Advanced Photon Source Strategic Plan

2025-2029

U.S. DEPARTMENT OF ENERGY | Office of Science

Argonne NATIONAL LABORATORY

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Foreword

The Advanced Photon Source (APS) is a world-leading synchrotron that has supported cutting-edge research for the past 28 years. As a key contributor to the Department of Energy's (DOE) mission, the APS has played an integral role in enabling scientific discovery and innovation, supporting the development of new energy technologies and ensuring U.S. security and prosperity. The APS user community stands as a global leader in synchrotron X-ray research, producing over 36,000 publications across diverse fields such as materials science and biology that have been cited more than 2 million times. Collaborations between the APS and its academic and industrial partners have resulted in over 33,000 protein structures deposited in the Protein Data Bank, and research conducted at the APS has led to three Nobel Prizes in chemistry, awarded in 2009, 2012 and 2024.

In the past decade, the APS, along with other light sources worldwide – which now includes over 30 synchrotrons and 6 X-ray Free Electron Lasers (FELs) – has undergone significant advancements. Technological innovations in multi-bend achromat design and superconducting accelerating structures have driven unprecedented increases in spectral brightness. Coherent light modalities traditionally confined to the optical regime are now thriving at X-ray energies, allowing for the exploration of matter at unprecedented length scales and time scales. This opens new possibilities for unraveling complexity in systems that are intrinsically heterogeneous or functionally dependent on complex hierarchical organizations. The APS has led the field of hard X-ray research at synchrotrons, leveraging modern optics nanofabrication, advances in solid-state detectors and electronics, and rapid developments in data science and artificial intelligence (AI) to enable new techniques that maximize scientific impact.

The future is exciting. After more than a decade of preparation, the upgraded APS has launched, establishing our new storage ring as the world's brightest fourth-generation synchrotron in the hard X-ray regime. We are embarking on an exciting journey with our user community to harness new X-ray instrumentation that will push the boundaries of research in their fields, and it is with great anticipation that we observe the early scientific endeavors at the renewed APS. Recognizing the importance of science and technology in advancing society and economic development, and conscious of our role in helping tackle the grand challenges facing our society, we seek to be a partner of choice in delivering basic scientific discoveries and supporting translational research for both our general users and our partner institutions.

More than ever, addressing the most demanding scientific questions will require an integrated research approach, and the APS intends to actively promote collaboration between light sources, neutron sources and nanoscale research centers at national laboratories to push innovation in data-driven science and AI, thereby promoting “big” science at scale.

Whilst the impact of machine learning (ML) and, more recently, generative AI was anticipated by the scientific community, the speed at which advanced scientific reasoning has evolved in recent years is truly remarkable. It will inevitably be a major driver and an accelerator of innovation, including at light sources, which are major generators of scientific data. Adapting to this new norm will require us to reframe our thinking and challenge ourselves in new ways. We have been early adopters of AI for science and ML, whether it is to achieve near-real-time data processing to accelerate discovery or to enhance controls of our X-ray instruments. In some disciplines, such as structural biology, information obtained by X-ray has been transformative. The data sets, well curated and annotated by the community, contain information that is easily tokenized, and they have led to major innovations, as recognized by the Nobel Prize in chemistry 2024. The scientific and economic impacts of such discoveries are vast. We are confident that our X-ray experts, our user community, and collaborators in computing science will soon imagine ways to expand this work in other areas of synchrotron-enabled science. They will eventually overcome the challenges associated with data heterogeneity and complexity to solve scientific problems that are currently intractable.

Equipped with the unprecedented X-ray brightness delivered by the new APS, with new instruments that can exploit it, and with the AI revolution underway, we are ready to boost scientific innovation for decades to come!

Laurent Chapon
Associate Laboratory Director for Photon Sciences

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Unveiling the Future: The Transformed Advanced Photon Source

The Advanced Photon Source is one of the 28 large-scale scientific user facilities built and operated by the Office of Science (SC) of the Department of Energy. It is one of 30 synchrotrons currently operating worldwide, and one of only five high-energy X-ray synchrotrons, with the European Synchrotron Radiation Facility (France), SPring-8 (Japan), Petra-III (Germany), and the recently built HEPS facility (China). In operation since 1996 as a third-generation synchrotron, the APS has served an increasingly large user community of almost 6,000 unique users in a typical year. The experimental facilities funded and operated by SC, together with those of our academic partners, and industry, have to date served hundreds of institutions from academia, government and industry. Its research output is of the highest rank in the world, with more than 36,000 peer-reviewed publications to date. The APS is the largest contributor (17%) of protein structures determined by X-ray worldwide.

In 2024, a new APS has emerged after a yearlong shutdown, delivering the most advanced fourth-generation storage ring in the world. Employing a hybrid multi-bend achromat lattice with a novel injection system, the upgraded APS's electron emittance has been lowered by almost a factor of 100 to 40 pm.rad. Our sources deliver unprecedented levels of X-ray brightness, increased by a factor of 500 compared to that of the original APS. The upgraded facility builds on the solid foundations established during nearly three decades of technological advances and cutting-edge research performed at the APS and at synchrotron facilities around the world. The comprehensive upgrade, conceptually imagined in 2010, includes nine new feature beamlines and 15 upgraded instruments that, upon completion, will transform the way we interrogate matter with X-rays and shed light on functions for the most complex systems that underpin today and tomorrow's technology. By ushering in a new era for X-ray imaging that can achieve nanometer precision, deploying new correlation techniques to probe systems out of equilibrium, and developing new tools to measure and possibly control new states of matter by exploiting the quantum property of X-ray light, we will empower our community for their most advanced research. Many areas of science - such as transformative manufacturing, microelectronics, quantum materials, circular economy, bio-preparedness, health, and environmental sciences - will be transformed.

Not only will our capabilities be augmented, but, at the completion of the beamline upgrade program, the renewed APS will have the largest capacity of any synchrotron in the world, operating 72 beamlines. Forty of them will be directly funded by DOE Basic Energy Sciences (BES) through the APS operations budget, 9 jointly or fully operated by the APS with other fundings, and 23 funded by partner institutions (Collaborative Access Teams – CATs).

Synchrotrons of the world (4th gen. (red), 4th gen. in preparation (orange), 3rd gen blue. Beamline capacity is proportional to the size of the symbols.

The Photon Sciences Directorate at Argonne

The prime responsibility of the Photon Sciences (PSC) Directorate at Argonne is to manage and operate the Advanced Photon Source, with a mission to remain at the cutting edge of X-ray enabled research. PSC also serves as a major innovation hub for X-ray instrumentation, accelerator technologies and data-driven science, and aims to maintain itself as the partner of choice for the development of existing and future light sources and integrated research infrastructures sponsored by the Department of Energy.

PSC benefits strongly from the vibrant scientific ecosystem existing within the DOE national laboratories. That environment attracts engineering and scientific talents across many disciplines in research areas such as physics, chemistry, materials science and biology, and also the leading expertise in accelerator technology, scattering instrumentation, data science and AI.

The APS has forged strong ties and collaborations with sister DOE light sources and the neutron sources at Oak Ridge National Laboratory (ORNL). Together, we created a community of practice that actively collaborates on technological developments relevant to our mission, and on continuously adapting our operational principles to boost scientific impact. Our partnership through the National Virtual Biotechnology Laboratory (NVBL) has been vital in addressing the challenges posed by the COVID-19 pandemic and prepares us better for future pandemics. Multilateral collaborations have been essential for the development of new accelerator technologies, new detectors and sensors, and X-ray optics. As a leading generator of scientific data alongside many other DOE facilities, we share a common vision for data science and a common need for an integrated data infrastructure. Achieving this vision will empower our users with new tools for real-time inspection of data, automatic and adaptive steering of experiments and integration of AI. Driven by the common needs and interests of our user community, the facilities will work with their communities to define how to efficiently aggregate annotated data to support frontier programs in artificial intelligence for science.

PSC is also strongly integrated in the local ecosystem at Argonne National Laboratory and the large number of local universities. The collocation of the six Argonne directorates has fostered many local interdisciplinary collaborations, from battery science to quantum materials research and biology. Beyond scientific research, strong synergies within the laboratory have been instrumental in developing technologies and attracting next-generation talent. For example:

- Establishing collaboration between the APS and the Center for Nanoscale Materials (CNM) has been critical for multimodal and cross-functional projects, and the development of nanoprobe techniques.
- Developing strong partnerships with the Argonne Accelerator Institute and attracting new talent through the Lee Teng fellowship program.
- Researching advanced acceleration techniques at the Argonne Wakefield Acceleration (AWA) facility in support of the High Energy Physics (HEP) mission, synergistic with light source needs. This drove the exploration of new concepts for multi-user soft X-ray Free Electron Laser (FEL) based on collinear Wakefield applications and the generation of bright electron beams for future light sources.
- Collaborating with experts in superconducting cavities for ion acceleration in the Physics Division. The bunch lengthening system, a vital technology to mitigate intra-beam scattering effects at the new APS, has been developed through this collaboration.
- Partnering with the Advanced Leadership Computing Facility and its divisions plays an instrumental role in deploying data analysis pipelines and methods using high performance computing (HPC) and AI training.

Organization and Governance

Argonne National Laboratory is managed by UChicago Argonne, LLC, a legal entity affiliated with the University of Chicago. UChicago Argonne, LLC appoints a Board of Governors that provides oversight for Argonne National Laboratory and the relationship with the U.S. DOE. The Board's role is to provide guidance, oversight, direction and advice to Laboratory management with respect to scientific and technical issues, long-range objectives, budget and facility plans, cooperative research and development, outreach, and technology transfer, as well as personnel and staffing matters, and the relationship with the U.S. Department of Energy under the Prime Contract.

Argonne counts five directorates alongside PSC: Advanced Energy Technologies (AET), Computing, Environment and Life Sciences (CELS), Physical Sciences and Engineering (PSE), Nuclear Technologies and National Security (NTNS), and Science and Technologies Partnerships and Outreach (STPO). Many scentific collaborations exist between these directorates and PSC, either directly in the programmatic areas or synergistically with other user facilities (CNM, AWA) and through the Argonne Accelerator Institute (AAI).

PSC counts three divisions: the Accelerator Systems Division (ASD), the APS Engineering Support (AES) Division, and the X-ray Science Division (XSD). The division directors, with the Associate Laboratory Director (ALD) for PSC, the Deputy ALD for Operations, and the Deputy ALD for Science & Technology, are responsible for the strategy and operations of PSC and the APS. The PSC ALD reports to the laboratory director.

The PSC senior management team is assisted by three advisory committees: the Scientific Advisory Committee (SAC), the Machine Advisory Committee (MAC), and a recently created Computing Advisory Committee (CAC). These advisory bodies meet bi-annually or annually. The Partner Users Council (PUC) is an advisory board to the PSC ALD that represents the interests of facility partners. The APS Users' Executive Committee (APS UEC) is an advocacy group for the APS and advises the ALD on matters affecting the user community. These groups meet quarterly with APS management.

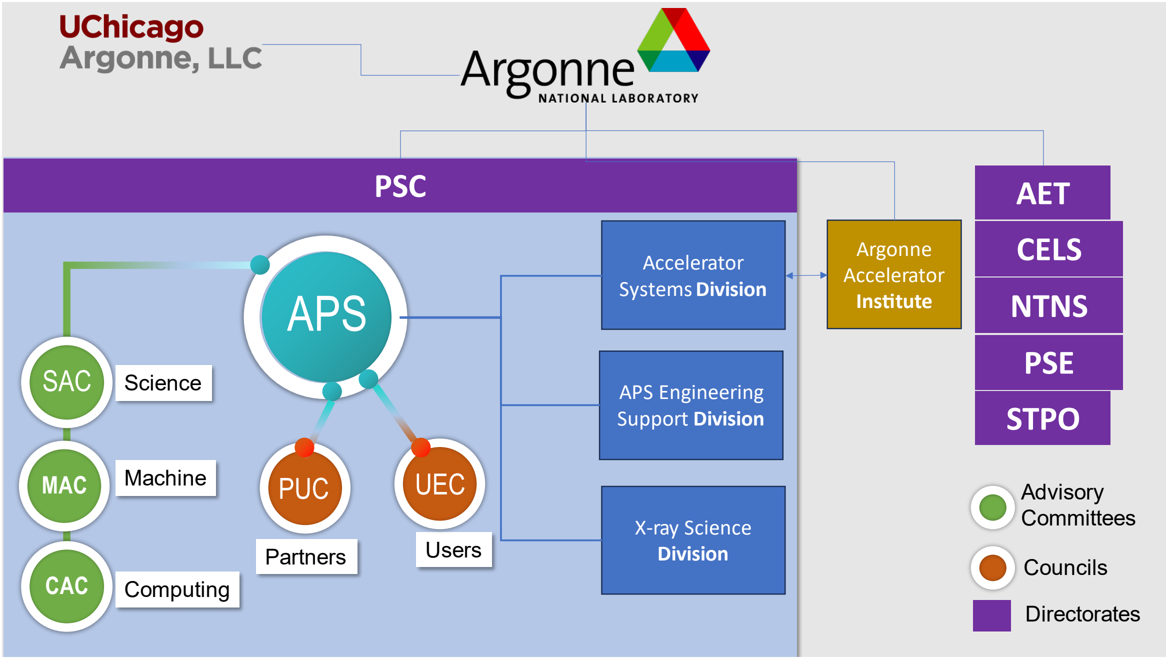


Figure 1: Organization structure of Argonne National Laboratory, divisional structure, and governance of the APS.

Vision Statement

Our vision is to drive a new era of scientific discovery, empowering breakthroughs through world-leading X-ray technology, AI innovation, and collaboration.

"Drive a new era of scientific discovery, empowering breakthroughs through world-leading X-ray technology, AI innovation, and collaboration"

In a rapidly evolving world, our vision guides us toward advancing scientific knowledge and solutions that impact society and help solve the most pressing scientific challenges. By combining cutting-edge X-ray capabilities with transformative AI and fostering an open environment for global partnerships, we are dedicated to empowering researchers to address today's challenges and shape the innovations of tomorrow.

Mission Statements

Our strategic plan is grounded in a multifaceted mission to advance the frontiers of scientific discovery through excellence in X-ray technology, innovation in artificial intelligence, and collaboration with the research community. Each of our mission statements reflects a core focus area, together forming a comprehensive approach to achieving transformative breakthroughs in science and technology.

- **To accelerate scientific discovery by providing world-leading synchrotron X-ray capabilities.**
  Our commitment to enabling groundbreaking discoveries is at the heart of our mission. By offering world-class synchrotron X-ray resources, we empower researchers with tools essential for exploring the most complex scientific questions. This mission emphasizes our dedication to supporting innovative research across diverse scientific disciplines, from materials science to biology.
- **To be a center of excellence for development of X-ray technologies for existing and future light sources.**
  As a global leader in X-ray technology, we continually invest in the development and refinement of X-ray capabilities, anticipating future scientific needs and challenges. The APS serves as a hub for pioneering advancements that keep us at the forefront of X-ray technology, ensuring that both current and next-generation light sources achieve their maximum potential for discovery.
- **To accelerate research by integrating AI in operations and X-ray science.**
  Recognizing the transformative potential of artificial intelligence, we are integrating AI-driven solutions into both our operational processes and scientific methodologies. This mission highlights our commitment to enhancing research efficiency, data accuracy and analytical capabilities, ultimately speeding up scientific advancements and enabling new insights.
- **To be a partner of choice for scientific collaboration.**
  We are dedicated to fostering a collaborative research environment, welcoming scientists, institutions and industries to join us in our mission. Our goal is to be the preferred partner for scientific collaboration, leveraging our expertise and resources to tackle challenges and drive scientific progress together.

Together, these mission statements define our commitment to advancing science and technology. By uniting leading-edge X-ray capabilities, innovative AI integration, and an unwavering dedication to collaboration, we create a strategic foundation for supporting scientific breakthroughs that will shape the future.

Core Values

PSC is committed to providing a safe, welcoming and inclusive environment and culture to support scientific discourse and discovery that operates in accordance with **Argonne's Core Values**. We strongly believe that mission success critically depends on fostering a culture that encourages creativity, integrity and respect between our staff, users, contingent workers and our numerous collaborators around the world. We believe in operating in a transparent manner and consciously building and maturing our culture.

Figure 2: Core Values at Argonne National Laboratory.

Scientific Opportunities

The upgraded Advanced Photon Source, with major improvements in X-ray coherence and brightness and transformative hard X-ray capabilities, is poised to address a wide array of scientific inquiries. Various research areas in the life and physical sciences, where critical societal challenges require rapid scientific and technological advancements, will benefit from the new capabilities of the upgraded APS. Such grand challenges include sustainable energy, environmental stewardship, circular economy, biomedical innovations, transformative computing and novel materials, just to name a few.

1. Mesoscale Engineering and Advanced Materials

The challenge in engineering advanced materials lies in understanding how microscopic structural features such as defects, dislocations, and grain boundaries influence such properties as strength, durability, and conductivity at larger scales. For high-performance applications, such as aerospace or renewable energy infrastructure, materials must withstand extreme stresses and temperatures without degrading. One key goal is to prevent fatigue and failure under cyclic stresses, which is vital for components like turbine blades or engine parts that experience continual stress fluctuations. Another significant challenge is optimizing the structure of energy storage materials like lithium-ion batteries, where even minor structural changes during charging and discharging cycles can cause capacity fade and failure. By understanding how nanoscale strain, defects and phase changes impact a material's performance over time, scientists can design materials with superior strength, longevity and energy capacity. This requires a comprehensive, multi-scale view, from atomic-scale interactions to larger structural behaviors, all observed under realistic operational conditions. High-energy X-rays are particularly relevant for addressing these challenges due to their ability to penetrate deep into samples and through vessels, allowing for *in situ* and *operando* studies of materials.

2. Soft Materials

Soft materials, including biological tissues, polymers, colloidal suspensions and gels, pose unique challenges due to their complex hierarchical organization and dynamic properties. These materials often exhibit self-assembly, where nanostructures organize into larger, functional forms that contribute to material properties. Understanding and harnessing this self-assembly is essential for creating next-generation materials with tailored properties, such as flexibility, biocompatibility or reactivity, but also crucial for advancing polymer recycling and upcycling. Additionally, dynamic interfaces—such as those found in biological membranes or polymer films—play a crucial role in the functionality of soft materials. They are sensitive to environmental changes and can respond to stress, temperature shifts or chemical stimuli, which affects the material's performance. Real-time studies of these dynamic processes are needed to explore applications like soft robotics and advanced biomedical devices. The challenge is to capture these rapid, small-scale changes as they happen to inform the design of adaptable, high-performance materials for diverse applications. Increased coherence from the upgraded APS is particularly relevant for these areas as it often leads to increased contrast and higher fidelity measurements with greater sensitivity, and thus reduced radiation damage concerns.

3. Biology and Life Sciences

A central challenge in life sciences is decoding complex molecular interactions that drive cellular functions and health. This includes understanding the roles of dynamic molecular structures, such as membrane proteins and DNA complexes, which regulate cellular communication, metabolism, and immune responses. These are often prime drug targets, but their fluidity makes it difficult to unveil their structures at physiological conditions. Additionally, understanding the molecular basis of disease—from protein misfolding in Alzheimer's to tissue changes in cancer—could enable earlier diagnoses and more targeted treatments.

Among human organs, the brain remains the least understood due to its immense complexity, containing around 86 billion neurons and trillions of connections. Connectomics, the mapping of neural connections, aims to reveal how these intricate networks underpin cognition and behavior, with implications for understanding such mental health disorders as schizophrenia and autism. However, capturing the brain's structure across scales—from individual synapses to entire circuits—requires advanced, high-resolution imaging.

Finally, understanding how tissue architecture functions in health and disease demands imaging across molecular and organ levels, especially for diseases such as cancer where structural disorganization disrupts normal function. Advancements in this area promise to revolutionize diagnostics, drug development and treatment monitoring, providing a more comprehensive view of health and disease mechanisms essential for tackling today's public health challenges.

Beyond direct application to human health, understanding complex biological systems and their interactions with the environment are critical areas of research. Advancing bioenergy solutions, such as engineering microbes and plants to produce biofuels, requires a deep understanding of cellular metabolism and gene regulation. Additionally, understanding how organisms, ecosystems and the biosphere respond to environmental changes, is critical to cope with a changing environment and requires multi-scale imaging and molecular insights into biological systems. For instance, understanding plant-microbe interactions at the molecular level is crucial for optimizing soil health and carbon sequestration.

The upgraded APS will advance these areas, with the increased brightness allowing for increases in measurement volumes while simultaneously improving resolution and sensitivity, as well as overall statistical sampling.

4. Chemistry and Catalysis

In catalysis and chemistry, a major challenge is to observe and control atomic-level processes that drive chemical reactions, as well as to design materials that optimize these processes for industrial applications. Catalysts are essential for a range of fields, from chemical manufacturing to energy production, but developing more efficient catalysts requires an intimate understanding of the reaction pathways and the relationship between a catalyst's structure and its function. This challenge is critical for artificial photosynthesis, where we aim to mimic natural photosynthesis to produce sustainable fuels. Additionally, synthesizing materials with precise structure-function relationships, like those found in zeolites or metal-organic frameworks, is essential for creating catalysts that selectively target specific reactions with minimal energy input. In energy storage, improving ion mobility and stability in batteries is crucial, as these properties directly impact efficiency and lifespan. Observing how lithium ions or other elements interact within battery materials at the atomic scale could lead to significant advances in battery technology, essential for such applications as electric vehicles and grid energy storage. *In situ* and *operando* measurements are particularly relevant for this field, and again uniquely enabled by the coherent hard and high energy X-rays delivered by the upgraded APS.

5. Earth Sciences and the Environment

Earth and environmental sciences face the grand challenge of understanding how materials behave under extreme pressures and temperatures, such as those found within Earth's core or in extraterrestrial environments. Replicating and studying these extreme conditions can reveal information about planetary formation, geophysical processes, and potential resource reservoirs. This knowledge is also essential for understanding geological risks, such as volcanic activity or seismic events, which have direct impacts on human life and infrastructure. Another challenge lies in understanding the long-term environmental impacts of nanomaterials, which are increasingly used in products from electronics to medicine. Understanding how these materials interact with ecosystems, especially in soil and water, is critical for evaluating their safety and environmental footprint. In climate science, a pressing issue is determining the role of trace metals in ocean ecosystems, which influence marine productivity and carbon cycling. Sustainable solutions in industry, such as reducing CO_2 emissions in cement manufacturing, require detailed knowledge of material properties under various processing conditions. These goals are essential for addressing climate resilience, resource management, and environmental protection. High brightness X-ray beams are key to expanding current capabilities towards higher resolution, higher sensitivity measurements and increased statistical relevance.

6. Condensed Matter Physics

In condensed matter physics, a key challenge is to explore quantum critical phenomena and the emergence of novel states of matter, such as superconductors, superfluids, and other strongly correlated electron systems. These materials hold transformative potential for applications in quantum computing, energy-efficient electronics and advanced sensors. However, understanding how these unique states arise and how they can be controlled remains a challenge, as they often exist only under specific conditions and are highly sensitive to external stimuli. Another grand challenge is in quantum device design, where stabilizing and scaling quantum bits (qubits) is critical for realizing practical quantum computing systems. Studying how localized strain or atomic-level defects affect qubits will help address issues like decoherence and error rates, which are obstacles to building stable, large-scale quantum computers. Additionally, as semiconductor devices approach physical miniaturization limits (in other words the end of Moore’s Law), understanding how strain, defects and atomic arrangements impact performance is crucial for future computing technologies. Designing materials that can leverage quantum properties and overcome physical limitations of traditional electronics remains a priority for advancing condensed matter physics and supporting next-generation technologies. X-ray techniques are uniquely suited to advance these areas because of their ability to probe materials from atomic to macroscopic scales with chemical, orbital, and spin specificity.

Executive Summary

The Advanced Photon Source (APS) at Argonne National Laboratory is a premier synchrotron facility that has been pivotal in advancing scientific research across various disciplines for nearly three decades. As part of the Department of Energy's mission, the APS has significantly contributed to scientific discovery, technology development, and national security and has established itself as a leader in synchrotron X-ray enabled research.

The APS has recently undergone a significant upgrade through the DOE funded APS-U project to create the world's brightest fourth-generation synchrotron for hard X-rays. The new storage-ring commissioned in 2024, and the new X-ray instrumentation being deployed offer unique experimental capabilities that will accelerate research and innovation in physical and life science.

The next five years will be a pivotal period for the APS as we build on our historical successes and recent technological innovation to advance the frontiers of science. Our strategic framework outlines four key goals:

Goal 1: Enable and Deliver Scientific Discoveries focuses on catalyzing science initiatives at the new APS by enabling new X-ray measurement modalities or improved capabilities offered by the upgraded facility. A key objective is to return the facility to the objective performance parameters defined by the APS-U project. We aim to enhance scientific support through increased staff levels on beamlines and investment in data infrastructure and data pipelines to create data analysis as a service for the most demanding science. We will achieve our objective by deploying a wide spectrum of technology, from edge computing to tight coupling to leadership-class computing on the campus and beyond. The final objective under this goal capitalizes on the APS-U investment under the program *Expand X-ray Capabilities with Extreme Light* (EXCEL@APS), an initiative that will augment our scientific impact by upgrading additional beamlines to more optimally exploit the significantly improved coherence.

Goal 2: Innovate and Advance Mission-Critical Technologies targets research and development that will keep the APS at the cutting edge of X-ray science and maintain PSC's position as an innovator for future light source technologies. We will develop novel ways to use extremely bright, coherent X-ray beams to give unprecedented insights into the structure and dynamics of matter. We will research how to increase the beam brightness at the APS by another order of magnitude by combining new sources and new electron optics. We will work at the frontiers of data science and AI to unravel the most intricate features arising from experiments and to boost the scientific productivity of our users. We will strengthen our facilities and retain our expertise to become global leaders and a valuable resource for other light sources in the areas of superconducting undulators (SCUs) and ultra-high vacuum (UHV) system cleaning, welding, assembly and certification.

Goal 3: Ensure Mission Success through Operational Excellence spans multiple objectives that target optimization of operations to enhance user experience, maintain high safety and security standards, continue to improve efficiency, reduce maintenance, and lower energy consumption of the APS. This includes a major objective to modernize our injector, accelerator and storage ring radio frequency (RF) systems. A second objective encompasses an integrated approach to preventive and predictive maintenance and management of spare components for the new APS. A third objective focuses on reducing the overall power consumption of the facility. Finally, we will continue to expand user access modes and pilot the deployment of context-aware AI systems to educate and guide researchers during experiments.

Goal 4: Foster an Innovative and Collaborative Environment that targets workforce development for PSC staff by supporting a strong culture of innovation in X-ray science, accelerator technology and data science. We will build a framework for training and education that supports agility in careers and opens transverse pathways for staff. We will launch an "AI for all staff" initiative in partnership with the laboratory, to ensure that the technology shift does not leave people behind. We will continue to build a culture that supports transparent and open communication and actively promotes collaboration with our partner institutions to imagine the future together and bring an integrated approach to support scientific excellence.

Goal 1: Enable and Deliver Scientific Discoveries

Objective 1.1: Maximally exploit X-ray capabilities offered by the upgraded APS

The APS currently provides the highest-coherence and brightest X-ray synchrotron beams in the world. These beam characteristics are enabling new types of imaging, microscopy (including coherent diffractive imaging), and correlative-dynamics experiments, which will make possible completely new measurements not currently feasible. For example, the increased coherence at higher energies delivered by the upgraded APS will provide a 4-to-6-order-of-magnitude increase in the time resolution of X-ray photon correlation spectroscopy (XPCS), revolutionizing the ability to probe the dynamics of systems in attenuating sample environments, such as electrochemical cells with applications to energy storage. With lensless imaging approaches, it will be possible to achieve high resolution in large three-dimensional fields of view. Likewise, the high-intensity, focused APS X-ray beams will provide the ability to obtain nanometer-size 3D voxels with chemical specificity in complex chemical environments. The APS-U project provided a suite of beamlines to exploit this dramatic improvement in the beam brightness and these capabilities will be significantly extended as part of the EXCEL@APS project.

Transform microelectronics metrology and research

Microelectronics play a pivotal role in the modern world, underpinning everything from household appliances, cars and consumer electronics to communications systems and advanced computing, including the compute resources for ever-growing demands of artificial intelligence. The sustained development of microelectronics is essential for pushing the boundaries of technological innovation, enabling faster, smaller, and more efficient devices that power today's and tomorrow's digital society. This progress involves not only scaling down to ever smaller structures but also advancing packaging technologies such as 2.5D and 3D integrated circuits (ICs), which are crucial for meeting the increasing performance requirements.

The upgraded APS dramatically improves lensless imaging techniques such as ptychography, which opens the possibility to routinely apply these techniques not only to fundamental research questions on novel materials, but also as a potential venue to qualify production-relevant processes as well as failure analysis. The key benefit of X-ray methods in this context is to be able to provide high spatial resolution in a large (3D) field of view on comparatively 'thick' samples, requiring minimal specific preparation. A dedicated instrument (LYNX) on the newly canted 31-ID-E beamline will provide opportunity to further develop the methods pushing the resolution boundary for 3D imaging of integrated circuits to the latest technology nodes and beyond (smaller than 5 nm), with large 3D field of view, 'natural' 3D registration of datasets and the ability for virtual delayering and statistically relevant analysis.

At the same time, as advanced semiconductor devices and their packaging become more 3D in their architecture, there is an ever-increasing need to develop advanced 3D metrologies that are non-destructive, can 'see through' packaging, and can probe devices during operation. Key challenges in 2.5D and 3D heterogenous integration include identification of defects arising during both fabrication and operation, as well as the need to understand what role these defects play in device performance and failure. The upgraded APS presents a unique opportunity to develop advanced metrology tools for microelectronics using high energy coherent X-rays. With the increased coherence at high energies provided by the upgraded APS, features buried in ever thicker device stacks can be imaged via phase contrast, which results in greater sensitivity than traditional absorption-based contrast. Furthermore, the penetrating power of hard X-rays can be exploited for *in situ / operando* characterization of 3D packaged semiconductor devices under relevant conditions. We will pursue projection microscopy as a tool for advanced 3D characterization of heterogenous IC integration. Here, the upgraded APS is used together with focusing optics to create a small source point. A sample is placed into the expanding X-ray beam and the X-ray projection collected by a detector further downstream, using the expanding beam to magnify the X-ray image of the sample. Coded aperture techniques can be used to visualize phase contrast in single-distance imaging for *in situ* studies at high sensitivities, with resolutions targeting the <50 nm regime, across significant areas of the ICs.

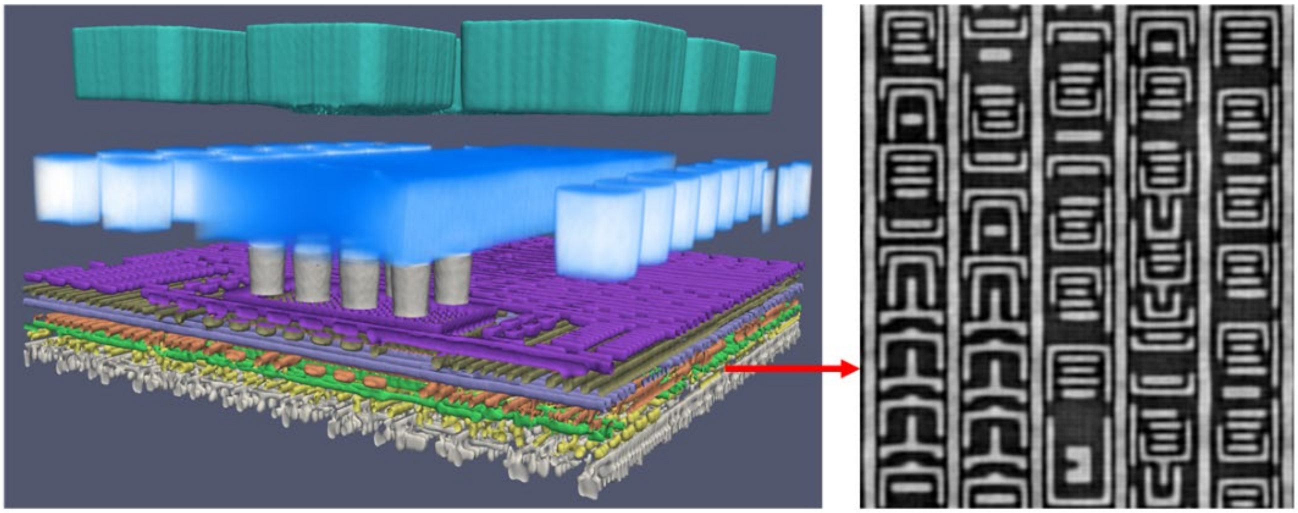


Figure 3: Left: Rendering of a 3D dataset from a 16nm FinFET device showing a 50-micron field of view of various metal layers and interconnects, using the LYNX instrument. Right: Metal layer 1, extracted from the full dataset by virtual delayering.

Beyond the characterization of devices and operation and failure mechanisms, the upgraded APS will uniquely enable the development of new materials and new processes for microelectronics. *In situ* X-ray scattering studies are uniquely well suited to unraveling the complexities of thin film growth and processing. Surface scattering measurements can distinguish between thin film growth modes and can track strain relaxation as films are grown beyond their critical thickness. Similarly, measurement of crystal truncation rods can reveal the complex interplay between stoichiometry, surface mobility and surface roughness. These *in situ* measurements aren't limited to synthesis. Processing steps such as etching, post-growth annealing and chemical reactions, such as oxidation, are fundamentally all surface and structure transformations that can be probed with X-ray scattering to better understand which processing steps are most critical in determining the properties of a material. *In situ* surface scattering and XPCS studies of deposition and etching processes at the CHEX (Coherent High-Energy X-ray) beamlines at 28-ID will provide insights into crystallization, defect formation and strain evolution during critical microelectronics fabrication steps.

In addition to development of synchrotron-based characterization tools for process development and device inspection, the opportunities afforded by the upgraded APS include the development of characterization tools for optics development for the microelectronics community. The shift to extreme ultraviolet lithography (EUVL) for micro- and nanoelectronic circuits with sub-10 nm nodes brings about new challenges, not just in fabricating nanocircuit patterns on wafers, but critically also for fabricating ultrahigh-precision optics and masks, where high-resolution metrology tools are critical. Since these often work in a reflection geometry, and relevant structures are numerous orders of magnitude thinner than the substrates they are fabricated on, we will explore reflective geometry-based coherent X-ray imaging, Critical-Dimension Reflective X-ray holography (CDRX-Holography), as the next-generation operando metrology tools for EUVL wafers and optics. This novel tool will fully utilize the high coherent flux of the upgraded APS, using the feature beamline Coherent Surface Scattering Imaging (CSSI) with its unique grazing incidence, reflection and scattering capabilities.

Lastly, the development of these methods goes hand-in-hand with the development of advanced software tools that allow for compressed sensing and AI/ML techniques to reduce required photon statistics. Those innovations, together with the development of the next generation of coherent X-ray sources with a smaller footprint, raise the possibility of eventual ‘in-line’ metrology tools for the semiconductor industry.

Understanding emergence of quantum states and decoherence mechanisms in quantum devices and systems

Materials for quantum information science and technology (QIST) exist at the interface between seemingly mutually exclusive materials properties. Qubits for quantum computing demand ultra-long coherence times, while the remarkable sensitivity of many quantum systems to external stimuli gives quantum-based systems a competitive edge in detection and sensing over classical-based systems. To fully harness the power of QIS, it is crucial to understand not only how quantum states and collective excitations emerge but also how these states interact with their surrounding environment. To this end, the APS will continue to expand its suite of techniques focused on discovering and characterizing materials with novel quantum states, as well as understanding the impact of defects, interfaces and external stimuli on quantum states and coherence times.

The DOE Roundtable on Next-Generation Quantum Systems summarizes this need as *“… the generation and stabilization of quantum states in a variety of materials systems.”* X-rays, with their unique ability to probe materials at both atomic and macroscopic scales while offering elemental, orbital and spin specificity across various time scales, have the potential to make revolutionary impacts in the field.

One of the biggest bottlenecks in QIST is the ability to scale up. Quantum circuits have unparalleled sensitivity to external stimuli, which is what makes them extraordinary as detectors and sensors. This is also what has limited the realization of large-scale quantum computing, due to decoherence and redundancy, and sophisticated error correction is required. Hard X-ray microscopy and imaging techniques, in both real and reciprocal space, enabled by the ultra-high brightness of APS X-rays, are ideally suited for *in situ* characterization of materials during synthesis and *operando*. This is crucial for identifying and classifying defects in materials and interfaces that contribute to the decoherence of entangled states.

Paradoxically, some naturally occurring defects in solid state systems can also serve as qubits themselves. Control of these defects and understanding how the local microstructure and local bonding environment affect the lifetime of coherent states is a potential pathway to room temperature quantum computers.

Many opportunities for transformational quantum technologies lie in the discovery of new materials, including those where the atomic structure itself leads to quantum states. Due to the symmetry of these states, they may be significantly less sensitive to specific types of defects or perturbations. Potential material classes include oxide-based high-temperature superconductors, two-dimensional heterostructures, and topological systems. X-ray spectroscopies, such as Angle-Resolved Photoemission Spectroscopy (ARPES) and resonant scattering, remain among the few definitive methods for identifying these new coherent states.

Dramatically improve our understanding of the brain

Despite significant advancements in neuroscience, much of the brain's complexity is still beyond our reach, and we are limited in our understanding of how it functions as well as how it fails. One of the challenges is simply the vast complexity of the brain's physical architecture. The brain is made up of billions of neurons, each capable of forming thousands of connections with other neurons. These connections, or synapses, create intricate networks, giving rise to complex functions like memory and decision making. This level of connectivity is orders of magnitude larger than for any other organ, making it extremely challenging to map and fully understand.

In addition, connections are made on local levels, but also connect different, physically separated brain regions to each other. To understand fully how the brain is wired up ('connectomics'), one would have to image the entire brain (to see how regions are connected) with enough spatial resolution and contrast to see individual synapses, and the ability to follow each neuron and see where it is connected to other neurons, ideally with spatial resolutions well below 10 nm and a 3D field of view of many mm. This presents a unique opportunity for hard X-ray imaging, with the intrinsic ability to achieve high resolution and large 3D fields of view. The upgraded APS, with its massively increased brightness, and the capabilities of new beamlines such as PtychoProbe for lensless imaging, will allow the further development of ptychography and sample preparation methods to image relevant brain volumes at the required resolution to improve our understanding of how the neural network is architectured.

Furthermore, future beamline upgrades (as outlined in EXCEL@APS) will enable high-resolution, phase-contrast-enhanced projection microscopy that will dramatically accelerate data acquisition, with minor reductions in spatial resolution. To work towards the 'holy grail' of imaging full brains of high-level organisms such as mammals, we will also develop and apply data analysis methods such as sparse sampling, enhance and exploit automated data analysis pipelines currently being developed and implemented, and make use of Argonne Leadership Computing Facility (ALCF) for data reduction and visualization.

To fully understand how the brain functions, it is not sufficient to 'just' understand it's physical structure and how it is wired. One also has to also understand brain chemistry. This becomes particularly important in understanding disease states, with obvious societal relevance. For example, neurodegenerative diseases (NDDs), such as Alzheimer's (AD) or Parkinson's (PD), are chronic disorders manifesting in the loss of function of nerve cells in the brain and peripheral nervous system. Caused by a combination of genetic predispositions and environmental factors, they manifest in deficiencies in cognition, mobility, strength, and other essential functions, ultimately leading to disability and death. Such conditions are estimated to affect ~50 million people worldwide and, as the population ages, the prevalence of neurodegeneration is expected to grow, adding significant burden to health systems. In 2017 in the U.S. alone, 7.5 million people were estimated to be affected by Alzheimer's and other dementias, with an annual cost estimate of $243 billion. The common trait of many neurodegenerative diseases is misfolding proteins and the toxic aggregates they form in brain tissue. Metals and the neurotoxicity caused by metal accumulation in the brain are correlated with neurological diseases in general.

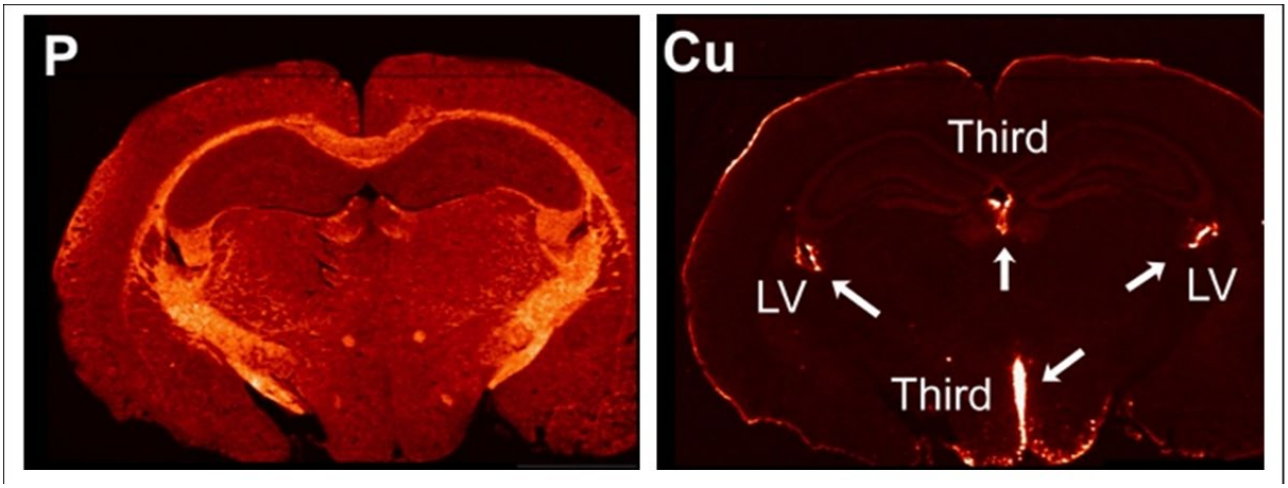


Figure 4: Elemental maps of phosphorous and copper content of a mouse brain section. Copper accumulation is visible around the lateral ventricle (LV) and the third ventricle, where the blood-brain barrier is located.

Understanding neurodegenerative diseases and developing possible therapeutics thus requires combined approaches on multiple scales using multiple contrast modalities, ranging from understanding the structural basis of proteins to the dynamics of protein aggregation, to the role of metals in these processes. The new capabilities afforded by the upgraded APS and its upgraded beamlines will be used to apply X-ray crystallography to determine protein aggregates *in-vitro*, use small angle X-ray scattering to study dynamics of aggregate formation (12-ID), as well as use the emerging application of X-ray photon correlation spectroscopy to study early phases of aggregation, including dimerization, thereby making use of the dramatically expanded capabilities of 8-ID. We will complement the above discussed new capabilities in X-ray imaging of brain structures in 3D with local trace-metal content and chemistry, using X-ray fluorescence contrast, X-ray scattering and nano-diffraction to characterize local aggregate architecture. We will develop methods to integrate the various data sources and scale up data analysis capabilities by utilizing leadership-class computation facilities such as Aurora and AI/ML-based approaches.

Expand nuclear materials research leveraging new hard X-ray capabilities and the Activated Materials Laboratory

Nuclear energy is the second largest source of power in the U.S. and the nation's largest source of clean power. The operation of current nuclear reactors and the development of advanced nuclear energy systems depend heavily on the performance of fuels and materials, which must endure extremely challenging environments. Structural alloys in modern nuclear energy systems are subjected to prolonged service times, intense neutron irradiation, mechanical stress, high temperatures, steep thermal gradients and various forms of corrosion. Nuclear fuel and cladding materials must support higher burn-up levels but face critical issues such as dimensional instability (swelling), fission product attacks, stress concentration and embrittlement. Understanding the microstructure-property relationships under reactor-relevant conditions is crucial for evaluating in-service performance and for developing advanced materials and fuels. Hard X-rays (at energies higher than 40keV) are particularly useful for this purpose, as they can penetrate these (often high-Z) bulk materials as well as necessary containment layers, and such can also be used for *in situ* investigations.

Driven by these needs and opportunities, both the High-Energy X-ray Microscope (HEXM) feature beamline at 20-ID and Activated Materials Laboratory (AML) were constructed during the APS Upgrade in the Long Beamline Building (LBB). HEXM will provide multi-modal high-energy X-ray data across a wide range of length and timescales, allowing users to zoom out (up to cm levels) and zoom in (on sub-micron levels) to materials using both diffraction and imaging. At least some version of these capabilities will also be present at other APS beamlines, including 1-ID, 6-ID and 11-ID, all of which have been successfully used to study nuclear materials prior to the upgrade.

The AML will be a centralized facility at the APS for radioactive specimen preparation and is located adjacent to the most distant HEXM end-station. This co-location in a building outside the APS main floor provides some risk reduction for experiments conducted at HEXM. The design and construction of the AML was funded by the DOE Office of Nuclear Energy, Nuclear Science User Facilities (NSUF). It will provide improved sample accessibility and flexible operation for all beamlines, minimizing the cycle time between samples, enhancing scientific productivity, and enabling the expansion of *in situ* testing capabilities. Since construction, the ANL-NE division, APS and NSUF have strategically developed a partner user proposal, which will provide multi-year beamtime for nuclear materials research at high-energy X-ray beamlines as well as operational funding to carry out the work safely and efficiently. This partnership will expand nuclear materials research to develop new - and benchmarking existing - materials and fuels. This will help enable continued use of nuclear energy to meet our nation's energy needs.

Figure 5: (a) An overview of the LBB at the APS which has three major components: the AML, the HEXM beamline, and the in situ nanoprobe (ISN) beamline; (b) the inside of the AML as of May 2023.

Advancing our understanding of non-equilibrium systems

Our understanding of nature is largely built upon the foundation of equilibrium systems, where statistical mechanics elegantly connects the probability of a state to its entropy. However, many systems that appear macroscopically stable are, at the nanoscale, constantly evolving across a vast range of timescales. While microstructure offers insights into equilibrium states, non-equilibrium behavior can be observed directly at the nanoscale, revealing fluctuations that signify deviations from equilibrium. Understanding these fluctuations, their evolution, and their role in reaching a steady state is crucial for comprehending the functionality and failure modes of materials. To explore these fluctuations in real time and across various scales, advanced tools such as the upgraded APS are essential.

The upgraded APS represents a major leap forward, with a more than 100-fold increase in X-ray beam brightness and coherence. This translates to a more than 10,000-fold enhancement in signal-to-noise for XPCS, enabling the study of non-equilibrium processes under real-world conditions. Coupled with external stimuli including electric, optical and mechanical excitation, driven dynamics that underpin the performance of quantum systems and microelectronics can be captured by time-resolved multimodal imaging and diffraction (TR-MMID) and driven XPCS measurements. With the upgraded APS we will be capable of measurements that span length scales from mesoscopic to atomic and timescales from 100 nanoseconds to 1000 seconds, bridging the gap in energy-momentum phase space for studying low-energy excitations in condensed matter. The suite of new and enhanced beamlines is designed to leverage the coherence enhancement in diverse areas of science such as electrochemical storage, catalysis, *in situ* growth and processing, quantum materials, energy efficient functional materials, complex fluids and biomaterials. The suite of beamlines (8-ID XPCS, 28-ID CHEX, 9-ID CSSI, 12-ID SAXS/XPCS and7-ID TR-MMID) will collectively utilize their subject matter expertise and wide energy range of operation, combined with a wide range of *in situ* and *operando* environments to offer complementary capabilities to the scientific user community.

The increased data complexity necessitates innovative approaches to data processing, where AI/ML becomes a powerful tool for real-time experimental steering and analysis. One of the technical challenges in realizing the full potential of XPCS is the need to handle the large amounts of data created and the need for real-time processing. To address this, the APS is pursuing AI/ML-guided experimental steering. In the first steps, we have leveraged AI/ML to classify the vast space of time correlation maps into groups of dynamical similarities and are successfully collaborating with the ALCF to leverage its supercomputing infrastructure with on-demand processing for the APS beamlines.

A central goal in materials science is to establish structure-property relationships in both soft and hard condensed matter. Despite the differing fundamental mechanisms between soft and hard matter, the technical developments can be agnostically applied between the two, often exhibiting similar underlying fluctuations, suggesting a broader universality class.

Hard Condensed Matter

Research in oxide based heterostructures for neuromorphic computing is closely tied to understanding the effect of oxygen ion/vacancy interactions and lattice strain, causing fluctuations far from equilibrium. Quantum materials exhibiting metal-insulator and superconducting transitions strongly couple to the underlying lattice. These transitions can occur under thermodynamic equilibrium or be driven by external electric fields through ionic liquid gating, making these materials attractive for next-generation microelectronics. At the atomic level, these gating-induced transitions are linked to changes in oxygen vacancies and modulation of the oxygen octahedral framework. Nucleation and growth of oxygen vacancies involve stochastic changes in the local structure, eventually developing into a larger defect framework. XPCS will provide crucial insights into the formation and propagation of these defects at the earliest stages by probing fluctuations across wider length and timescales.

Nanoscale ion dynamics in the next-generation superionic solid electrolytes is an area that can lead to significant energy storage gains. The highly enhanced coherent flux will enable diffuse scattering measurements decades into the tails of the Bragg peaks probing the order-disorder in the material that is critical to the understanding of the functioning of batteries.

Thin film growth and processing under various synthesis conditions such as chemical, plasma and atomic layer growth and etching are areas where spatio-temporal heterogeneities play a crucial role in the non-equilibrium evolution of the microstructure in 3D. Linking atomic-scale process with mesoscopic properties has been a long-standing challenge in condensed matter physics. Utilizing grazing incidence and wide angle XPCS, the impact of surface roughness and mobility, surface and bulk defects and island formation on the device performance can be elucidated.

Soft Matter

Soft materials are essential in diverse fields, including oil recovery, cosmetics, biomaterials, polymer upcycling and circular economy. Such materials inherently possess hierarchical structures spanning nanometers to micrometers and exhibit dynamics across nanoseconds to seconds and beyond.

Rheology of complex fluids is an area where the material properties are tailored to the applications by studying the effect of shear forces on the microstructure and nanoscale flow. Rheology-XPCS capability, which is unique at the APS, combined with the development of a first-principles approach to characterizing nonequilibrium dynamics in soft matter, will be leveraged to vastly improve our understanding of nonequilibrium dynamics by connecting microscopic insights into macroscopic properties. Other related areas of research include the study of dynamics of stress relaxation to enable performance enhancements in rubbers for energy saving car tires, polymers with dynamic bond exchange for improved polymer upcycling, and building an understanding of frictional dissipation in shear thickening fluids. Combining complementary microstructural capabilities in the USAXS, SAXS and WAXS regimes with dynamics at small and wide angles will lead to an improved structure-function understanding in functional materials.

In the area of biomaterials, microsecond-resolved XPCS, another technique pioneered at the APS, enables the study of rapid fluctuational dynamics in engineered biomacromolecules (e.g., artificial protein polymers and virus-like particles) when they self-assemble into functional hierarchical structures. Furthermore, the more than 100-fold increased coherent flux of the upgraded APS at higher energies greatly minimizes radiation damage in biological samples, facilitating studies of deformation dynamics in solid biomaterials such as cartilage and other soft tissues in their native environment. This will ultimately aid in designing new biomaterials with enhanced properties, including increased strength, pharmaceutical effectiveness and biocompatibility.

eBERlight: A program to expand biological and environmental research

The APS is set to transform biological and environmental sciences with its upgraded capabilities. One of our strategies is to expand the user community engaging with these fields by leveraging the enhanced X-ray techniques to conduct comprehensive studies of complex Earth systems, addressing societal challenges in sustainability and climate change.

To achieve an in-depth understanding of complex biological, Earth and environmental systems, it is essential to integrate genomic science, computational analyses, field studies and laboratory experiments, including multimodal X-ray techniques. Foundational knowledge of biological structures and functions is crucial for leveraging natural processes in energy production and developing high-value bioproducts. Imaging biological systems and determining their three-dimensional structures is vital for understanding the relationships between sequence, structure, dynamics, function and phenotype. Similarly, a deep understanding of environmental systems, such as soils or aerosols, is necessary for sustainable agriculture, and water management strategies. 3D visualization and investigation of dynamics, chemistry and interactions of complex soil or aerosol particles with the rhizosphere form the basis for ecosystem-level modeling of Earth processes.

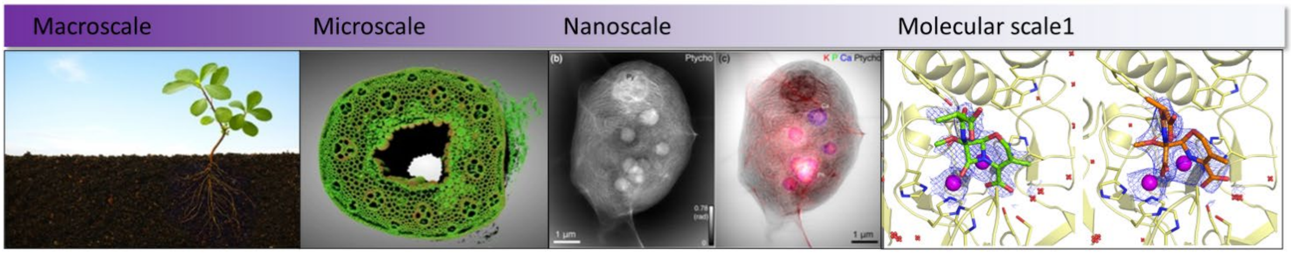


Figure 6: Bridging the different spatial dimensions with eBERLight.

Launched in FY24 and funded through FY27 by the Department of Energy's Biological and Environmental Research (BER) program, the eBERlight program is designed to maximize the upgraded APS's impact in bioenvironmental science. It addresses barriers in the scientific community, such as knowledge gaps, lack of suitable experimental envelopes, and overcoming barriers to entry. Through comprehensive user support, outreach and R&D activities, the initiative accommodates novice users and novel experiments. eBERlight offers coordinated access to APS beamlines and support facilities, improving sample preparation and data collection and processing efficiencies. The core capabilities include, in a distributed manner, macromolecular crystallography, X-ray full-field imaging, X-ray fluorescence microscopy (XRF), X-ray absorption spectroscopy (XAS), and scattering techniques.

The users can apply for eBERlight-supported beamtime directly via the APS, but the program also supports inter-facility collaborations to better serve the researchers tackling BER mission-related projects. The program works closely with major BER user facilities, such as the Environmental Molecular Sciences Laboratory (EMSL) and the Joint Genome Institute (JGI). With these collaborations in place, scientists can work with the APS through the Facilities Integrating Collaborations for User Science (FICUS) program, which grants access to multiple facilities through a single proposal. Such an approach not only simplifies the application process but also allows for a more synergistic approach, combining information from different X-ray techniques with genomics and biogeochemical analytics (e.g., soil organic matter characterization, bulk isotope analysis, mass spectrometry mapping). The eBERlight program supports individual users and large initiatives such as the Molecular Observation Network (MONet at EMSL) that focuses on high-throughput, comprehensive studies of soil.

Enable protein crystallography at physiological conditions

The primary goal of structural biology is to understand the relationship between the 3D structure of proteins and DNA molecules and their function. Knowledge of 3D structures is essential to understanding how biomolecules perform their normal functions in living systems, how mutations in some proteins cause cancer progression, how drugs bind to their target proteins, how receptor proteins respond to external stimuli and transmit information from outside to inside the cell, how pathogens evade detection by our immune system, and how our proteins detect infection by pathogens. Other economically and environmentally important applications include engineering proteins for the bioremediation of toxins in the environment, bioproducing important chemicals, or to modify genotypes to express desired phenotypes in plants. However, most structures in the Protein Data Bank (PDB) were determined from crystals of biomolecules at cryogenic temperatures far from physiological temperatures where most function occurs. Understanding the mechanism behind the function often requires mapping out active site structures with selective genetic mutations, chemical trapping, or freeze trapping. In addition, biomolecule crystallization has long been a bottleneck in determining structure. Many researchers report having crystals that are only a few microns in size and, therefore, too small for data collection.

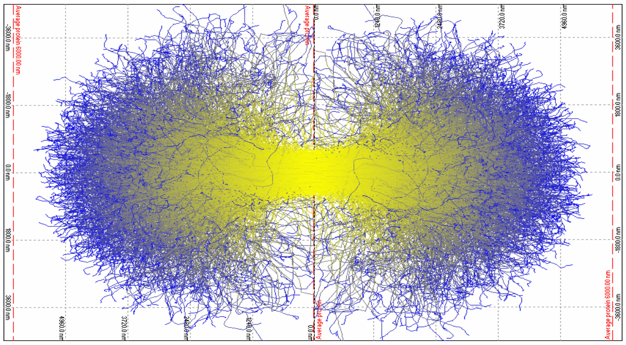


Figure 7: Photoelectron escape in a protein crystal.

To truly understand and control the structure-function relationship of biomolecules, experiments must be performed at a more relevant physiological temperature. The upgraded APS, combined with state-of-the-art X-ray optics, will deliver unprecedented X-ray brightness to the sample. Users will tailor the beam properties to match the scientific needs of their challenging biomedical problems. They will be able to rapidly and reliably select a beam size between 1 and 50 µm over an energy range of 5 – 35 keV (2.48 to 0.35 Å). The beam will be more than 100-fold brighter at the sample than before the upgrade. Users will control the sample temperature between room temperature and 100 K. Most data will be collected in serial crystallography mode, where each crystal is exposed to the beam for only a few milliseconds. Datasets will be assembled from the diffraction recorded from many crystals. Samples will be presented to the beam via either high-precision rapid scanning goniometry or a viscous-injector jet. High count rate, fast-framing, low-noise detectors will enable users to fully exploit the transformative new beamline capabilities. Detectors with high quantum efficiency (QE) at high X-ray energy will allow users to mitigate primary radiation damage by selecting the optimal energy based on the ratio of elastic to inelastic scattering, photoelectron escape from micron-sized beams, and detector QE. This will enable high-quality diffraction data to be collected from small, weakly diffracting crystals, such as those of membrane proteins.

Objective 1.2: Enhance scientific capabilities and mission performance

Deliver objective performance parameters, stable and reliable operation of the upgraded APS accelerator

The objective performance parameters for the project are shown in Table 1. The storage ring has been operating at 6 GeV energy since April 2024, and to date with beam current as high as 160mA for user operation. The next target is a beam current of 200 mA, which will be delivered to users at the beginning of June 2025. Our current ramp-up is in line with this objective. The primary challenges to reaching 200 mA are the short beam lifetime and the beam-induced heating of vacuum components. Both issues are mitigated by operating the bunch lengthening system, a passive superconducting higher-order harmonic cavity, which stretches the electron bunches longitudinally. This system is already operating and will be run at increasing voltage to reach optimal stretching and enable the nominal 200mA current.

The subsequent performance parameter is the horizontal emittance of the electron beam at 200 mA. We have already successfully demonstrated an emittance of 43(3) pm.rad at 50 mA, closely matching the design specifications. With full coupling, i.e. round beam, an emittance of 29(3) pm.rad has been achieved. We do not anticipate any emittance blow-up when the current is increased to 200 mA. Therefore, meeting this requirement should simply involve repeating the emittance measurements once we reach 200 mA.

Key Performance Parameters	
Storage ring energy	6GeV
Beam current	200 mA
Horizontal emittance	≤42 pm.rad at 200 mA
Brightness (20 keV)	≥1.10^{22} ph/s/mm²/mrad²/0.1%BW
Brightness (20 keV)	≥1.10^{21} ph/s/mm²/mrad²/0.1%BW

Table 1: Objective Key Performance Parameters of the APS-U Project.

The final two performance parameters are the X-ray beam brightness at 20 keV and 60 keV. Achieving these will require the installation of in-line SCUs. The first in-line SCU is scheduled for installation in May 2026, after which brightness measurements will be conducted on the relevant beamline. The brightness is expected to surpass the objective KPP brightness by a factor of 3 to 4. If, for any reason, the SCUs are not available for installation, we can still meet the brightness requirements using a hybrid permanent magnet undulator with a 14 mm period and a 6.5 mm magnetic gap. This alternative would provide a safety margin, delivering brightness at least twice the required value.

Additional parameters are critical to deliver successful science, for example achieving ultra-stable beam positions. Given the very small beam sizes in the storage ring, stability in beam position and divergence is essential in allowing users to take full advantage of the high X-ray brightness. The Fast Orbit Feedback System (FOFB), initially planned as part of the APS Upgrade project, is being pursued in the operation phase. It will operate at an unprecedented rate of 22 kHz, allowing suppression of motion up to ~1 kHz. This is expected to easily deal with the beam motion seen in the ring today. Initially, a prototype system will be installed in a single sector. Once this is functioning as expected, similar independent systems will be installed in all sectors. Finally, the independent systems will be tied together using a high-speed network into a global feedback system. Since development is expected to take until Q1 of 2026, we will continue searching for the sources of beam motion and, if possible, eliminating these.

In parallel with meeting performance targets, we will prioritize enhancing machine availability and increasing the mean time between faults (MTBF). Achieving this requires a comprehensive, multi-faceted strategy. This will include conducting detailed post-mortem analyses to identify root causes of faults, implementing clear and thorough operating procedures to minimize human error, and employing both predictive and preventive maintenance practices. Additionally, each technical group will have a dedicated downtime budget to ensure resources are appropriately allocated for improving reliability.

Deliver timing mode at the upgraded APS

The APS has developed strong established programs in ultra-fast X-ray scattering, spectroscopy and imaging for probing dynamic phenomena on time scales of hundreds of picoseconds to milliseconds. High-speed imaging of single-event processes such as dynamic compression or additive manufacturing has gained significant user interest over the past decade. The continued viability of these programs relies on a filling pattern with sufficient charge per bunch as well as a long intra-bunch time interval (~75 ns). The upgraded APS's "timing mode" would provide 200 mA stored current in 48 evenly spaced bunches, which requires an average stored charge per bunch of 15.3 nC, meeting the needs of this community. Accounting for transfer losses, the required charge from the Particle Accumulator Ring (PAR) is 20 nC per cycle. The PAR has demonstrated this performance by accumulating 20 shots of 1 nC each from the linear accelerator (linac). However, at this level, bunch-lengthening occurs in the PAR, which prevents efficient capture in the booster.

To overcome the challenges, the beam energy from the PAR will be raised from the present 425 MeV to about 500 MeV. A prioritized plan has been developed to accomplish this, the primary components of which are:

- Increase the beam energy from the linac to 530 MeV by adding three accelerating structures between the linac and PAR. Time for delivery of the structures is 12 months after reception of order. Installation of the structures and related equipment would take place in the nearest following one-month shutdown after receipt.
- Purchase new power supplies for two PAR-area magnets that cannot presently support the higher energy. Time for delivery is 120 days after reception of order.
- Commission the digital low-level RF system for the booster. Estimated completion by May 2025.
- Purchase and install high-power couplers in the booster RF cavities. We are partnering with European Organization for Nuclear Research (CERN) to finalize the design. Estimated delivery is Jan. 2026.
- In addition, the plan contains a prioritized list of injector improvements needed to maintain reliable operation at higher energy with consistently high charge.

In addition to delivery of high-charge bunches from the injector, full timing mode operation will benefit from achieving and maintaining optimized injection efficiency and lifetime, optimization and closed-loop (voltage-regulated) operation of the bunch lengthening system (BLS), continuous monitoring of the bunch length and longitudinal distribution, routine use of the bunch-to-bunch transverse feedback systems, and careful assessment of any chamber-heating issues that may emerge.

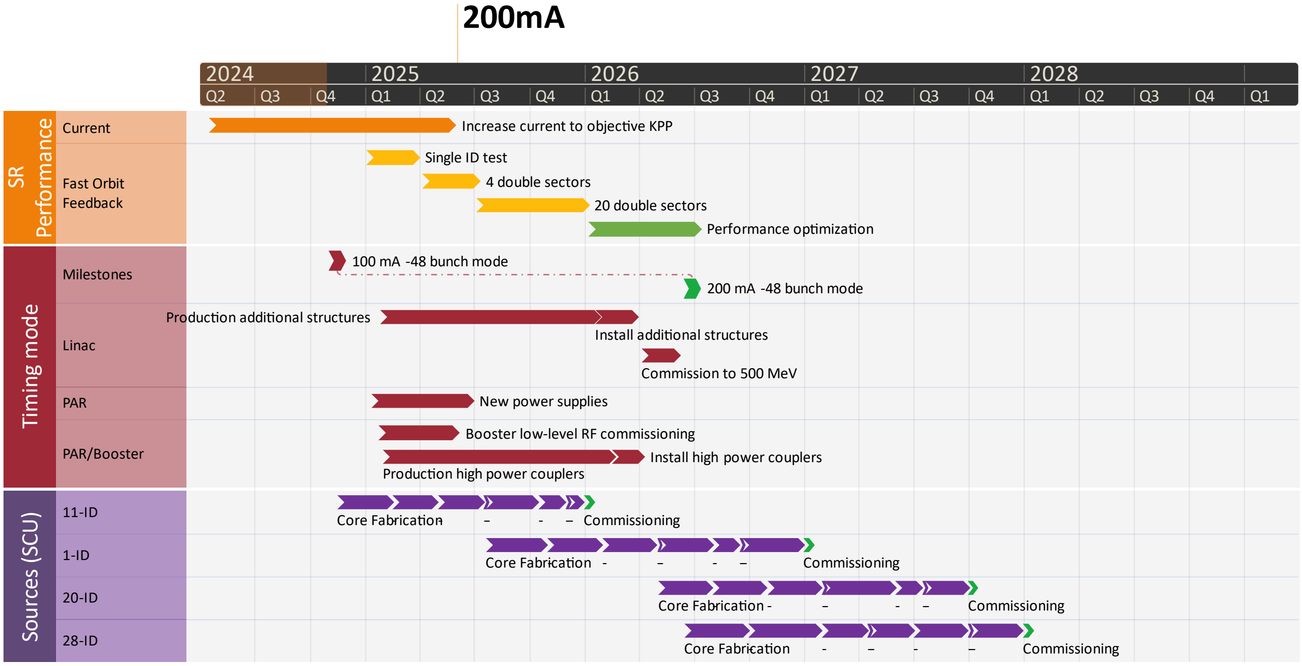


Figure 8: Accelerator and sources performance plan.

Deliver superconducting undulators for upgraded APS beamlines

The upgraded APS has provided users with increased radiation brightness and coherence by over two orders of magnitude. Compared to conventional hybrid permanent magnet undulator (HPMU) radiation sources, SCUs will further boost photon brightness by a factor of three at energies exceeding 50 keV. The APS is the world leader in superconducting undulator technology and has successfully operated NbTi SCUs at the original APS. We also delivered the first Nb_3Sn SCU in 2023. The APS-U plan included construction and installation of 8 SCUs on four straight sections of the storage ring by the middle of 2024. This included two 1.5-meter-long, 16.5-mm period SCUs in canted configuration at Sector 11, two pairs of 1.9-meter-long, 16.5-mm period SCUs in inline configuration at Sectors 1 and 20, and two 1.3-meter-long, 18.5-mm period SCUs in canted configuration at Sector 28.

The cryostats have been successfully delivered, and multiple cores have been fabricated and successfully trained. However, the new design with long cores and reduced period lengths has led to reliability challenges that present significant risks for operation, delaying installation. The technical challenges have now been overcome on a new prototype core design, and the development and fabrication of final SCU magnets is currently underway. The plan is to install the first pair of SCUs at Sector 11 at the end of 2025. The next 6 SCUs will be fabricated and installed at the upgraded APS storage ring in 2026-2027.

Implement a sustainable staffing model for beamlines

In normal operations the APS provides 5000 hours per year for X-ray experiments distributed over 3 run cycles, with beamlines typically scheduling experiments for 1-6 days depending on the technique involved. Effectively supporting these experiments for the 24-hour 6-days-a-week operation during each cycle places significant burden on experimental support staff on beamlines. Upon completion of the APS Upgrade the facility will operate ~4 additional beamlines requiring additional beamline scientific staff. Furthermore, experiments are becoming increasing complex, with rapid scanning, more demand for *in situ* sample environments, multiple detector streams, large data volumes, and need for remote operations and monitoring, placing an increasing need for additional specialized engineering support staff.

Over the past few years, the APS has embarked on a strategy to address these critical staffing needs. With the increase in the base operations budgets, the APS has been able to recruit staff for the new APS-U beamlines, supplement staff on existing beamlines that were in critical need and bring on additional support staff, particularly in data sciences and high-performance computing. The overall goal of this program is to increase the number of staff directly supporting beamline operations by at least one full-time equivalent (FTE) on average across all APS-operated beamlines, to enable improved scientific discovery and provide beamline staff with sufficient time for innovation for instrumentation and methods development, so that the APS can remain at the forefront of synchrotron science.

Recapitalize existing beamlines to maintain technological and scientific leadership

Upon completion of the APS-U, the APS will operate 40 of the 72 beamlines using base APS operations funding. Ten of these are new or completely refurbished beamlines included in the APS-U project that provide optimized capabilities for exploiting the world-leading coherence and brilliance of the new upgraded APS source. While the upgrade also included optics enhancements to 15 additional APS- and CAT-operated beamlines to more fully exploit the brilliance of the APS source, critical gaps exist on many APS beamlines in their optical component performance, instrument design, compute infrastructure and detector systems. These gaps prevent them from fully realizing the scientific potential of the new source.

The APS has a multi-pronged approach to address these critical gaps. First, we recently received CD-0 authorization for the EXCEL@APS major item of instrumentation project. This project specifically targets instrumentation and optics upgrades for 8 additional beamlines, that will place them at the forefront of high-brilliance-driven techniques. Further, the project includes vital compute infrastructure to handle the volume and speed of data acquisition realized from these upgraded instruments. Secondly, we continue to prioritize funding for ongoing beamline recapitalization within the base operations. Increased operations funding has allowed us to better address obsolescence issues on many beamlines through increasing investment in environmental control systems, support laboratories, energy efficient measures, sample environments and detector upgrades. Longer term, we are developing a new beamline recapitalization proposal to deploy an additional suite of new and upgraded beamlines that will maintain APS's technological and scientific leadership in high-energy, high-brilliance synchrotron X-ray characterization. To define the scope of this proposal, we will engage with the APS user community in a series of workshops that will form the basis for the proposed beamline and instrumentation package.

As the APS Upgrade nears completion, with many new and enhanced beamlines, the improvement focus will shift to recapitalizing the remaining beamlines. This transition aims to fully utilize the improved brightness of the upgraded APS beam. Since the facility has been in operation since the mid-1990s, many of the beamline scientists who originally developed, built, and maintained the beamlines are now retiring or approaching the end of their careers. To address the risk of an expertise gap in the future, and to ensure continuity in updating and upkeeping beamlines, a dedicated AES beamline technician team will be established to support these critical tasks.

Objective 1.3: Transform data analysis to accelerate scientific discovery

A primary goal for the APS, articulated in detail in the APS Scientific Computing Strategy, is to accelerate scientific discovery by harnessing the unprecedented power of computing and data science. More than ever before, advanced computational approaches and technologies are essential to fully unlocking the scientific potential of the new facility. The upgraded source opens the door for new measurement techniques and increase in throughput, which, coupled to technological advances in detectors, new multi-modal data and advances in data analysis algorithms, including AI/ML, will open a new era of synchrotron light source-enabled research. In particular, the high brightness and increase in coherent X-ray flux at the new APS is leading to significant increases in data rates and experiment complexity that can only be addressed with advanced computing. Advances in this area will empower APS users by providing the cutting-edge tools needed to continue to produce world-leading science.

Develop high-performance & AI-accelerated data analysis tools

High-performance data reduction, reconstruction, and analysis tools play a crucial role in enabling high-speed discovery. The APS is focusing data analysis algorithm and software development in the areas needed to answer novel scientific inquiries enabled by the renewed APS. These areas are techniques driven by coherence, imaging, and high-energy, as well as multi-modal techniques.

Algorithms and software are being developed to analyze and reconstruct massive data volumes, bridge across length and time scales, combine and understand data from multiple modalities, identify and classify features and patterns, and provide feedback to experiments dynamically. Data reduction and analysis will rely heavily on the use of high-performance computing (HPC), utilizing appropriate technologies such as multi-threading, General Purpose Graphics Processing Units (GPUs), edge devices, and distributed computing environments to obtain results with near real-time completion.

The APS has already made key developments in high-performance software that meet the initial needs of APS-U feature beamline techniques, including high-performance Bragg Coherent Diffractive Imaging (CDI), fluorescence mapping, GI-SAXS, high-energy diffraction microscopy near-field and far-field diffraction, Laue depth reconstruction, ptychography, reciprocal space mapping, tomography, and XPCS software. The APS will continue to focus its efforts on software for the APS-U feature beamlines and enhancement projects, and EXCEL@APS beamlines, including new algorithms and HPC software for multi-modal analysis, such as fluorescence tomography, fluorescence ptychography, magnetic ptychography, tomography diffraction, and Bragg CDI and ptychography.

The APS will develop and leverage advances in physics-aware AI and generative AI for fast data inversion and analysis, real-time streaming algorithms and EdgeAI for feedback during experiments, and multi-modal data fusion and analysis. This will be partially enabled through the APS's participation in the X-ray & Neutron Scientific Center for Optimization, Prediction, & Experimentation (XSCOPE), Intelligent Learning for Light Source and Neutron Source User Measurements Including Navigation and Experiment Steering (ILLUMINE), and Actionable Information from Sensor to Data Center (AISDC) projects.

Deliver sustainable solutions for storage and high-performance computing resources

The APS is developing and executing sustainable plans to deliver data storage and high-performance computing resources required to accelerate scientific discovery. The APS is stabilizing investment in storage and computing resources through regular upgrades, ensuring the facility keeps up to date with emerging technologies aligned to its needs within a sustainable budget framework.

The APS is in the procurement process for a new high-performance data buffer for APS beamlines. The system will be installed in phases over four years, resulting in a system with approximately 50 PB of storage and hundreds of GB/s of aggregate throughput available with GPFS. The system is a hybrid NVMe SSD/spinning disk system, where NVMe SSDs provide a high-speed landing space for data and spinning disks provide storage capacity. The first phase of this storage will be in operations use during the first quarter of calendar year 2025 and provide approximately 12 PB of usable storage with 300 GB/s of aggregate throughput. The storage capacity and throughput will increase as future phases are installed annually through the end of calendar year 2028.

The APS is heavily leveraging supercomputers, especially the Polaris supercomputer, at the ALCF for its high-performance computing needs. The APS currently accesses the ALCF through Director's Discretionary allocations. The APS is working to secure expanded future access to the ALCF Polaris supercomputer through a planned ALCC proposal, and continued participation in Integrated Research Infrastructure (IRI) activities. Additionally, the ALCF and APS have issued an RFP for computing systems that would provide dedicated computing resources for APS applications hosted at and managed by the ALCF. The APS and ALCF will evaluate RFP responses and develop a path forward early in calendar year 2025.

Deploy state-of-the-art data pipelines

The APS is deploying state-of-the-art data pipelines connecting APS instruments to ALCF supercomputers in order to provide near real-time data processing. These workflows use the APS Data Management System and the Globus Compute framework to run HPC-enabled software at the ALCF and return results quickly. The APS has already developed over 30 workflows for 10 data processing techniques that are being used as beamlines are commissioned.

The APS will harden existing data pipelines and develop new ones as beamlines return to operation. The priority is to deploy workflows for beamlines and techniques most enabled by high-energy, high-brightness, and coherent X-rays, namely all of the APS-U feature beamlines followed by the APS enhanced beamlines and beamlines delivered as a part of the EXCEL@APS project. As an IRI Pathfinder project, the APS will leverage IRI developments to create more advanced pipelines and deploy data pipelines and workflows at other supercomputer facilities, such as National Energy Research Scientific Computing Center (NERSC), Oak-Ridge Leadership Computing Facility (OLCF), and the future High Performance Data Facility (HPDF).

The deployment of advanced controls infrastructure and tools is critical to unlocking exceptionally challenging experiments and capabilities. Additionally, for the beamlines, advanced experiment control systems will enhance the user experience and better empower users to realize the full potential of the APS.

To this end, a number of solutions were proposed and vetted with the beamline community and will be rolled out to an increasing number of beamlines over the next five years: a network-based motor motion system, networked industrial input-output (IO) devices, and an internally designed field programmable gate array (FPGA)-based synchronization and triggering system (deployable either as a commercial FPGA DAQ appliance for the largest installations or as a smaller locally-packaged toolset for more routine installations).

In addition to these hardware and firmware solutions, we will advance the software controlling the accelerator and beamlines. First, we will continue transitioning to Experimental Physics and Industrial Control System (EPICS) v7 [https://epics-controls.org/], a large-scale distributed control system that facilitates data integration and streaming. A key motivator for the switch to EPICS v7 is the pvAccess protocol, which enables the manipulation and transport of structured data over the network. pvAccess will form the bridge between instruments and the high-performance data stores and data reduction tools. Second, we will roll out Bluesky [https://blueskyproject.io/bluesky-slides/] to more beamlines over the next five years. Bluesky is an open-source Python framework designed for instrument control and data acquisition. It provides a structured way to manage and automate experiments, making it easier to handle complex data workflows. It provides comprehensive meta-tagged data collection so that we can deploy AI/ML-enabled autonomous discovery at selected beamline experiment end stations.

Objective 1.4: Expand research capabilities to meet the national needs

Develop and implement the EXCEL beamline project to boost 4th generation synchrotron capabilities

To keep a competitive advantage on the international stage for the foreseeable future, we propose expanding the APS-U impact by modifying or constructing new instruments and optics to leverage the new beam characteristics. The first phase of this investment, which covers the period 2025-2029, is proposed through the EXCEL@APS (Expand X-ray Capabilities with Extreme Light) project. The EXCEL@APS project aims to magnify the impact of APS-U by expanding the improvements to 8 of our key experimental facilities. It also includes scope to provide advanced computational and storage capabilities for data-intensive beamlines, a key part of the computing ecosystem that will enable real-time data analysis capabilities at scale. Through the project EXCEL@APS, targeting the enhancement or transformation of existing beamlines to take further advantage of the bright, highly focused and coherent X-ray beams, we are proposing to build a unique research facility that will multiply the impact of the upgraded APS for research in micro-electronics and quantum materials, high-throughput materials discovery programs, battery research and advanced manufacturing.

Specifically, this project will provide unprecedented capabilities for characterizing nano-scale strain in both single- and poly-crystalline materials through Bragg Coherent Diffractive Imaging; enable microscopic mapping of light elements under *in situ/operando* conditions by increasing the throughput of hard X-ray Raman spectroscopy by a factor of >80; shedding light on the rapid structural changes of engineered materials on millisecond time scales and length scales from the atomic to millimeters; and exploring the dynamics of topological and quantum information science materials through spatially resolved inelastic X-ray scattering.

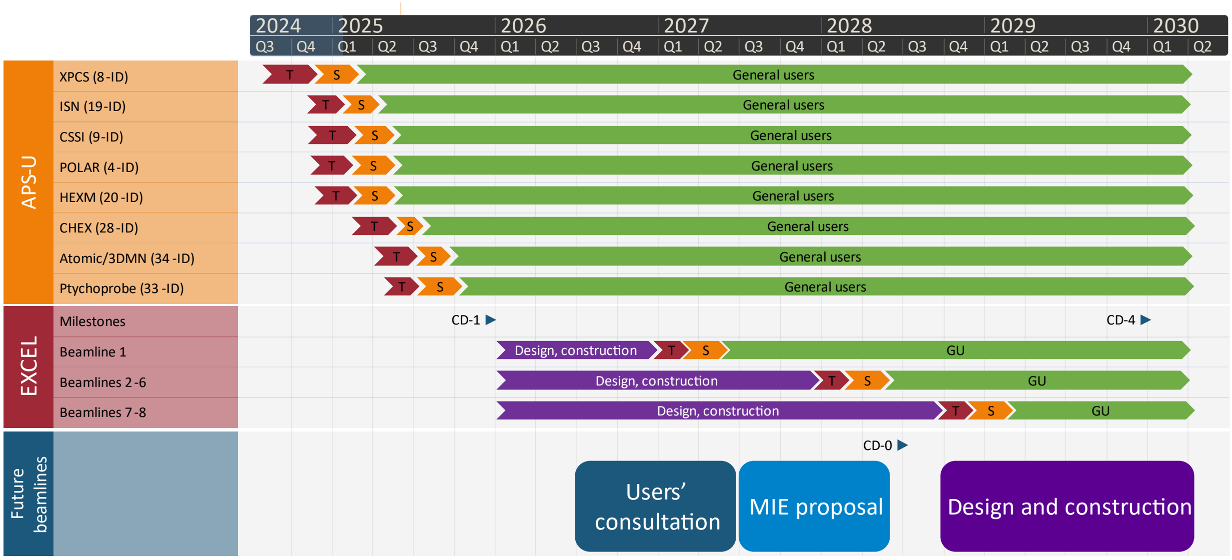


Figure 9: Beamline deployment plan at APS-U and future beamline upgrade plans

Horizon planning for next generation capabilities

The light source community is not standing still. On the international scene, many facilities are being upgraded and improved. Retaining scientific and technical leadership in synchrotron science requires continual refurbishment of the APS beamline portfolio. Longer term, the APS is proposing a follow-on beamline renewal project that builds upon on the capabilities realized in the APS-U and EXCEL@APS projects. In order to develop the scientific case and explore technical requirements, we foresee a series of workshops late in 2026, with the intent of building out a full instrumentation and beamline portfolio package to include in an MIE proposal that could be submitted in late FY27. In particular, we will explore capability gaps of the current APS beamline suite for addressing developing scientific areas. If successful, beamline and instrument design could start in late FY28 as EXCEL@APS nears completion, with construction and deployment starting in FY29.

Expand characterization capabilities in support of the NNSA mission

The National Nuclear Security Agency and Argonne National Laboratory recognize the strategic importance of the Advanced Photon Source to meeting the broad range of missions that DOE/NNSA supports. The upgraded APS storage ring creates an ideal capability that improves NNSA's ability to predict how changes in microstructure impact the performance goals in materials critical to the NNSA mission. Enhanced high-energy characterization techniques developed by beamlines such as the High Energy X-ray Microscope (HEXM) will be used to further enhance the experimental techniques that are available to NNSA sponsored programs.

In addition to the X-ray capabilities, the APS will continue to enhance the safety and security framework around the conducting of these experiments within the limits of the current APS facility. This includes increased explosive limits to characterize the explosives themselves and also to act as drivers for dynamic compression experiments. The APS will continue to support the security infrastructure needs of NNSA to support sensitive experiments. The APS is prepared to support strategic investments from NNSA in support of the Defense Materials Science Sector should the Sector be funded and approved as a DOE 413.3B project. This facility will provide NNSA capabilities with enhanced safety and security that are not practical to achieve inside of the existing APS facility.

Goal 2: Innovate and Advance Mission-Critical Technologies

Objective 2.1: Enhance X-ray capabilities through innovative techniques

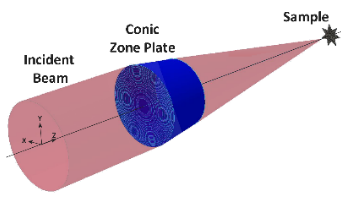
The world-leading brightness provided by the APS source opens up a wealth of new opportunities for X-ray characterization of materials at unprecedented spatial and temporal scales. To realize this potential, however, requires targeted research activities by APS staff to develop the instrumentation and methods that realize all the advantages of the upgraded source. Much of this work is done collaboratively with other DOE user facilities in response to technical Funding Opportunity Announcements (FOAs), particularly in development of optics, detectors and AI/ML applications for accelerator and beamline optimization. We leverage high-performance computing capabilities and expertise both within Argonne and across the DOE complex for comprehensive and timely analysis of large, complex, and multi-modal data sets.

Further, the APS exploits Argonne's specialized capabilities in nanofabrication and engineering for the development of state-of-the-art optics (e.g., Zone plates, micro-electro-mechanical systems (MEMS)-based choppers) and advanced detectors (e.g., Transition Edge Sensors (TES) high energy-resolution detectors). Lasty, APS staff leverage Argonne's Laboratory Directed Research and Development program for more exploratory research, including exploring novel X-ray methodologies, development of new core capabilities for attracting untapped user communities, and realizing advanced applications of AI/ML and HPC for data handling and analysis.

With its record small source emittance and 100-fold increase in coherent flux, the upgraded APS provides the impetus to push the frontiers of optics that will exploit the new APS characteristics to explore uncharted areas of scientific research. To take advantage of the new characteristics, the APS optics strategy is centered on three main areas which are described below.

Focusing high-energy X-rays for micro- and nanoscale resolution

Several APS beamlines are being developed to incorporate efficient and higher-resolution focusing optics, with the Ptychoprobe setting a goal of 5 nm resolution for routine user operations. The APS Optics Group will pursue two complementary solutions to address future needs: fabrication of conic zone plates (CZPs) and depth-graded multilayer mirrors. Like a multilayer Laue lens (MLL), a CZP is a volume diffractive element that provides 2-D focusing with a single circular optic, unlike two orthogonal 1-D MLL optics.



For CZPs, our objective for the next four years is to develop the tools and procedures to fabricate these optics further. We built a first-generation deposition system through a Laboratory Directed Research and Development (LDRD) project. In FY 2025, we will demonstrate focusing with a CZP made in this deposition system. In FY 2026, we will optimize the bi-material systems and deposition parameters to produce a nano-focusing optic for an insertion device beamline in FY 2027. The fabrication will incorporate AI/ML for optimization and automation of the process. Achieving resolution approaching 1 nm and theoretical diffraction efficiency will require an advanced fabrication tool, such as atomic layer deposition (ALD), combined with sub-Angstrom-resolution *in situ* metrology. To validate our hypothesis, in FY 2025, we will work with a vendor to show that ALD can achieve the necessary structure definition, interlayer roughness, and X-ray transmission. If successful, we will develop the scientific and technical case for building a full-scale custom-made ALD system incorporating metrology in FY 2026.

The APS has developed and demonstrated the basic methodology to produce depth-graded multilayer mirrors in the Kirkpatrick-Baez (KB) geometry. These mirror systems provide broadband focusing (high flux) and large working distances. To optimize X-ray performance, we will refine this process in the coming years by including *in situ* metrology in the modular deposition system and leveraging research results obtained for low-stress reflective multilayers. In FY 2025 and FY 2026, we will test *in situ* metrology with velocity profiling and profile etching in the modular deposition system. These results will guide us toward demonstrating a fully functional and automated system for the deterministic fabrication of high-quality single- and multilayer KB mirrors in FY 2028.

Developing advanced optics for wavefront conditioning, manipulation and control

One requirement for the EXCEL@APS project is to deploy a fully operational zoom mirror system for the ATOMIC beamline within four years. Accordingly, this initiative focuses on advancing adaptive optics systems and at-wavelength diagnostic tools to achieve precise wavefront engineering and control for X-ray beamlines. We will prioritize creating deformable mirror systems capable of dynamic bending, beam shaping, zooming, and real-time wavefront control. We will accomplish this by working with vendors to fabricate advanced optics systems, particularly hybrid mirrors that combine mechanical benders and bimorph structures.

In FY25, we will augment our AI-driven autofocus and wavefront optimization tools by leveraging additional deployments and training on the APS's upgraded beamlines. The advancement of at-wavelength diagnostic tools will enhance real-time feedback control and enable minimally invasive solutions for diagnostics across multiple beamlines. In parallel, we will develop user-friendly software to enhance the accessibility and usability of our diagnostic tools, to continue advancing ML-based data analysis for real-time 2D nano-focused beam wavefront sensing, and to improve the precision and speed of diagnostics. Together, our developments will enable more accurate alignment and optimization of complex optical systems.

Advancing enabling technologies, including crystal fabrication and metrology

Crystal Optics: To better deliver upgraded APS X-ray coherence to beamline end stations, we will develop new procedures to reduce the rms surface roughness of Si single crystals from 0.5 to < 0.3 nm and Ge crystals to ~ 0.5 nm. First, we will equip the polishing lab with needed metrology tools by acquiring a standard surface roughness microscope in FY 2026 and deploying an existing compact interferometer for flatness measurements. Second, we will implement new pitch polishing and crystal mounting procedures in FY 2025 and FY 2026 using the new tools for feedback on our process improvements.

Optical metrology: Over the past 30 years, the surface figure error of meter-long mirrors has improved from 5 to < 0.1 micro-radians root-mean-square (rms), and surface roughness has been improved from ~ 0.5 to ~ 0.1 nm rms. Metrology of focusing mirrors with tight curvature remains challenging, especially in the mid-spatial frequency range. These currently unmeasurable mirror errors induce unwanted structures in the transmitted beam. In FY 2025, we will focus on improving the method to account for systematic errors of <50 nrad. In FY 2026, we will explore a new type of slope sensor with the potential to reduce the size of the probe beam from 2.5 mm to ≤1 mm and angular resolution to ≤ 25 nrad. A prototype to test the concept will be built using commercial components, with testing in FY 2028 and validation in FY 2029. 2D shape-error measurement, used for more demanding mirrors for coherent beams, is typically done with sub-aperture stitching for surfaces larger than the interferometer aperture. Here, the accuracy is limited to a few nanometers peak-to-valley for a mirror measuring > 0.5 m. In FY 2025, we will explore solutions to build a stitching platform capable of achieving < 1 nm accuracy. Design will start in FY 2026, with a prototype built, tested, and validated in FY 2028 and FY 2029.

Advancing detector sensing and electronics

Detectors are an integral part of scientific discovery. From Wilhelm Röntgen's barium platinocyanide screen to Georges Charpak's multiwire proportional chamber, detectors allow scientists to see far beyond human limits. Biochemistry has been transformed first by the development of megapixel detectors for X-ray crystallography and more recently using high frame rate detectors to correct for drift and enable atomic resolution structure determination in cryo-electron microscopy. The mission of the XSD Detectors group is to deliver cutting-edge detectors to APS beamlines via the APS Detector Pool and detector R&D projects. With the advent of data-driven intelligent detector architectures, the involvement of computational and beamline scientists will be critical.

In the coming years, we plan to continue this approach to push computing towards detector silicon (i.e., on-chip technologies and at the edge), emphasizing minimizing memory transfer bottlenecks and latencies between sensors and computing units. At the APS, detector development is an interdisciplinary activity involving detector developers and computational and beamline scientists. This has been exemplified by the SparkPix-RT detector, developed from an enduring strategic partnership with SLAC. The SparkPix-RT detector consists of a charge-integrating analog front-end with user-selectable on-chip digital lossless and lossy compression algorithms co-designed with computational and beamline scientists. A 192x168 SparkPix-RT detector (i.e., "SparkPix-RT2-32k") with Si, CdTe and $CsPbBr_3$ sensors running at 100kHz full-frame readout will be deployed and tested at several APS beamlines starting in FY25. Looking beyond SparkPix-RT, we plan to use the concepts and methods learned from SparkPix-RT to move in the MHz frame rate regime in a joint project with SLAC named SparkPix-ED. A conceptual design will be finalized by the end of FY25, and preliminary designs and prototypes will be developed in FY26 with megapixel detectors in FY27. Finally, we are engaged in forward-looking microelectronics R&D. For example, XSD Detector staff are co-PIs in two DOE-funded Microelectronics Science Research Centers (MSRCs) projects which are focused on energy efficiency: Adaptive Ultra-Fast Energy-Efficient Intelligent Sensing Technologies (AUREIS) and BIA: A Co-Design Methodology to Transform Materials and Computer Architecture Research for Energy Efficiency.

In addition to developing pixel detectors, the APS has a long history of developing and deploying superconducting sensors for resolving X-ray photons with eV-scale precision. In the coming years, we will continue efforts to exploit this detector technology to enhance techniques in the soft and very hard X-ray regimes. In collaboration with the National Institute of Standards and Technology (NIST), we plan to deploy two science-grade TES detectors in FY25 – one at 29-ID for resonant soft X-ray scattering (RSXS) and another at 11-ID for high-energy spectroscopy. Looking further ahead, we also see an opportunity to leverage this expertise in developing low-noise microfabricated superconducting sensors to explore the development of experimental sample platforms for multi-modal measurements. We have recently developed a nano-calorimetry sample platform for *in situ* heat capacity measurements. In FY25, nano-calorimetry sample platforms will be deployed at 6-ID and 29-ID. This platform will be available to all APS beamlines. In FY26 and beyond, we plan to build upon this platform to integrate more measurement modalities.

Engineering over the next five years

Over the next five years, beamline engineering will transition from work almost exclusively in service to APS-U to delivering on a more diverse set of facility needs and objectives. First, we will execute the EXCEL@APS MIE. Two significant tasks (among many) will be augmenting capabilities of the end stations for the 3DMN and ATOMIC beamlines. Secondly, we will deliver additional major beamline projects, which are significant upgrades of existing beamlines, and provide engineering support for new initiatives in collaboration with our partners. We also anticipate additional engineering support needed to further optimize and fine-tune the APS-U beamlines as experience is gained with the new source characteristics and the new beamline infrastructure.

Another priority will be furthering automation capabilities at relevant beamlines. This will facilitate remote operations, autonomous discovery and high-throughput experimentation. Another area of focus will be sample environments. Work in this area will allow the new source's unique high-energy and nano-focusing properties to be fully leveraged for *in situ* and *operando* science. A final emerging priority will be exploring opportunities in mechatronics to enable scanning over large areas or volumes with high fidelity and speed.

Digital twins are transforming complex experiments by creating virtual replicas of physical systems that enable safer, more efficient research and development. By providing a virtual testing ground, these digital counterparts allow researchers to rapidly test thousands of parameter combinations and optimize experimental conditions before physical experimentation. They enable real-time monitoring and adjustment of experiments, integrate data from multiple sources, and help predict long-term outcomes that would be impractical to observe physically. The APS is in the midst of developing capabilities to simulate every aspect of beamline experiments, and this work will continue over the coming years.

Objective 2.2: Push boundaries of X-ray brightness at the APS

The reduction of horizontal emittance at the upgraded APS is truly transformative, offering up to a factor 500 increase in X-ray brightness. Opportunities exist to push the hard X-ray brightness levels by another order of magnitude in the next 5-10 years by optimizing electron focusing on the storage ring straights to better match the electron and photon emittance ellipses, reducing the undulator gaps further, and developing new generations of superconducting undulators. Theoretically, a photon brightness approaching 10^{23} ph/s/mm^2/mrad^2/0.1%bw is within reach, not only offering new opportunities for coherent X-ray applications at higher photon energies but also bridging the gap in average brightness available at synchrotrons and X-ray Free Electron Lasers (XFELs), opening new complementarities for time-resolved experiments from the attoseconds available at XFELs to ps and beyond at storage rings. Remaining at the forefront of hard X-ray science technologies is mission critical. By supporting a comprehensive program of R&D in this area, we will ensure that APS continues to play a leading role on the international scene and retain world-leading capabilities for research.

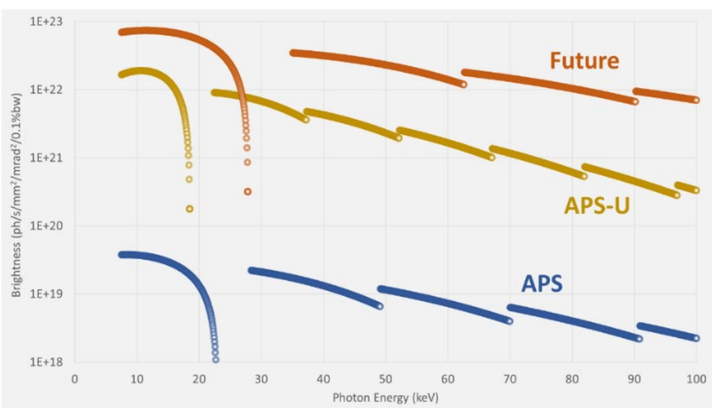


Figure 10: Brightness curves for superconducting undulators at the original APS (blue), APS-U, and future SCU with optimized beta functions and reduced vertical gaps.

Develop new small-gap and compact undulator technologies

In the development of future insertion devices (IDs), innovative designs like Force Neutral Adjustable Phase Undulators (FNAPUs) and X-undulators (XUs) with force compensation are gaining significant traction. These compact, lightweight devices offer cost-effective and scalable solutions for X-ray production. With their modular, stackable design, FNAPUs and XUs can be efficiently scaled from 3 to 5 meters in length, or even beyond, to meet the specific needs of various applications. This multiplexing capability enables the production of a broad energy range or multiple X-ray beams, making them ideal for advanced research facilities.

XUs, in particular, exhibit exceptional performance characteristics. Their precise polarization control and rapid switching capabilities make them well suited for round beam storage rings such as the APS and FEL facilities. Moreover, XUs can be configured as Knot or Figure-8 types to minimize thermal load and optimize photon delivery, further enhancing their versatility and efficiency.

The development of a 2.4-meter-long undulator array with 27 mm and 17.2 mm period lengths for FNAPUs is due for completion in 2025. A one-meter-long prototype XU with a 30 mm period length has been designed and fabricated, with tuning and characterization to be completed the same year. Additionally, two 2.2-meter-long XUs are planned for the POLAR beamline at the APS.

Develop cryo-free small gap superconducting undulators with high-temperature superconductors

The development of APS undulators—the primary radiation source of the user facility—is critical for further advances in the increased brightness and flux delivered to users' experiments. The obvious path to that goal is advancing undulator technology toward smaller undulator periods without sacrificing undulator performance in terms of its spectral tunability. Also, undulators with smaller periods would compensate for the loss of high-energy X-ray flux in the transition from 7 to 6 GeV of APS storage ring operation.

Currently there are two technologies that support construction of small-period (less than 20 mm) undulators: hybrid cryogenic permanent magnet undulator (CPMU) technology and SCU technology. Many CPMU devices are used at various synchrotron radiation facilities, but their theoretical and practical limit extends to 14-mm-period IDs with an undulator K-value less than 1.5. The SCU technology, on the other hand, theoretically and very likely practically can achieve 10-mm-period IDs with an undulator K-value equal to 2, which is important for non-interrupted X-ray energy coverage for one undulator.

The APS is the world leader in the development of SCU technology and has every intention of maintaining this leadership. The path toward smaller-period SCUs includes a) development of small-period undulator magnets; b) development of a thin-wall vacuum enclosure for the electron beam, which will allow us to minimize the SCU magnetic gap; and c) use of high-temperature superconductors (HTSs) to achieve record high small-period undulator magnetic fields. Additionally, the cryogenics of these novel devices will rely on liquid helium-free technology.

In the first of these developments, the 14-mm-period Nb3SN-based SCU with a magnetic gap of 6 mm will be built with the goal to demonstrate that such an SCU could be superior to any existing CPMUs. This development will be accomplished in FY2025-27. The second step will be to design and build 12-mm-period and then 10-mm-period SCUs using HTS technology. These devices should achieve an undulator K-value of 2 while maintaining a magnetic gap of 5 mm or higher. This development will be accomplished in FY2026-29.

Research electron optics to reduce beta functions

X-ray brightness can be increased by reducing the electron beam emittance, which was the main objective of the APS-U storage ring upgrade, but also by reducing the electron beam beta functions in the straight sections to more closely match the ideal (radiation-matched) beta functions. For a 4.8-m-long device, the ideal beta functions are about 0.8 m, which is much smaller than the APS-U electron beam values of 5.2 m in the horizontal and 2.4 m in the vertical.

Reducing the electron beam beta functions to 0.8 m is not feasible due to other constraints, such as the deleterious impact it would have on the effective physical aperture of the ring. In addition, reducing the beta functions is not necessarily compatible with maintaining low emittance, long lifetime, and good injection efficiency. However, preliminary studies performed during development of the APS-U lattice indicated that reducing the horizontal beta functions to as low as 3 m may be possible while maintaining similarly low vertical beta functions. In addition, it may be possible to obtain even smaller values by breaking the optical symmetry of the ring, e.g., by having 20-sector symmetry instead of the present 40-sector symmetry.

Exploration of these options will first be undertaken using simulations. In particular, we will use a multi-objective genetic algorithm to optimize X-ray brightness while maintaining adequate injection and momentum acceptances. The initial goal will be to deliver the same brightness to all beamlines. If this proves elusive, we will also explore the possibility of delivering smaller beta functions for some beamlines, e.g., at uniformly spaced locations around the ring. Assuming the simulations yield a positive result, machine studies will be undertaken to verify the configuration and, if successful, deliver it to user operations.

Objective 2.3: Research technologies and improve processing facilities for future light source applications

Towards compact XFELS: Research high-gradient acceleration technology for future compact light sources

Argonne is uniquely positioned to lead the development of compact XFELs, leveraging its expertise in beam dynamics, insertion devices and high-gradient acceleration technologies. The envisioned compact XFEL will likely combine short-period undulator innovations from APS with cutting-edge high-gradient accelerating structures [e.g., structure-based Wakefield acceleration (SWFA)] and bright photoemission electron sources under development in Argonne's HEP division.

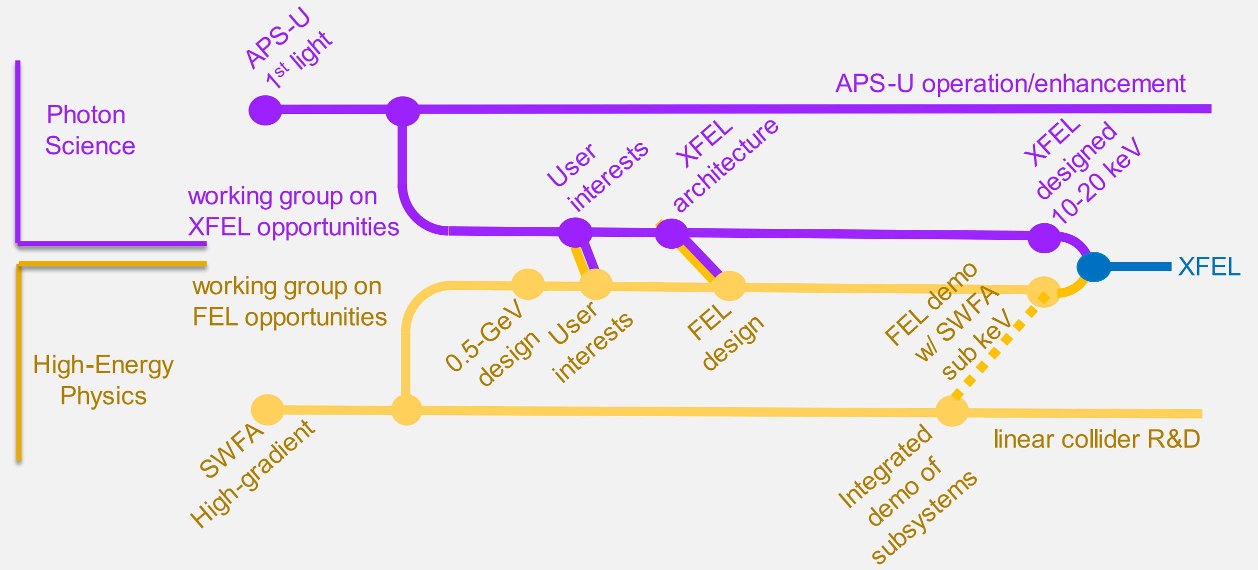


Figure 11: Roadmap showing synergies between PSC and HEP at Argonne.

A key focus of this research is addressing a recent recommendation from the Basic Energy Sciences Advisory Committee (BESAC) by developing new technologies for a green-field future light source. This effort will advance photon-pulse-on-demand capabilities, enabling programmable photon pulses with tailored shapes or spectra, ideal for next-generation XFEL applications. These capabilities will rely on advanced electron-beam conditioning methods, laser-electron-beam interactions, and precise stabilization and synchronization. Much of this work will be experimentally developed at the Linac Extension Area (LEA) facility, utilizing bright photoinjected electron bunches enabled by the planned photoemission-laser upgrade of the APS linac photoinjector.

A first phase will demonstrate the integrated operation of a soft X-ray FEL in the water-window regime, comprising a 1-GeV linac with a 5-m long 10-cm-period undulator. This FEL will leverage advancements in short RF-pulse acceleration techniques, supporting GV/m-class acceleration fields and enhancing energy efficiency, thus paving the way for more sustainable accelerator technologies. An advantage of this approach is the potential to utilize existing facilities at Argonne and implement a two-beam acceleration scheme to generate arbitrary RF waveforms and frequencies, allowing for design refinement of the accelerator components and integrated testing before committing to the development of dedicated short-pulse klystrons. A follow-up phase will scale the concept and focus on the design of a hard X-ray FEL with photon-energy in the 10-20 keV range.

This research not only positions Argonne at the forefront of FEL development but also creates exciting opportunities for the PSC staff and bridges expertise across Argonne by fostering inter-directorate collaboration. Additionally, some of the expertise developed could open new opportunities for the APS storage ring and its accelerator complex.

Cavity-Based X-ray Free Electron Laser (CBXFEL)

PSC has been partnering with SLAC to develop a Cavity-Based X-ray Free Electron Laser (CBXFEL) since 2019. The CBXFEL concept, originally proposed by staff at PSC, will produce longitudinally coherent pulses with improved spectral brightness. The project is in its final production phase, with a current focus on the successful installation of the CBXFEL concept in LCLS-II at SLAC. PSC will support the installation, scheduled for summer 2025, as well as commissioning and subsequent beam studies. This work will guide potential future CBXFEL-based sources operating at over 1 MHz, as envisioned by the DOE.

Key R&D activities in support of a comprehensive CBXFEL include designing, prototyping and testing diamond X-ray optics that can withstand high heat loads; developing cryogenic cooling and precision temperature control for diamond mirrors and related components, including the design and construction of a UHV, 50K, 20-W cooling power enclosure with 20-nrad and 1μm stability for beam tests at the APS; establishing at least one U.S.-based manufacturer for diamond mirrors and other crucial components; developing novel materials and treatments for detectors and diagnostics; creating and testing radiation-hard encoders for nano-positioning systems; and developing hydrocarbon-free, bakeable components to replace those currently used at APS and CBXFEL.

Beam simulations to optimize the design of a future facility will be planned, considering a superconducting RF or compact normal conducting linac as the driver, a long undulator system, an X-ray switchyard, and more. Argonne will focus on the original bow-tie design and optimize for the XFELO rather than the regenerative-amplifier FEL (RAFEL) configuration, based on user preferences.

We will consult the community during a dedicated workshop to capture future requirements and identify the best way forward to mature CBXFEL technology.

Develop the Linac Extension Area as a test stand for accelerator technology

The APS LEA is an approximately 50-meter-long shielded tunnel located at end of the APS linac. Within the tunnel, a 15-meter electron beamline has been installed including quadrupoles, steering magnets, various electron beam diagnostics stations, and a beam dump. A designated area in the middle of the beamline includes two gate valves on either side to facilitate the installation of equipment for different experiments. At the end of the tunnel, a Class IV laser room is ready to accommodate lasers used in experiments conducted in the LEA. Adjacent to the LEA enclosure, an S-band RF station capable of delivering 50 MW RF power is available.

An electron beam can be supplied to the LEA either directly from the APS linac or from the PAR with accumulated linac bunches. The electrons are generated either by a photocathode RF gun or by thermionic cathode RF guns, offering a wide range of bunch charge (from 50 pC to 20 nC), normalized emittance and peak current. Beam energy can reach up to 500 MeV. A magnetic electron bunch compressor in the linac can be used to compress the electron beam when high peak current is required for specific experiments in the LEA. The first electron beams were delivered to the LEA in 2023. The APS linac has been commissioned to operate in an interleaving mode, allowing electron beams to be injected into the storage ring on demand while directing them to the LEA when they are not needed for storage ring injection.

Figure 12: The Linac Extension Area Beamline.

With the possibility of a high-brightness, high peak current photoinjector beam at several hundred MeV, along with the availability of a laser room and an S-band RF station, the LEA is poised to become a unique test stand for advanced accelerator technology and beam physics. This includes novel undulator testing such as tapered undulator system for energy extraction, interactions between electron beams and laser beams such as Compton, and structure-based Wakefield acceleration, among other possibilities.

The recently established BeamNetUS collaboration has garnered significant interest from the accelerator community. As of October 2024, BeamNetUS includes 10 facilities for accelerator beam-based research. The beam parameters simultaneously achievable at the LEA are unique and not available at any of these other facilities. This presents a golden opportunity for the LEA to join BeamNetUS and become part of the accelerator test stand community. The advancements in accelerator technology and breakthroughs in beam physics possible at the LEA are going to attract exciting projects and talented people to the APS at Argonne.

Improve the UHV assembly, welding, cleaning and certification facility

Since the inception of the APS, the PSC team has been a leader in the light source community, particularly in UHV chamber science and technology. We have supported numerous accelerators in their chamber development, manufacture, cleaning, assembly, and certification since completing the initial APS. Looking ahead, we plan to re-establish our leadership in this field by expanding our current capabilities and offering them to our colleagues. As part of this commitment, we will revitalize our chamber production facilities by upgrading to a new welding machine with enhanced tolerances and safety features and a new vacuum certification oven with increased throughput. We will expand and improve our cleanrooms, vacuum cleaning, and vacuum certification areas. We will leverage our experience with the recently upgraded storage ring bakeouts to include automated controls and software monitoring throughout our certification process. Drawing on our team's extensive knowledge of past UHV chambers, we will envision, design and certify the next generation of vacuum chambers, while also enhancing expertise through training from both internal and external experts. Our strategy would support the DOE particle accelerator community as we embark on the development of the next generation of accelerators.

Objective 2.4: Accelerate Scientific Frontiers by harnessing Data and AI

The development of new X-ray characterization techniques has historically depended on the simultaneous invention of algorithms and mathematical models. These computational tools are vital for analyzing and interpreting the data each new technique generates. For instance, several synchrotron imaging techniques, such as ptychography and tomography, owe their feasibility to specific computational imaging methods and the development of accelerated computing. While numerical algorithms have historically enabled groundbreaking science at synchrotron sources, the next-generation light sources pose significant computational challenges that many current algorithms may struggle to meet due to the sheer volume of data expected in the upgraded APS era.

In response to these challenges, AI/ML techniques are emerging as powerful tools. They not only accelerate X-ray data analysis but also enhance the robustness and expand the potential applications of these methods. At the APS, AI is being used to speed up data analysis, automate operations, improve scientific knowledge extraction, and assist users in experiment planning and execution.

AI for analysis, steering and knowledge generation

The overarching motivation of leveraging AI at the APS is to unlock new scientific capabilities from existing instruments while improving and enhancing the users' experience and scientific productivity.

This is being made possible by R&D efforts in:

- AI4Analysis: As synchrotron experiments increase in complexity and detector capabilities grow, the computational demands of X-ray data inversion become overwhelming, making real-time feedback during experiments unfeasible with traditional iterative methods. To address this, we are implementing machine learning data inversion across various X-ray characterization methods at the APS. This approach enables real-time analysis where conventional methods can take days or months, and sometimes more precise data inversion compared to conventional methods. We will continue the development of AI-accelerated analysis methods for high-data rate instruments including multi-modal analysis.
- AI4Steering: As the complexity of instruments and experiments grows, manually steering experiments or optimizing beamlines has become impractical. We are progressively utilizing ML in various aspects of accelerator control, beamline tuning, and intelligent, guided experimentation. We will extend demonstrations of adaptive sampling in imaging and XANES experiments to more challenging acquisition protocols including 3D fly-scanning imaging.
- AI4Knowledge: As instruments have become multi-modal and multi-faceted, extracting scientific insight from very large, complex multi-modal datasets is becoming an increasing challenge. AI generated latent spaces provide scientists with the ability to quicky identify patterns in massive, high-dimensional datasets and correlate observations at the nano and mesoscale with macroscopic phenomena. We will continue to develop AI solutions for knowledge extraction from raw X-ray science data, reducing the time from observation to scientific insight.

In addition to domain-specific ML and Deep Learning (DL) methods being developed over the last few years, we will increasingly generative AI in coordination with DOE initiatives as described below.

Large Language Models (LLMs) as scientific co-pilots

Large language models (LLMs) have transformed how scientists conduct their research, offering powerful tools for literature review, experimental design, and data analysis. While these AI assistants help researchers quickly synthesize information from vast numbers of papers, generate hypotheses, and draft manuscripts, they also present important challenges around reliability and research integrity.

The APS is developing sophisticated AI co-pilots grounded in appropriate context to enhance scientific experimentation. The Context-Aware Language Model for Science (CALMS) serves as an intelligent assistant for light source instruments, combining a large language model with access to facility documentation and control systems. This enables CALMS to both answer queries about experimental capabilities and directly assist with instrument operations through natural language interaction. Similarly, the Ptychographic Experiment and Analysis Robot (PEAR) has been developed to automate complex imaging processes. PEAR employs multiple specialized AI agents to mimic expert decision-making in ptychography, a computational imaging technique used across optical, X-ray, and electron microscopy. Through natural language interaction, PEAR gathers experimental parameters, generates reconstruction scripts, diagnoses issues, and iteratively optimizes results. This system makes expert-level ptychographic imaging more accessible and efficient by automating parameter selection and experimental design while maintaining transparency in its decision-making process.

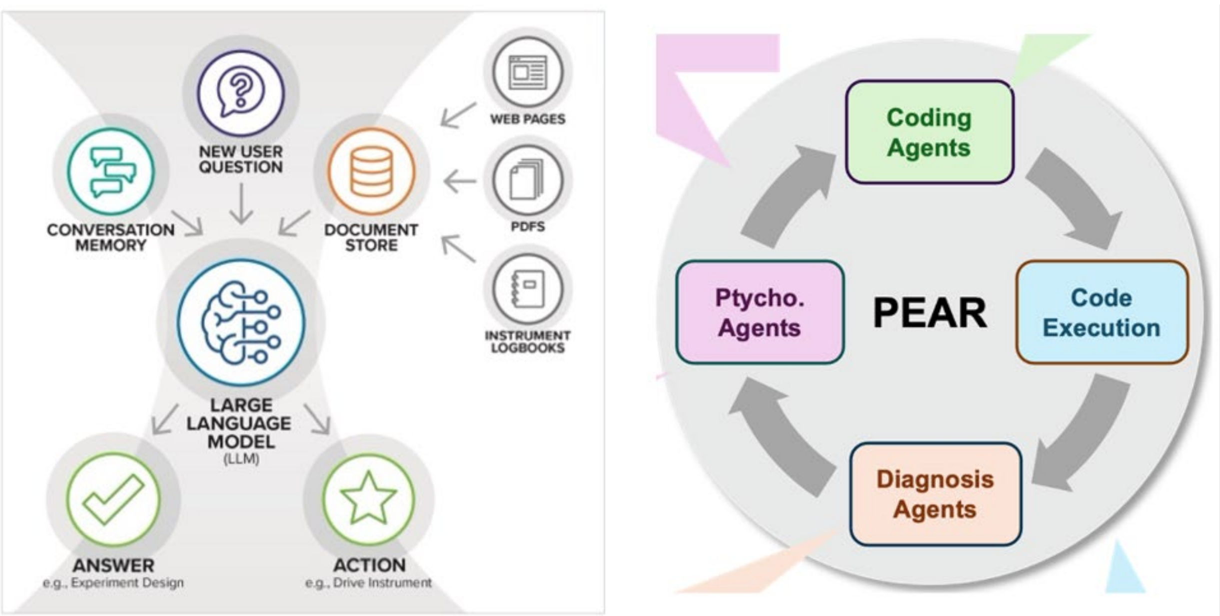


Figure 13: Left: Overview of CALMS, a context-aware language model that uses conversational memory, document stores and access to experimental tools to answer user queries or take action to drive an instrument. Right: Ptychography Experiment and Analysis Robot (PEAR) which uses multiple language model agents to guide users through reconstructing challenging ptychography datasets.

We will continue to expand these systems' capabilities and integration. Priorities include enhancing the AI models' ability to handle more complex experimental scenarios and developing more sophisticated error detection and correction mechanisms. Additionally, efforts will be made to extend these AI co-pilot systems to other experimental techniques and instruments, creating a more comprehensive ecosystem of intelligent scientific assistants. The ultimate goal is to democratize access to advanced scientific instruments while maintaining the highest standards of experimental quality and reproducibility.

Leverage data and foundational models for new science

The DOE's leadership in frontiers of artificial Intelligence for science, security and technology represents a groundbreaking effort to develop the world's most powerful integrated scientific AI systems. This proposed initiative also aims to revolutionize how we conduct scientific research by creating advanced AI infrastructure that can handle and learn from the enormous volumes of data generated by DOE, including the APS.

The integration of AI infrastructure with facilities like the APS will involve establishing sophisticated infrastructure to automatically channel experimental data into AI training pipelines. This system will not only process data from regular scientific experiments but may also utilize beamlines specifically as dedicated data generators, creating rich, quality-controlled datasets for AI model training. Conversely, we will develop ML Operations (MLOps) infrastructure that can effectively leverage AI-driven foundational models for APS science applications as well as provide automated model evaluation and testing. This symbiotic relationship between DOE's investment in artificial intelligence and the APS's experimental facilities promises to accelerate scientific discovery by enabling more novel, multi-modal data analysis; pattern recognition using data from different facilities; and experimental guidance in complex scientific experiments. The resulting AI-powered research ecosystem could dramatically enhance our ability to tackle challenging scientific problems across multiple disciplines, from materials science to biological research.

Goal 3: Ensure Mission Success through Operational Excellence

As a major national user facility serving hundreds of scientific organizations across the nation and the world, we strive to provide access to X-ray instrumentation operating at optimal performance, with the utmost stability and reliability. We aim to stay at the forefront of technological innovation in support of operational excellence and to modernize our most critical infrastructure by employing strategic foresight. Targeted investments in infrastructure modernization projects and long-term planning of maintenance and obsolescence mitigation strategies are key elements of our overall strategy and integral to the success of our scientific mission.

Safe and secure operations are a pillar of our mission. We work with discipline in all areas, from implementing the new DOE accelerator safety order to maturing our integrated safety management practices, to deploying a secure network for our accelerator and beamlines.

We actively target measures that reduce the overall energy consumption of the facility, and we routinely evaluate their effectiveness to adjust our operational practices. Energy efficiency, reduced power consumption, and will be integrated into our strategy with initiatives prioritized by a dedicated committee established in 2024.

We will continue to expand the modes of access for scientific users by leveraging the modularity of the recently launched Universal Proposal System. In partnership with our APS User Organization, we will launch new visioning workshops to prepare the future of the APS beamline suite for the EXCEL-II program. We will continue to train our community through schools and workshops and aim to use the power of LLMs to provide context-aware virtual assistance during experiments.

Objective 3.1: Modernize mission-critical accelerator and beamline infrastructure

Modernize RF power systems

Since 1995, the APS has operated using 352-MHz, 1-MW continuous-wave (CW) klystrons as the RF power source for the storage ring and booster. While these klystrons have been highly reliable, contributing to RF system downtime as low as 0.2%, changing market conditions have rendered 1-MW CW klystrons commercially unavailable. In addition to klystron obsolescence, the associated high-voltage power supplies are nearing the end of their reliable service life, and many of their components are facing similar obsolescence challenges. Recognizing these risks, the APS is transitioning to solid-state RF technology for its 352-MHz RF sources, with the goal of completing the conversion before depleting its stock of spare klystrons.

The transition began with the purchase of a 200-kW solid-state amplifier (SSA) prototype from R&K Company Limited. After extensive on-site testing of this prototype, a contract was signed for the purchase of twelve 160-kW SSAs from the same supplier. Deliveries are scheduled to occur every two months starting in November 2024. The installation schedule has been carefully planned to minimize disruptions to the overall RF system, and it includes significant modifications to the space and infrastructure.

The first batch of four amplifiers will be installed in Sector 36 to power four cavities, with completion targeted for FY25. Simultaneously, modifications in Sector 40 will begin to accommodate the next batch of four amplifiers, with installation there expected to be completed in FY26. Sector 37 will undergo modifications last, with the plan to complete installation by FY27. This phased approach optimizes the cost of infrastructure upgrades while keeping RF system interruptions to a minimum.

The modernization of the booster RF system will utilize SSAs similar to the ones being purchased for the storage ring. Overall, the booster modernization will require 4 amplifiers. Contract signing for the booster SSA purchase is expected in FY26 with deliveries in FY27.

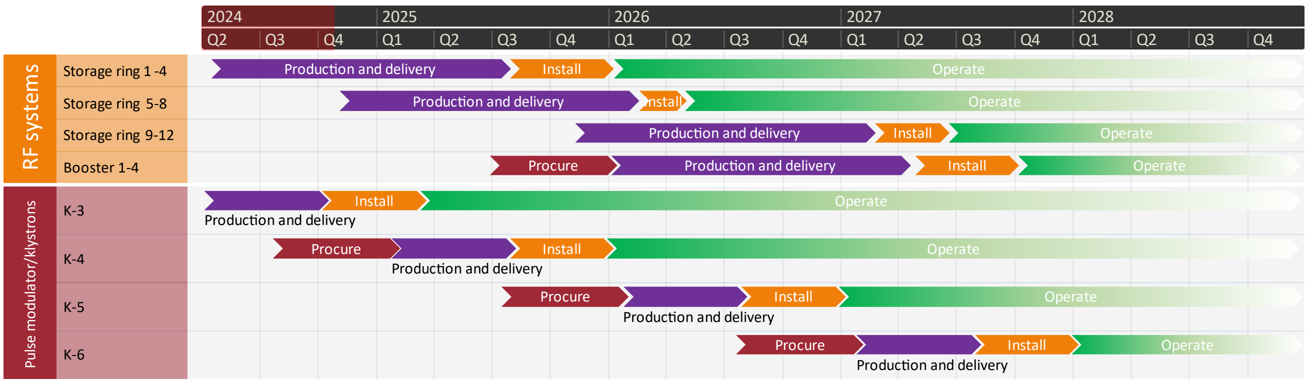


Figure 14: Modernization program for RF systems in the LINAC, booster, and storage ring.

Reduce accelerator maintenance by replacement of LINAC components

The APS linac, currently powered by six 30-MW pulsed RF stations, has been in operation for 30 years. Each RF station consists of a high-voltage modulator, pulsed klystron, and low-level RF controls. To address obsolescence of these systems, the APS initiated a modernization program several years ago. Each RF station is being upgraded to a 50-MW pulsed system with new solid-state high-voltage modulators, klystrons, and digital low-level RF systems. These new stations are not only more powerful but also offer significantly lower RF phase noise, easier maintenance and troubleshooting, and lower electricity consumption.

The first such system was purchased as a test prototype. After successful testing, a second system was purchased and installed in the linac, now powering section L2. The next RF station has recently arrived and is being installed in section L5. Moving forward, the APS plans to purchase and install one new RF station per year. The original prototype will be repurposed to power the RF test stand. After these upgrades, all APS RF systems will be fully modernized and equipped to power the APS accelerators for next 25 years.

Many of the power supplies serving the linac magnets are nearing the end of their operational life. To address this, a two-phase plan for their replacement was developed. Phase one focuses on upgrading the bipolar power supplies, which is currently underway. These were prioritized because their replacement will enable the automation of linac transmission tuning, thereby improving overall linac performance. Phase two will focus on replacing the larger unipolar power supplies, ensuring a comprehensive renewal of the linac's power supply infrastructure.

Develop a comprehensive spares strategy for the upgraded APS

A spares strategy is necessary to provide high reliability, minimize machine downtime, increase MTBF, and manage costs. The upgraded APS included a considerable number of spare parts for the storage ring components, and we will build upon the number of spares, but also the inventory management system - called the component database (CDB) - to manage the inventory of accelerator and accelerator supporting equipment spares. As we update our injector complex, we will identify necessary spares, procure those spares and manage the inventory via the component database. The CDB will allow us to review demand and determine use cycle for our spare parts for reordering or evaluation of different materials for the parts. The database enables our ability to rapidly locate the spare parts when needed for use and includes barcode technology for ease of use to update our inventory. Our spare management will include automated processes to order replacement parts as spares are used, kitting of all parts needed for a major spare replacement (O-rings, gaskets, nuts, bolts, bellows, etc.) included with the spare part, as well as having parts cleaned, tested, and ready for install when needed. The management of our spare parts would be integrated with our preventative maintenance strategy. We will store some large accelerator parts in the associated area (LINAC, PAR, Booster, Storage Ring) to allow for efficient installation.

Execute an integrated program of preventive maintenance to ensure reliable future operation

As a user facility our goal is to reliably provide X-rays for experimental use on our many beamlines, and a data-drive preventative maintenance program is one supporting method. After many years of operating the APS accelerator and supporting equipment, we have extensive knowledge in preventative and corrective maintenance. We have leveraged that experience into planned maintenance; however, these plans are manual and require physical updates in lieu of leveraging technology to help determine our planned/preventative maintenance cycle, schedule, repair parts, and expected costs. We will assess multiple preventative maintenance software platforms including those in use elsewhere onsite as well as local systems (e-Traveler) and the possible integration with the component database to help manage our spare parts inventory. Our integrated system will function across all of PSC and allow us to minimize downtime of equipment by scheduling maintenance on one system for multiple work groups at the same time. It will allow improved metrics tracking including MTBF, mean time between repair (MTBR), ratio of planned to unplanned maintenance, common failure mode and effects analysis (FMEA), systemic failures, etc. with dashboards to easily interpret the data. The preventative maintenance program can monitor performance via sensors and utilize AI/ML to enhance monitoring and prompt for scheduling. We will assess integrations with our work request system to provide for improved coordination and planning of work.

Enhance user engineering support via 3D printing and collaborative design

The Photon Sciences staff, users, and Collaborative Access Teams (CATs) require special or one-off parts be fabricated for use on beamlines, on the experiment hall floor, or for accelerator support systems. In many cases, additive manufacturing (3D printing) can be used to meet their needs. Additionally, 3D printing of mock-ups is a cost-effective approach to ensure the fit of parts or necessary modifications before moving to metal machining, and in some cases the fit-up piece may be able to be used in lieu of metal parts depending on the use. We plan to increase the 3D printing capability (as we saw an increased demand prior to the APS shutdown in April 2023) and bring the service closer to the experiment hall floor by repurposing some select user shops into additive manufacturing shops. This is a step toward a long-term vision of satellite 3D printing shops that the PSC team can utilize, with some oversight from the AES division. We will use our history of printing demand data to inform our decisions on equipment to purchase and service locations for on-demand printing with a user-friendly self-service platform. In keeping with the Argonne Core Value of safety, training and other safety precautions will be taken to mitigate risks and cost control measures will be implemented to prevent unnecessary use. We will continue to assess the best methods of implementing our design and drafting engineering support including use of AI/ML as a tool to improve efficiency, effectiveness and empowering our team to work differently.

Deploy a modern IT infrastructure that supports science and accelerator systems

The APS computer room, co-located with the main control room (MCR), has served PSC well for nearly 30 years. However, with advances in detectors, data acquisition, processing, and accelerator and beamline controls, a modernized approach to APS's IT infrastructure is now essential. The IT infrastructure must include high-speed, low-latency networking to ensure that data is transferred quickly between detectors, storage, and HPC systems. The APS Scientific Computing Strategy outlines the path forward, and an upgraded IT infrastructure is critical to supporting this vision. We plan to invest in a state-of-the-art computer room/data center to house all non-accelerator operational IT storage, hardware, and backups. This facility will feature redundant power and cooling systems with high fault tolerance to maximize reliability, with considerations for reusing waste heat to lower our energy footprint. We will evaluate several options for the new data center, including:

- Expanding and relocating equipment to the lab's Enterprise Data Center (EDC) in the 300 area of the Argonne campus.
- Building and relocating IT equipment to a local data center within the APS/400 area.
- Overhauling the current computer room and the injector control room (ICR), where many of our backups are currently stored.

The management of our IT systems will enable the use of cloud computing and AI/ML, and facilitate agile reconfiguration and upgrades as technology evolves, allowing PSC to continue advancing its IT capabilities and leverage enhanced technologies.

Objective 3.2: Maintain safe, secure and efficient operations

Develop and implement effective safety policies and procedures to meet new science needs

In 2023 and 2024, the APS installed and commissioned the new multi-bend achromat (MBA) storage ring. The work occurred within the existing operational facility where operational readiness, especially configuration management, needed to be maintained. This resulted in PSC reexamining practices to more effectively manage interfaces within the operational areas and between operations and project work. We utilized overall readiness concepts to ensure that people, processes and equipment are ready with the appropriate level of rigor to ensure safe, secure, and efficient operations.

The readiness framework used in PSC is derived from the DOE accelerator readiness review framework and we will continue to use it to improve our safety and operational processes. This framework also helps ensure that Integrated Safety Management is built into how we perform operations. This approach was validated through the successful restart of the APS LINAC and Booster as well as the storage ring through the DOE Accelerator Readiness Review process. Recommissioning of the APS beamlines is also following this framework. Operational practices include a plan of the week meeting driven through written work requests which provides visibility to staff and management. Daily toolbox talks and closeout meetings provide for higher levels of situational awareness across the facility and encourage collaboration around work planning. Integrated management team meetings were used during the APS-U installation phase to help manage interfaces and resolve issues not directly within scope of operations or project work.

These more informal Human Performance tools augment the more formal readiness constructs such as training. Argonne's work planning tools and our design review processes help ensure that our processes and equipment are also ready. These proven practices will continue and be improved during facility operations and will ensure smoother integration with other large projects that come into the facility, such as the EXCEL@APS project and future potential projects in partnership with other organizations, such as the Defense Materials Science Sector.

As we continue to advance the safety of our facilities, improvements in safe and secure operations reduce overall cost and enhance mission effectiveness. In an era where operational excellence and employee safety are paramount, our organization is committed to enhancing operational and safety processes and reporting through innovative technology and management engagement. We will continue to modernize our software tools, following a recent rewrite of our Behavioral-Based Safety Observation system (BBSO). We aim to investigate and implement software and hardware solutions that leverage artificial intelligence to streamline processes and help identify trends.

These include:

Tighter system integration with Laboratory Subject Matter Experts (SME): While the majority of the experiments that are conducted at the APS pose limited risk, the APS will accept higher hazard experiments provided that the hazards and risks are appropriately mitigated. In some cases, mitigation requires integrating with other Laboratory safety and emergency management programs. Early notification of these experiments is important to ensure all stakeholders have the chance to review and develop their part of the mitigation portfolio. We will develop toolkits to provide input to Laboratory SMEs at the proposal stage in order to obtain early feedback.

Lowering the barrier of reporting and comprehensive data analysis: By working with the Laboratory to consolidate the collection of field observations as well as mining APS performance and safety data, we will use machine learning tools to help identify targeted focus areas for operational and safety improvements.

AI-enhanced risk-based experimental reviews: The APS has an extensive database of experimental and safety information. We will explore solutions that utilize this data set with machine learning algorithms to predict potential safety risks and incidents, hereby leveraging the extensive experimental experience of the APS into the future.

Real-time Monitoring: By leveraging the existing control system infrastructure at the APS, we will evaluate system improvements that extend our real-time insights into safety compliance, incident reporting and operational efficiency, thereby providing greater insight into emerging issues. These include improvements to our real-time radiation monitoring, which not only ensures personnel safety but provides insights into accelerator machine performance and will include significant investments into new area radiation monitors, personnel safety systems and equipment protection systems that provide safety interlocks to protect both personnel and equipment. Many of these systems are original or near-original design and are increasingly becoming obsolete.

Leveraging Human Performance Improvements (HPI) We will focus on solutions that offer intuitive user interfaces, ensuring easy adoption and engagement from all employees. This includes a comprehensive approach that includes strong visual cues in the work environment, and enhanced use of HPI tools at the APS.

Remote operations: APS users access the facility both onsite and offsite. When operating offsite, access to beamline control systems needs to meet increasing cybersecurity requirements. The APS will continue to work with Argonne and DOE cybersecurity professionals to create an offsite control environment that protects DOE assets and minimizes complexity to the user community. In the near term, multifactor authentication for remote access of beamline equipment including an efficient and compliant way to distribute multifactor keys will be implemented.

Information security: While the APS is primarily an open science facility, the APS also has proprietary and national security program users. National security users, in particular, need to collect and manage data with different levels of sensitivity from Controlled Unclassified Information to higher levels of information control. The APS will continue to develop processes and protocols to collect and manage information protection needs of our user community. This includes the collection and management of CUI data required by our national security program users.

Through these objectives, we aim to foster a safer work environment, improve compliance with safety regulations, and ultimately drive organizational performance through informed decision-making and enhanced operational agility. This initiative will involve collaboration across departments, ensuring that the selected solutions align with our safety goals and organizational values. We are keenly aware that the safety and operational culture we adopt has impact with our users and when done well extends the tools of operational excellence into the cultures of our user organizations.

Modernize business systems

The APS strives to continuously improve efficiency and effectiveness. Advancing our business systems is a key pillar of our strategy, to improve agility, to provide consistent and data-driven decision-making processes, to support short and long-range planning, and to deliver various data analytics to our stakeholders and sponsors.

We will pursue two strategies:

- Enabling data-driven performance management by building powerful dashboards, KPIs and balanced scorecards that are tracking key performance of the APS facility, PSC strategic initiatives and risks. A modern performance tracking system will also ensure consistent communication flow across the directorate and provide the necessary alignment beyond common goals.
- Ensuring that PSC staff spend their time or high-value tasks by migrating the most time-consuming and manual processes into automated tasks and, where possible, to integrated AI tools to enhance operation support.

Five key projects are targeted:

- We will mature our portfolio management system by providing real-time access to project performance in the form of cloud-based project portfolio dashboards. We will transition to a two-stage project request workflow that will enforce structured and common review processes across divisions and limit manual tasks.
- We will modernize our accounting information system by transitioning entirely to database solutions. This will provide real-time reporting capabilities and support a more agile management of strategic and operation investments.
- We will deliver a user publication data system that is capable of automatically searching and aggregating user publications by using multiple APIs for research information and tracking scientific output of the APS in close to real time. This system will be capable of classifying research output using various open and proprietary taxonomies.
- We will improve processes and tools used to manage the collection and storage of user publications by leveraging our access to persistent identifiers such as Digital Object Identifiers for publications, and Research Organization Registry (ROR).
- We will incorporate a performance monitoring solution to assess the health of our software applications, network and system performance in real-time to identify bottlenecks and improve detection of security issues. The system will provide greater visibility on a large spectrum of applications and facilitate seamless and continuous user experience.

In addition, we will perform a comprehensive review of all business systems to enhance efficiency and drive innovation. The review will include a survey of applications and provide recommendations for long term cost savings and appropriate distribution of responsibilities that include both user-facing and back-end systems. The review will also consider the adoption or expansion of systems developed through the APS Upgrade for potential use in inventory management and record keeping. The review will also assess our incorporation of new technologies, including new design technologies, new hosting technologies, and the use of modern design toolkits.

Objective 3.3: Transform user services and communication to enhance engagement and support

Mature and expand the Universal Proposal System

The Universal Proposal System (UPS) has been developed as a common platform for the management of user scientific proposals across multiple facilities and was launched at the APS after the upgrade of the facility in December 2023. It is a collaboration between the APS at Argonne National Laboratory, the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory, and the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory. The APS is committed to actively support this collaboration in the future and help extend it to other scientific user facilities where applicable.

Given the high volume of user proposals received each year at the APS, our primary objective is to focus on continuously supporting and maturing the platform experience for users and reviewers. Given the wide adoption of AI in the ServiceNow platform, on which the application is built, we expect to continuously roll out new features that will streamline the submission and review process.

The second objective is to capture data analytics that support reporting requirements from DOE and leverage the provision of consistent, persistent user identification in the form of ORCID (Open Researcher and Contributor ID) to channel data collected to relevant Argonne management system owners. The system will be enhanced as other forms of persistent identifiers become widely used and recognized, for example ROR to be able to perform automatic searches and breakdown of data as needed. We will also connect this platform to other tools to meet current and future needs related to the management of risks inherent to a SUF, for example export control and information security.

In the next five years, we will partner with other DOE facilities who have expressed an interest in joining the collaboration to expand the UPS beyond the initial 3 founding labs. Particular attention will be paid to the governance to identify synergies and to ensure long-term success.

Website redesign and social media targets to increase engagement

Following the recent comprehensive upgrade to the APS, it is essential that our digital presence mirrors this state-of-the-art transformation. The APS five-year strategic plan includes a redesign of the APS website to enhance communication of scientific discoveries enabled by the upgraded APS and expand our reach to new communities of users from academia and industry. By improving functionality and accessibility issues and providing a better classification of knowledge through science and technology taxonomies, we aim to be at the forefront of the light source global community when it comes to communication. A redesigned website also aligns with the facility’s strategic goals to enhance communications with our key stakeholders, keeping them apprised of the new and innovative research at the APS.

Our five-year social media strategy focuses on increasing and expanding our key audiences – primarily the science community with an emphasis on users and potential users – and fostering engagement through content creation and interaction. We launched the APS LinkedIn channel in November 2023, and it will play a pivotal role in our future social media strategy. We will explore opportunities to engage more APS employees, who may serve as ambassadors to not only increase public awareness of their own research but also to elevate the APS. We will prioritize platforms used by our audience and consider new platforms that may gain traction with key audiences in the coming years. We will develop content based on our expertise and scientific impact, and build engagement through interactive campaigns and real-time conversations, as appropriate.

Objective 3.4: Embedding energy efficiency into operation

Energy savings and environmental sustainability

In 2022, PSC performed a review of the energy impacts of the facility, with the aim to drive improvement in power efficiencies and integrate best practices into the operations of the facility. To foster a shared understanding of energy efficiency, we are aligning the current practices at the laboratory, DOE and PSC. This will be achieved by improving renewable energy usage and incorporating energy efficient practices into both facility operations and accelerator infrastructure. We will leverage existing updates to our operating equipment, such as the transition from RF klystrons to solid state amplifiers and the installation of variable frequency drives for the processed water system, to continue to lower our energy use and carbon footprint. We will also integrate environmental impact, and (where applicable) environmental resiliency, as part of the criteria for project delivery and procurement strategies.

PSC started implementing energy reduction measures in May 2022, including a risk-based decision to not operate “hot spare” klystrons. More measures were introduced during the APS shutdown in 2023 with the installation of variable frequency drives (VFDs) on processed water systems. These two initiatives resulted in energy savings of 9.200 GW-hr/year. In section 3.1, we described our Linac modernization program updates including new modulators based on SSAs. The recently installed station reduces energy by 800 MW-hr./year and once the project is complete, it will save 4.8 GWh/year compared to the original APS.

The PSC environmental sustainability committee is coordinating with the lab on energy improvement projects to replace our Storage Ring mezzanine lights with LEDs, corresponding to an energy savings of 120 MW-hr./year.

The new storage ring operating at 6GeV instead of 7GeV offers an opportunity to reduce the energy consumption further as it requires only 1.2 MW of RF power instead of the 1.6MW of the old machine. That will correspond to an additional 2.5 GWh/year saving. The SSA replacement project will also increase power efficiency since SSAs run typically at 60% efficiency.

The combined energy efficiencies and reductions result in an anticipated 19.3% decrease by 2020 (see Figure 15).

Other activities are being coordinated with the laboratory, most notably the installation of a recovery system, reusing the waste heat from the storage ring magnets to reduce the steam load from the central heating plant. The project is in construction with planned completion in FY25, with an anticipated energy savings of 2.4 GWh/year to the laboratory.

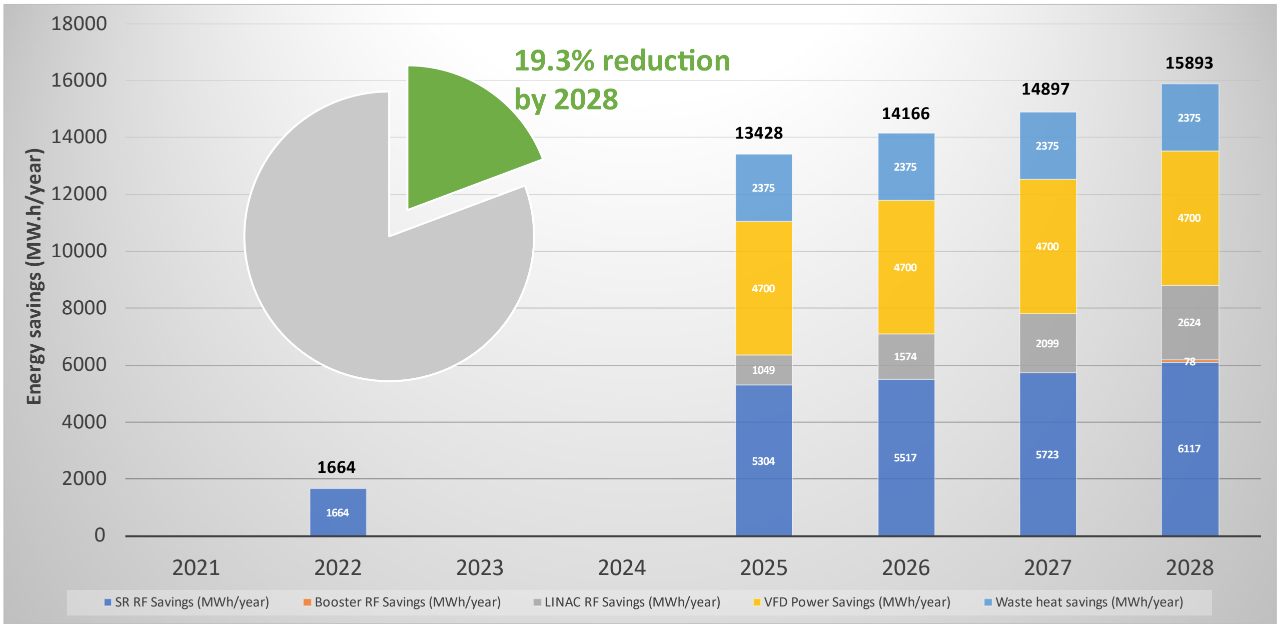


Figure 15: Energy savings anticipated in the period 2025-2028.

We will continue to drive energy improvements through investments to our systems as identified in section 3.1 above, through PSC projects as well as lab-funded initiatives. We have identified potential significant improvements for chilled water, compressed air and low temperature hot water systems and are executing a plan to replace the chillers that were part of the initial APS design. In conjunction with our Infrastructure Services directorate, we will continue similar large equipment improvements with a focus on energy efficiency.

A comprehensive waste reduction, reuse and recycling program will continue to be implemented and promoted to increase cost savings and minimize waste. In close coordination with the laboratory, we are piloting the lab's recycling and composting signage at multiple areas within our facility that will improve Argonne's ability to recycle and compost (see image below).

The PSC committee is working closely with the lab to develop and implement sustainable supply chain management processes, as we want to improve our team's ability to procure items with a lower cost and lower carbon footprint and understand the impacts of sustainable purchasing.

We are in the very early stages of a PSC water conservation program that will help reduce waste and improve overall efficiency in resource usage. We have assessed which PSC areas have the highest demand and will plan improvements moving ahead.

Minimizing He consumption

Finally, we are targeting a major reduction in helium consumption and an increase in recycling. PSC uses a significant amount of liquid helium (LHe) to operate magnets on beamlines (up to 9 Tesla field) and for superconducting undulators. To mitigate the usage of this critical resource, we have recently implemented a recycle and reuse program that includes:

- A LHe liquefier in sector 4-ID, commissioned in August 2022 and utilized during the October-December 2022 and February-April 2023 run periods. The liquefier was able to recover approximately 1800 L of LHe in this period.

- We recently received a new magnet for the POLAR beamline, which will use twice the LHe per run. We plan to mitigate this additional consumption by upgrading the LHe recovery to 2400L/run or 7200L/year.
- Other investments made in 2023 include purchases of helium closed-cycle refrigerators for beamlines 3-ID, 6-ID and 27-ID. We estimate that these improvements will yield an 800L/year LHe saving.
- We are working closely with the laboratory to improve the LHe recycling capabilities at a nearby magnetic devices' facility with a LHe recycling plant that could service multiple beamlines at the APS in addition to the facility itself. When operating, we estimate that approximately 15,000L of LHe/year up will be recycled.

Goal 4: Foster an Innovative and Collaborative Environment

Objective 4.1: Empower the user community

Deliver new user access modes to accelerate time to discovery

The access model at scattering facilities (light sources, neutron sources) has evolved over the years to best respond to new demands from the user communities. Rapid access modes now available at most facilities are designed to streamline and expedite access for researchers requiring quick turnaround times. It allows scientists to access beamtime or other experimental resources without the lengthy, competitive application and scheduling processes. It accelerates science by de-risking larger and more complex experiments or providing fast measurements of critical measurements to complete studies. The APS has been operating with Rapid Access for a number of years.

In addition, many facilities have developed Block Allocation Group (BAG) access. A Block Allocation Group is a collaborative access model to optimize the allocation and utilization of beamtime among multiple research groups. In this framework, several independent principal investigators (PIs) or research teams form a consortium to submit a joint proposal for a collective beamtime allocation. It enhances scheduling flexibility by pooling beamtime requests since BAG members coordinate and prioritize experiments more effectively, accommodating the varying needs and timelines of each group. This flexibility is particularly beneficial for projects requiring regular or frequent access to beamlines. It also fosters collaboration facilitating the sharing of expertise and methodologies, which can lead to more comprehensive and impactful scientific outcomes. The APS will use the newly developed UPS system to expand access models and accommodate BAGs in the next 2 years. We will engage with the community to understand and accommodate user needs.

In addition to understanding the best modalities and implementation strategies for BAGs, one of the important topics of discussion will be centered on AI for science. As a significant provider of scientific data, the APS user community is in a leading position to leverage the power of generative AI and large language models for scientific applications. AI will require improvement in data annotation and curation, as well as innovation to understand how to best tokenize knowledge for exploitation of data by AI. These tasks are domain specific, which suggest that the best way to ensure common frameworks and discipline is to engage user communities around missions, i.e. experimental campaigns, that share a unified framework for data collection and curation. A BAG can promote data AI-compliance and leverage the required expertise in the community. We will be working with our APS User Executive Committee to organize workshops with the user community to explore the best avenues and changes in policies required to make the most of the AI revolution.

Develop context-aware AI models to boost user support experience

Large Language Models (LLMs) can significantly enhance the experience of domain scientists using the APS by providing 24/7 assistance, streamlining knowledge acquisition and supporting complex experimental processes. In addition, LLMs can significantly reduce the overhead in performing an experiment at the APS. Mirroring broad trends in industry, we will leverage generative AI and LLMs to provide end-to-end assistance for the APS users, allowing them to focus on their scientific questions. Pre-arrival support could include proposal writing assistance, generating example proposals, beamtime allocation guidance, sample preparation requirements, site access procedures, and identifying the right combination of beamlines to address a particular scientific question. On-site support could include real-time access to equipment manuals, troubleshooting off-hours, recommending appropriate analysis tools and scripts, and generating code for bespoke analysis and visualization, etc. Post-experimental support could include data retention and access guidelines, offline analysis assistance, guidance to obtaining additional computing time and others.

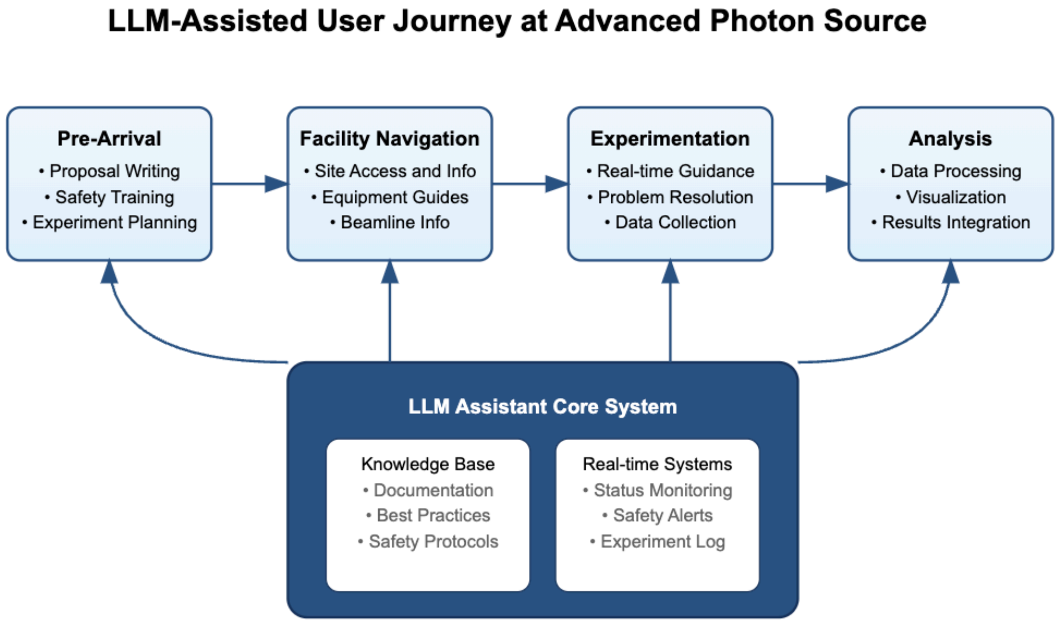


Figure 16: Future AI assistance for APS users.

Objective 4.2: Cultivate and attract a talented workforce

Train the next generation of scientists and users

Since 1999, the APS and Oak Ridge National laboratory have supported the National School on Neutron and X-ray Scattering (NXS). This is an educational program designed to train graduate students in utilizing major neutron and X-ray facilities, offering lectures and hands-on experiments to provide participants with practical experience in scattering techniques. Applications are open to graduate students enrolled in North American universities who are pursuing experimental degrees and plan to incorporate neutron and X-ray techniques into their research. The APS remains committed to educating the community though this program and will fund this course in the future.

APS will partner with the AAI to attract the next generation of accelerator physicists. The effort is rooted in the Lee Teng Undergraduate Fellowship in Accelerator Science and Engineering, an AAI effort that consists of a competitive, paid summer program designed to immerse undergraduate students in the field of accelerator science and technology. Established in 2008 by the Illinois Accelerator Institute, the fellowship was set up as a collaborative effort between Argonne National Laboratory, Fermi National Accelerator Laboratory (Fermilab), and the U.S. Particle Accelerator School (USPAS). The fellowship, spanning ten weeks during the summer, pairs participants with physicist or engineer mentors at Argonne, aligning student skills with specific research projects. Students engage in hands-on research, gaining exposure to various aspects of accelerator science beyond their individual projects.

The APS has also invested in other opportunities to develop early-career talents, such as those offered by the national GEM Consortium, a U.S.-based non-profit organization that provides graduate fellowships to students in the fields of STEM. Over the last three years, the APS has tripled the number of GEM students (from 3 to 12 a year). We aim to maintain this level of engagement for future years.

Education and training opportunities for staff

In partnership with the Argonne Leadership Institute, we offer mentoring and networking resources for all employees, including professional development programs, assistance in connecting with mentors, and guidance on becoming a mentor. Mentoring is strongly encouraged in PSC to actively build a strong community of talents.

PSC will work Argonne to continue to provide training and upskilling for staff in AI through a lab-wide initiative that aims to democratize access to cutting-edge AI technologies. The institutional computing strategy includes access to some of the most advanced LLMs that can be operated behind the Argonne firewall. Our vision is to build a culture where AI is fully integrated in our operations and research activities. PSC will, alongside the rest of the lab, assist employees as they incorporate AI in their daily work, by identifying AI experts to partner with staff and provide guidance. Starting in 2025, we will augment the program by integrating a buddy system to support education and cross-training in AI Mentors will be needed to cover a range of skill levels – novice, advanced beginner, competent, proficient, expert – as well as many types of assistance including general productivity, research acceleration, and code development.

Beyond AI, we will work in collaboration with the other DOE light and neutron sources to create a common framework for workforce development. The topic of workforce development was one of the cross-cutting themes identified at the recent Basic Research Needs workshop for accelerator-based technologies. The global shift in physics and engineering workforces is of particular interest. The taskforce we created aims to identify the workforce development needs to support the long-term mission of DOE light and neutron sources and understand the gaps that are critical for the successful operation and innovation mission in the shorter term. The APS is also a contributor to other collaborative initiatives such as the recently launched Accelerator Science & Engineering Roundtable Meeting organized by DOE on this topic.

Transitioning from the APS-U project environment back to full operation offers the unique opportunity to transfer knowledge to a new generation of technicians, engineers, and scientists. Mentoring and shadowing programs will be supported in key areas to facilitate knowledge transfer between outgoing staff and early career staff. We will also offer formal training to our technical groups from outside vendors to build up knowledge.

Improve communication avenues and cultivate a culture where it is safe to speak up. This goal focuses on enhancing communication between employees and management, and addressing employee concerns.

- **Lower the barriers to access jobs at PSC by providing new talent pipelines and enhancing job postings.** This goal focuses on improving job descriptions to attract talents, enhancing access to job postings through partnerships and pilot projects, and incentivizing staff to participate in new talent pipeline programs.

- **Develop career pathways and communicate opportunities for professional development.** This goal aims to enhance employees' knowledge of career development opportunities and pathways, promote management advocacy for employee professional development, improve onboarding experience and education on policies and resources, and foster open dialogue between staff and senior leaders to drive continuous improvement.

Objective 4.3: Enable and enhance R&D partnerships at Argonne, with partner institutions and with industry

From its inception, the APS has partnered with external organizations to enhance the scientific impact of the facility. These include the original CATs, which created a long-term relationship between the APS and external organizations to provide scientific direction and operation of individual beamlines, and the current practice of engaging in the more limited-scope Partner User Proposals, which provide access to peer reviewed programs in exchange for investments that benefit the facility and the General User Program. These relationships have increased the reach of the APS into targeted communities. The APS will collaborate with the Laboratory's Science and Technology Partnerships and Outreach Directorate to seek out beneficial R&D and educational partnerships that enhance and extend the impact of the APS. In addition, the APS will continue to enhance existing CAT and Partner User relationships to ensure mutual beneficial institutional engagement.

Implement the new BES light source partnership model

Operations after the APS Upgrade come with changes in the operation model of the facility for our partner institutions (CATs), required to provide 50% of the beamtime available on their beamlines to General Users (GU), compared to 25% at the original APS. The partners will, however, qualify to openly compete for GU beamtime. The APS realizes that this change in access model introduces opportunities for the general community and some risks when it comes to the optimal utilization of beamtime. It is APS's overall responsibility to ensure that beamtime is maximally exploited and results in high-quality scientific output. Given this change in policy, we will work with our SAC to ensure that beamline reviews in the next two years (2025-2026) target beamlines where the introduced changes are expected to have the greater impact, in order to inform APS management early about effectiveness of the new partnership model.

Promote collaborations with industry through new strategic partnerships

The Advanced Photon Source is uniquely positioned to foster collaborations with industry by establishing new strategic partnerships that leverage its cutting-edge capabilities. With the recent upgrade and the dramatically enhanced beam brightness and coherence, the facility can offer industry access to state-of-the-art research tools that can help drive innovation and create competitive advantages in various sectors.

Industry partners, particularly those in fields such as pharmaceuticals, energy, aerospace, advanced manufacturing, chemical engineering and microelectronics, can greatly benefit from the APS's advanced X-ray techniques. For instance, high-resolution X-ray imaging, X-ray fluorescence, and X-ray scattering provide detailed insights into battery and solar cell materials, offering crucial information on elemental composition, structural changes and nanoscale features, both in static conditions and during their operation. Advanced metrology capabilities are relevant not just for understanding processes for manufacturing of devices, but also for packaging and 2.5D and 3D stacking of integrated circuits. In addition, advanced metrology and measurement capabilities can be used to build better digital twins, as well as validate performance of industry relevant models. These capabilities enable companies to accelerate product development cycles, optimize manufacturing processes, and design new materials with targeted properties.

Strategic partnerships can include collaborative R&D projects, dedicated beamline access for proprietary research, and joint projects (CRADAs) to tackle scientific questions of interest. These engagements are facilitated by the APS's world-class expertise in synchrotron science, complemented by strong ties to computational resources and data analytics through collaborations with the ALCF.

We will continue to work with existing partners in these areas as well as seek opportunities to further expand the breadth of our collaborations.

Imagine a bio-imaging and innovation hub at Argonne National Laboratory

Biological research is a vast field of natural sciences that has an immense societal and economic impact. The immense complexity of biology, in terms of length scales (molecules, cells, organisms, and entire ecosystems); the existence of extensive conformational spaces; and the complex dynamic evolution key to biological function represents a massive phase space in which lies a formidable set of scientific challenges.

U.S. light sources and their partner institutions have contributed more than 27% of the 223,790 protein structures available in the Protein Data Bank, with more than 50% of the U.S. contribution coming from the APS alone. AI prediction of protein folding structures from an input sequence of amino acids, recognized by the Nobel Prize in chemistry in 2024, was simply an intractable problem historically until deep learning methods were developed and trained on these datasets.

Beyond isolated proteins, and because of the inherently complex biological organization landscape, there is consensus in the scientific community that the future of the field lies in integrated approaches combining data at different levels of biological organization with generative AI. Such approaches are data and compute intensive, which plays perfectly into the strengths and capabilities offered by leading SUFs available at Argonne – in particular, electron microscopy at CNM, structural biology and X-ray imaging at the APS, and the development of foundation models at ALCF. Even with these state-of-the-art facilities, the growing scientific demands in biology call for a rapid expansion of the laboratory's experimental capabilities and the creation of an integrated biology platform. This platform will promote technological innovation and drive synergies between Argonne directorates, and with partners from academia and industry.

Argonne is extremely well positioned to launch a major initiative in biological sciences that will leverage world-leading capabilities at the APS and the ALCF, along with the significant existing infrastructure. A proposal for a significant investment in cryo-EM will be developed to augment the experimental capabilities and create a world-class center for integrated structural biology and imaging. Cryo-EM would provide near-atomic or atomic resolution microscopy for proteins and complement X-ray crystallography. Cryo-electron tomography (cryo-ET) will be used to study macromolecular complexes in their native environment, which is not currently possible.

Partner with CNM to explore MEV-UED at Argonne

Ultrafast electron diffraction using MeV-energy ultrafast electron probes (MeV-UED) has a growing range of applications, including the study of photochemical processes, capturing light-induced transient states in quantum materials, and imaging the dynamics of electronic and nuclear structures. Deploying an MeV-UED system on the Argonne campus would complement X-ray scattering capabilities at the APS, extending the suite of quantum probes available to users of the EXM/EMM center. To advance this effort, a task force composed of PSC and PSE staff—including users, electron microscopists, and accelerator physicists—has been formed to explore potential MeV-UED configurations and the parameters required to execute potential transformative experiments envisioned by users.

The goal of this task force is to define a set of parameters for the MeV electron probe that will guide the high-level conceptual design of a potential beamline configuration by the end of FY25. One approach under consideration involves designing an experiment with existing hardware to locally gain experience with MeV-UED, providing a foundation for a future proposal to establish a user facility. This would expand the range of instruments available within the PSC and PSE facility portfolio, further enhancing research capabilities.

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Acronyms

- AAI: Argonne Accelerator Institute
- AD: Alzheimer's Disease
- AES: APS Engineering Support Division
- AET: Advanced Energy Technologies
- AI: Artificial Intelligence
- AISDC: Actionable Information from Sensor to Data Center
- ALCF: Argonne Leadership Computing Facility
- ALD: Associate Laboratory Director
- ALD: Atomic Layer Deposition
- AML: Activated Materials Laboratory
- ANL: Argonne National Laboratory
- APS: Advanced Photon Source
- APS-U: Advanced Photon Source Upgrade
- ARPES: Angle-Resolved Photoemission Spectroscopy
- ASD: Accelerator Systems Division
- AUREIS: Adaptive Ultra-Fast Energy-Efficient Intelligent Sensing Technologies
- AWA: Argonne Wakefield Accelerator
- BAG: Block Allocation Group
- BER: Biological and Environmental Research
- BLS: Bunch Lengthening System
- BES: Basic Energy Sciences
- BESAC: Basic Energy Sciences Advisory Committee
- CAC: Computing Advisory Committee
- CALMS: Context-Aware Language Model for Science
- CAT: Collaborative Access Team
- CBXFEL: Cavity-Based X-ray Free Electron Laser
- CDB: Component Database
- CDRX-Holography: Critical-Dimension Reflective X-ray Holography
- CELS: Computing, Environment, and Life Sciences
- CERN: European Organization for Nuclear Research
- CDI: Coherent Diffractive Imaging

- CHEX: Coherent High-Energy X-ray
- CNM: Center for Nanoscale Materials
- CPMU: Cryogenic Permanent Magnet Undulator
- cryo-ET: Cryo-electron tomography
- CSSI: Coherent Surface Scattering Imaging
- CW: Continuous-Wave
- CZP: Conic Zone Plate
- DL: Deep Learning
- DOE: Department of Energy
- EDC: Enterprise Data Center
- EMSL: Environmental Molecular Sciences Laboratory
- EPICS: Experimental Physics and Industrial Control System
- EUVL: Extreme Ultraviolet Lithography
- EXCEL@APS: Expand X-ray Capabilities with Extreme Light at APS
- FEL: Free Electron Lasers
- Fermilab: Fermi National Accelerator Laboratory
- FICUS: Facilities Integrating Collaborations for User Science
- FMEA: Failure Mode and Effects Analysis
- FNAPU: Force Neutral Adjustable Phase Undulator
- FOA: Funding Opportunity Announcements
- FOFB: Fast Orbit Feedback
- FPGA: Field Programmable Gate Array
- FTE: Full-Time Equivalent
- GU: General User
- GPU: Graphics Processing Unit
- HPDF: High Performance Data Facility
- HEXM: High-Energy X-ray Microscope
- HPC: High-Performance Computing
- HEP: High Energy Physics
- HPC: High-Performance Computing
- HPI: Human Performance Improvements
- HPMU: Hybrid Permanent Magnet Undulator
- HTS: High-Temperature Superconductor

- IC: Integrated Circuit
- ICR: Injector Control Room
- ID: Insertion Device
- ILLUMINE: Intelligent Learning for Light Source and Neutron Source User Measurements Including Navigation and Experiment Steering
- IO: Input-Output
- IRI: Integrated Research Infrastructure
- ISN: In Situ Nanoprobe
- JGI: Joint Genome Institute
- KB: Kirkpatrick-Baez
- LBB: Long Beamline Building
- LCLS: Linac Coherent Light Source
- LDRD: Laboratory Directed Research and Development
- LEA: Linac Extension Area
- LHe: Liquid Helium
- LINAC: Linear Accelerator
- LLM: Large Language Model
- LV: Lateral Ventricle
- MAC: Machine Advisory Committee
- MBA: Multi-Bend Achromat
- MCR: Main Control Room
- MeV-UED: MeV-energy ultrafast electron probes
- ML: Machine Learning
- MLL: Multilayer Laue Lens
- MLOps: ML Operations
- MONet: Molecular Observation Network
- MSRC: Microelectronics Science Research Center
- MTBF: Mean Time Between Faults
- MTBR: Mean Time Between Repair
- NDD: Neurodegenerative Disease
- NERSC: National Energy Research Scientific Computing Center
- NSUF: Nuclear Science User Facilities
- NTNS: Nuclear Technologies and National Security

- NVBL: National Virtual Biotechnology Laboratory
- NSLS-II: National Synchrotron Light Source-II
- NXS: Neutron and X-ray Scattering
- OLCF: Oak-Ridge Leadership Computing Facility
- ORCID: Open Researcher and Contributor ID
- ORNL: Oak Ridge National Laboratory
- PAR: Particle Accumulator Ring
- PDB: Protein Data Bank
- PD: Parkinson's Disease
- PEAR: Ptychographic Experiment and Analysis Robot
- PI: Principal Investigator
- PSC: Photon Sciences Directorate
- PSE: Physical Sciences and Engineering
- PUC: Partner User Council
- QE: Quantum Efficiency
- RAFEL: Regenerative-Amplifier FEL
- RENEW: Reaching a New Energy Sciences Workforce
- rms: Root-Mean-Square
- ROR: Research Organization Registry
- RF: Radio Frequency
- RSXS: Resonant Soft X-Ray Scattering
- SAC: Scientific Advisory Committee
- SC: Office of Science
- SCU: Superconducting Undulator
- SLAC: Stanford Linear Accelerator Center
- SME: Subject Matter Expert
- SSA: Solid-State Amplifier
- STEM: Science, Technology, Engineering and Mathematics
- STPO: Science and Technologies Partnerships and Outreach
- SWFA: Structure-Based Wakefield Acceleration
- TES: Transition Edge Sensor
- TR-MMID: Time-Resolved Multimodal Imaging and Diffraction
- UEC: Users Executive Committee

- UHV: Ultra-High Vacuum
- UPS: Universal Proposal System
- USPAS: U. S. Particle Accelerator School
- VFD: Variable Frequency Drive
- WDTS: Workforce Development for Teachers and Scientists
- XAS: X-ray Absorption Spectroscopy
- XFEL: X-ray Free Electron Laser
- XPCS: X-ray Photon Correlation Spectroscopy
- XRF: X-ray Fluorescence
- XSCOPE: X-ray and Neutron Scientific Center for Optimization, Prediction, and Experimentation
- XSD: X-ray Science Division
- XU: X-undulators