Approximately 4.9M gal/yr (a savings of $64,000) of potable water is saved annually by reusing discharge water from the Test Lab ultra-pure water system as a make-up water supply source for a nearby cooling tower. A project to provide an additional 50M gal/yr of reuse water from a nearby stormwater lake to evaporative cooling towers has been partially funded and is currently in the conceptual design phase. Expansion of this water system has even been planned to compensate for projected future HPDF water demands.

Recent legislation such as the Energy Act of 2020 and Executive Order 14057 are actively being integrated into TJNAF campus and sustainability planning efforts. In FY22, TJNAF began conversations with the TJSO and Federal Energy Management Program to pursue the establishment of performance contracts that will further assist in reaching energy savings, net-zero, decarbonization, and greenhouse gas reduction goals. A Vulnerability Assessment and Resilience Plan will be completed in FY22, which will enable TJNAF to identify, prepare for, and meet the challenges posed by climate change.

Electricity Usage and Cost Projections

The figure below shows TJNAF's historical and projected electricity usage and costs. Projections are based on scheduled operations for FY23 of 33 weeks and, for FY24 and beyond, 34 weeks. Additional projections related to a proposed new high-energy, mission-specific facility (HEMSF)—a data center—are also included from FY26 forward.



	FY08	FY09	FY10	FY11	FY12	FY13	FY14	FY15	FY16	FY17	FY18	FY19	FY20
New HEMSF - Data Center													
Existing HEMSF - CEBAF	105	118	128	114	104	42	85	121	141	130	152	162	164
Site Base	18	20	18	21	22	47	25	25	24	24	25	27	25
Cost ($M)	$5.8	$8.6	$7.7	$7.0	$7.6	$5.1	$6.2	$8.4	$10.	$8.4	$11.	$10.	$11.

	FY21	FY22	FY23	FY24	FY25	FY26	FY27	FY28	FY29	FY30	FY31	FY32
New HEMSF - Data Center						96	96	96	96	159	159	159
Existing HEMSF - CEBAF	114	203	210	210	210	210	210	210	210	210	210	210
Site Base	22	27	27	27	27	27	27	27	27	27	27	27
Cost ($M)	$8.7	$15.	$15.	$15.	$16.	$23.	$23.	$23.	$24.	$29.	$29.	$29.

Figure: Electricity Usage and Cost Projections

APPENDIX 1
SCIENCE AND ENERGY CORE CAPABILITIES

The Programs reporting to the Under Secretary for Science and the Under Secretary for Energy have together identified twenty four categories of core capabilities that comprise the scientific and technological foundation of its national laboratories. There are three criteria to define core capabilities. They must:

- Encompass a substantial combination of facilities and/or teams of people and/or equipment;
- Have a unique and/or world-leading component; and
- Be relevant to a discussion of DOE/NNSA/DHS missions.

Below is a table of the core capabilities that have been affirmed by DOE at each of the thirteen Science and Energy national laboratories. The following pages give a detailed definition of what each core capability encompasses.

Figure: Distribution of Core Capabilities across the Science Laboratories

	Core Capabilities	AMES	ANL	BNL	FNAL	LBNL	ORNL	PNNL	PPPL	SLAC	TJNAF
1	Accelerator Science and Technology		✓	✓	✓	✓	✓			✓	✓
2	Advanced Computer Science, Visualization, and Data		✓	✓	✓	✓	✓	✓		✓	✓
3	Applied Materials Science and Engineering	✓	✓	✓		✓	✓	✓	**NEW**	**NEW**	
4	Applied Mathematics		✓	✓		✓	✓	✓			
5	Biological and Bioprocess Engineering		✓			✓	✓	✓			
6	Biological Systems Science			✓		✓	✓	✓		**NEW**	
7	Chemical and Molecular Science	✓	✓	✓		✓	✓	✓	E	✓	
8	Chemical Engineering		✓	✓		✓	✓	✓			
9	Climate Change Science and Atmospheric Science		✓	✓		✓	✓	✓			
10	Computational Science		✓	✓		✓	✓	✓	E		
11	Condensed Matter Physics and Materials Science	✓	✓	✓		✓	✓	✓	E	✓	

	Core Capabilities	AMES	ANL	BNL	FNAL	LBNL	ORNL	PNNL	PPPL	SLAC	TJNAF
12	Cyber and Information Sciences		✓			✓	✓	✓			
13	Decision Science and Analysis		✓			✓	✓	✓			
14	Earth Systems Science and Engineering					✓	✓	✓			
15	Environmental Subsurface Science					✓	✓	✓			
16	Large Scale User Facilities/Advanced Instrumentation		✓	✓	✓	✓	✓	✓	✓	✓	✓
17	Mechanical Design and Engineering					✓	✓		✓		
18	Nuclear and Radio Chemistry		✓	✓		✓	✓	✓			
19	Nuclear Engineering		✓	E			✓	✓			
20	Nuclear Physics		✓	✓		✓	✓				✓
21	Particle Physics		✓	✓	✓	✓				✓	
22	Plasma and Fusion Energy Science					✓	✓		✓	✓	
23	Power Systems and Electrical Engineering			E		✓	✓	✓	✓		
24	Systems Engineering and Integration		✓	✓		✓	✓	✓	✓		

✓ = DOE Endorse Core Capability E = Emerging Core Capability NEW = Core Capability Proposed in FY 2022

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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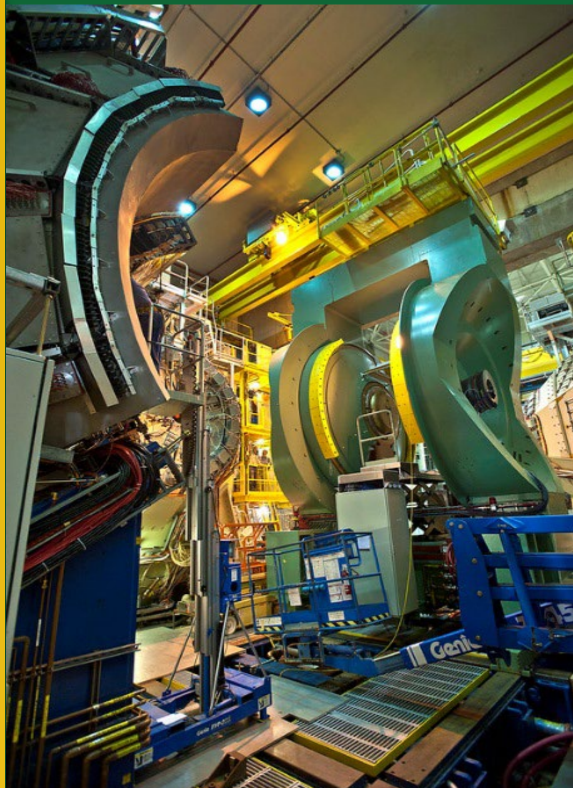

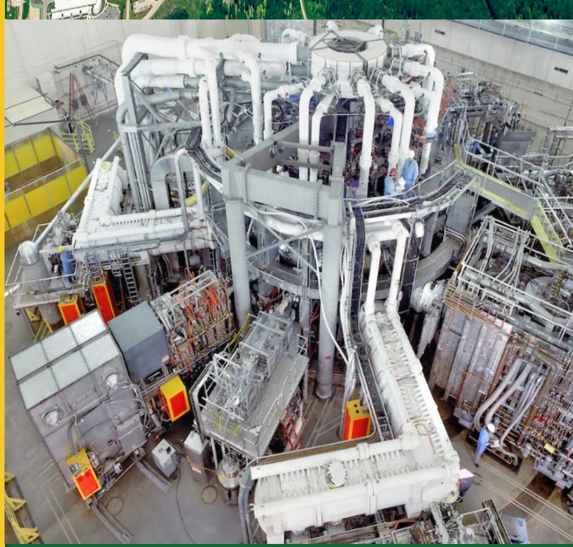

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