APS Scientific Computing Strategy

December 9, 2022

Table of Contents

1 Overview

1.1 Introduction

The ongoing APS Upgrade (APS-U) will replace the entire APS storage ring with a ring based on a reverse bend multi-bend achromat (MBA) lattice design. The new storage ring will increase the APS's brilliance by factors of 100-1,000s depending on x-ray energy and make the APS the brightest hard x-ray synchrotron source in the world. Moreover, because of both ongoing developments at the APS in superconducting undulators and the fact that the APS is the highest energy storage ring in the western hemisphere, the APS-U will continue to be world-leading in high energy x-ray capabilities. A one-year shutdown is required for removal and replacement of the storage ring to achieve these revolutionary gains; the one-year shutdown period is scheduled to begin on April 17, 2023. This date provides context and a timeline for the ongoing and needed developments described below.

As part of the APS-U project, feature beamlines were selected for new installation and/or complete replacement based on their promise to best exploit the capabilities of the new source, namely brightness, coherence and high energy x-rays. In addition, based on similar criteria, several beamlines were selected for major enhancements. Because of the greatly enhanced brightness, coherence, and signal at high x-ray energies along with new state-of-the-art high-bandwidth commercial detectors that are part of these projects and amplify these gains, the feature and enhanced beamlines require significant improvements in networking, controls and data acquisition, computing, workflow, data reduction, and analysis tools to operate effectively. For the most part, these needs are not part of the APS-U project but, instead, must be developed as part of APS Operations. The purpose of this document is to summarize the assembled needs, the plans in place to address these needs, and document remaining gaps and proposed next steps.

All aspects of APS operation depend on computation, but data analysis software and beamline control and computing infrastructure are of particular importance for facility productivity. Demands for increased computing at the APS are driven by new scientific opportunities, which are enabled by new measurement techniques, technological advances in detectors, multi-modal data utilization, and advances in data analysis algorithms. The priority for the APS is to further improve our world-class programs that benefit most from high-energy, high-brightness, and coherent x-rays. All of these require advanced computing. The revolutionized high-energy synchrotron facility that APS-U will deliver will increase brightness and coherence, leading to further increases in data rates and experiment complexity, creating further demands for advanced scientific computation.

Over the next decade, the APS anticipates a multiple-order-of-magnitude increase in data rates and volumes generated by APS instruments. This necessitates 10s of PFLOP/s of on-demand computing resources and increased data management and storage resources to process and retain this data and analyzed results. Advanced data processing and analysis methods will be required to keep up with the anticipated data rates and volumes and to provide real-time experiment steering capabilities. The key elements of this strategy and plan include:

- Upgrading networking infrastructure within the APS and between the APS and the Argonne Leadership Computing Facility (ALCF)
- Deploying state-of-the-art experiment control software at beamline instruments
- Expanding the capabilities and use of common data management and workflow tools and science portals
- Deploying sufficient local and edge computing resources, and utilizing the Argonne Leadership Computing Facility (ALCF) for large on-demand data processing and analysis tasks
- Developing high-speed, highly parallel data processing and analysis software, and extensively applying novel mathematical and AI/ML methods to solve challenging data reduction and analysis problems
- Collaborating with the BES light sources, the ASCR computing and networking facilities, the APS User community, and the larger DOE landscape

The APS and ANL are poised well to employ advanced computing to maintain a world-leading position in the synchrotron community. The APS has a world-class photon science program with a large and diverse user base, and ANL is home to world-leading supercomputing infrastructure and computer science expertise in the Computing, Environment, and Life Sciences directorate (CELS). This co-location provides an unprecedented opportunity for collaboration.

The APS collaborates closely with the other BES light sources, and the ASCR computing and networking facilities and ASCR researchers. With the other BES light source facilities and ASCR computing and networking facilities, the APS co-developed a common vision for the future of computing at the light sources and for the light source user community. This common vision is a transformative computational fabric that covers the full lifecycle of data generated at the BES light Sources. It facilitates all aspects of the data lifecycle across the BES light sources, including theory, modeling and simulation, experiment design, data generation at the light sources, data reduction and processing, data analysis and interpretation, and publication and dissemination of scientific knowledge. In this vision, the over 200 current and planned instruments at the light sources are seamlessly connected to a multi-tiered computing landscape that includes edge and local systems, laboratory and campus computing resources, the ASCR facilities, and sustainable and discoverable scientific data repositories. These capabilities will advance the science of the over 10,000 annual light source users. The APS and the other BES light source facilities have partnered with the ASCR computing and networking facilities to take steps toward realizing this shared vision.

The APS has organized the core groups required to achieve these goals under the X-ray Science Technologies (XST) umbrella within the X-ray Science Division (XSD). The XSD Beamline Controls (BC) group is responsible for beamline data acquisition, through control and operations systems and software. The XSD Computational X-ray Science (CXS) group is mainly responsible for the development of theory, mathematical models, algorithms, and software for interpreting x-ray measurements. The XSD Scientific Software Engineering & Data Management (SDM) group is responsible for software engineering for data analysis applications and data management tools, enabling high-performance computing (HPC). The management and support of information technology resources within the APS is handled by the APS Engineering Support (AES) division Information Technology (IT) and Information Solutions (IS) groups.

The outline of the rest of the document is as follows. The remaining sections provide a beamline-independent overview of plans for networking architecture & infrastructure (see 1.2), controls, data acquisition, and detector integration (see 1.3); data management, workflows, and science portals (see 1.4); computing infrastructure (see 1.5); data reduction and analysis (see 1.6); effort funding and collaborations (see 1.7); and priorities for the upcoming fiscal year (see 1.1.1). Specific needs and plans for the APS-U feature beamlines are documented in 2.

1.1.1 FY 2023 Priorities

In FY 2023, the APS is focusing its efforts in scientific computing on those items most important to ensuring the success of the APS-U project. High-level priorities for each area are:

Network Architecture and Infrastructure

- Complete detailed network designs and plans for APS-U Feature beamlines
- Begin procurement of APS-U Feature beamline network components and services
- Complete installation of APS-U Feature beamline networks as per APS-U schedule

Controls, Data Acquisition, and Detector Integration

- Complete detailed plans for, and complete procurement of identified, controls hardware for the APS-U Feature beamlines
- Develop plans and implementations for fast scanning and feedback systems, fast detector acquisition, and integration of multiple data streams, for example interferometer data and detector data, for scanning probe APS-U Feature beamlines
- Create a strategy for addressing known gaps related to fast scanning, feedback, and data acquisition tools
- Identify and begin procurement of detectors for APS-U Feature beamlines

Data Management, Workflows, and Science Portals

- Demonstrate production implementations and routine use of two or more additional on demand workflows using the Polaris supercomputer for APS-U Feature beamlines

Computing Infrastructure

- Demonstrate operationally ready use of the Polaris supercomputer, including consistent account utilization, facility-wide projects and allocations, and end-point administration
- Begin developing a strategy for short-term and long-term data storage

Data Reduction and Analysis

- Continue developing high-speed, highly parallel data processing and analysis software, and extensively applying novel mathematical and AI/ML methods to solve challenging data reduction and analysis problems focused on techniques enabled by high-energy, high-brightness, coherent x-rays provided by the APS-U

Effort, Funding, and Collaborations

- Continue collaborating with the BES light sources, CAMERA, the ASCR computing and networking facilities and ASCR researchers, the APS User community, the larger DOE landscape, and international partners

In addition to these priorities, each support group maintains its own detailed documents and plans describing goals for the current and next fiscal year:

- Beamline Controls Group: https://www.aps.anl.gov/files/APS-Uploads/XSD/XSD-Strategic-Plans/BC-FY22-FY23-Plan-2021-08-31.pdf
- Computational X-ray Science Group: https://www.aps.anl.gov/files/APS-Uploads/XSD/XSD-Strategic-Plans/CXS-FY22-FY22-Plan-2021-08-31.pdf
- Detector Group: https://www.aps.anl.gov/files/APS-Uploads/XSD/XSD-Strategic-Plans/DET-FY22-FY23-Plan-2021-08-31.pdf
- Scientific Software Engineering & Data Management Group: https:///www.aps.anl.gov/files/APS-Uploads/SSG/SDM-FY23-FY24-Plan-2022-10-01.pdf

1.2 Network Architecture and Infrastructure

As data rates and volumes continue to grow (see 1.4), greater demands will be placed on the APS network. This is especially true for the APS-U feature and enhanced beamlines. The APS is updating its network architecture and infrastructure to better serve the beamlines as it enters the APS-U Era. The APS Network Integration Team has been working over the past years to develop a network architecture and infrastructure plan and to implement that plan. Figure 1-1 depicts the APS-U Era network architecture and infrastructure plan.

The center of the APS network consists of a pair of core switches (HPE Aruba 6410) located in the APS data center. These Tier 1 switches provide all routing to beamline subnets and to other parts of the APS, Argonne and the Internet via ESnet. The core switches are configured in a redundant active/active configuration. The core switches provide multiple 10/40/100 Gbps ports. These core switches are connected via 4 x 40 Gbps uplinks to the APS Tier 2 firewall, which in turn connects to the Argonne Tier 1 firewall with 2 x 100 Gbps uplinks. The Tier 1 Argonne firewall connects to the Internet via ESnet using 2 x 100 Gbps uplinks. The APS core switches also connect directly to the Argonne Leadership Computing Facility via 2 x 100 Gbps uplinks. The same core switches connect to the storage systems for the APS Data Management System (see 1.4), sector data storage systems, the dservs that host beamline control system configurations and software, and the APS accelerator network.

Each sector at the APS has a Tier 2 switch (HPE Aruba 6410) that serves to connect beamline devices and to connect the beamline to the core APS switches. The Tier 2 switches connect to beamline computers, control system EPICS IOCs, detectors and data acquisition servers, wireless access points, cameras, and controls hardware. Each Tier 2 beamline network switch will provide line rate 10/100/1000 Mbps ports for many of devices at the beamline, as well as high speed line rate 10/40/100 Gbps ports for data acquisition where needed. Uplinks to the APS Tier 1 core switches will be sized appropriately based on beamline needs.

A Tier 3 managed switch with 48 x 10/100/1000 Mbps ports may be deployed at each experiment hutch for controls hardware stations to provide a dynamic cabling environment and to isolate beamline controls hardware traffic.

The APS will adopt a Supervisory Control and Data Acquisition (SCADA) architecture for the APS-U beamline control system network. Controls and data analysis network traffic will be separated and isolated from outside networks for maximum performance and security. Wireless access points can also be provided inside the hutch to support, for instance, advanced sensors or augmented reality headsets.

Each APS-U feature beamline will have a 10 Gbps copper cabling infrastructure (CAT 6A) from beamline stations to the sector network switch. An additional 96 pairs of single mode fiber have been installed from APS data center to each of the Laboratory Office Module (LOM) network closets; 768 pairs in total. This additional fiber infrastructure will provide sufficient network bandwidth from the beamlines to the data center for the next decade.

The APS-U project scope is responsible for networking at the Tier 2 and Tier 3 levels for the APS-U feature beamlines, including the Tier 2 and Tier 3 switches and optics modules, and all cabling in the sector and hutches. APS Operations is responsible for Tier 2 and Tier 3 networking for all other beamlines. APS Operations is responsible for all networking from the Tier 2 sector switches to the Tier 1 core switches, and to other systems at the APS. Argonne Operations is responsible for networking from the APS Tier 1 switches to the Internet, and to the Argonne Leadership Computing Facility (ALCF).

The upgraded Tier 1 core switches were installed in the spring of 2021. Each APS-U feature beamline network upgrade will follow the beamline upgrade schedule. Fiber optic cable upgrades have been completed from the APS data center to LOMs 431-438. The APS Network Integration Team is working with beamline staff to identify requirements for and procure Tier 2 and Tier 3 switches and beamline cabling, components, and jacks for the feature and enhanced beamlines. Argonne's central networking team is responsible for maintaining the network between the APS and the ALCF and to the Internet. Networking between the APS and ALCF will be upgraded to terabit/s over the next decade.

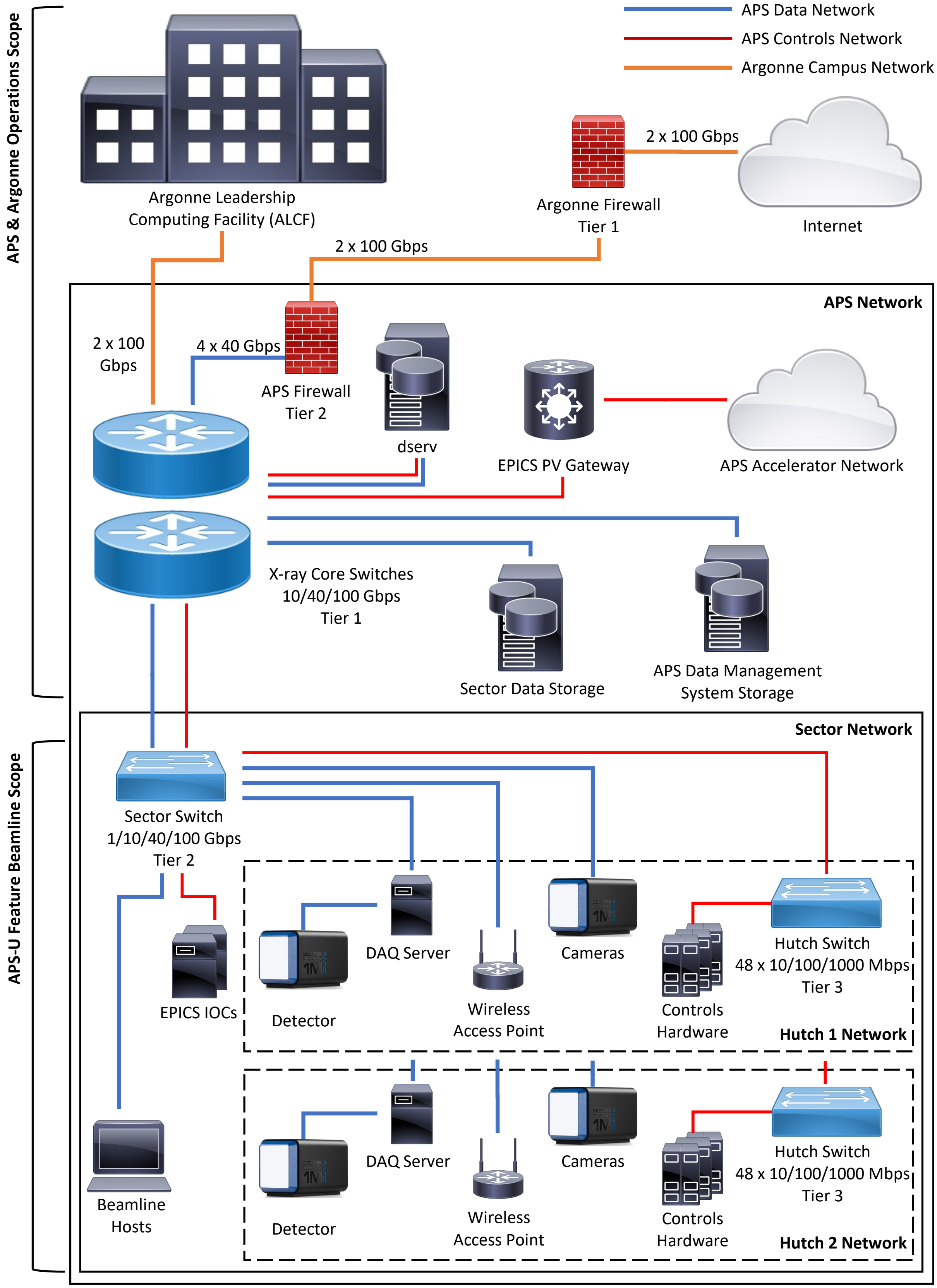

Figure 1-1 The APS-U Era network architecture and infrastructure.

1.3 Controls, Data Acquisition, and Detector Integration

The Beamline Controls (BC) Group will provide direct engineering, installation and commissioning support for APS-U beamline machine control, data acquisition and experimental process control systems. Maximizing system operability, maintainability and adaptability while providing state-of-the-art performance are the goal of all system engineering decisions.

To achieve those goals for APS-U beamline controls engineering will rely on a standards-based approach, with a strong preference for open-source or commercial-off-the-shelf components, where possible. Unique controls capabilities are engineered in-house or in collaboration with a vendor with the goal of being adaptable to multiple beamline uses.

The APS-U scope, a combination of new and rebuilt beamlines with significant improvements in data acquisition performance, requires a multi-tiered strategy for implementation of the control system. The BASE tier of beamline controls will apply to all APS-U beamline controls systems. This tier will receive the upgraded SCADA network layout, EPICS V7 capable IOCs, *bluesky* experimental control and data handling (when appropriate) and replace end-of-life hardware, as funding permits. Beamlines/hutches that are adding instruments that require additional control system functionality (ENHANCED tier) will have necessary components upgraded or systems added to meet performance goals. ADVANCED beamlines are ones that are completely rebuilt or built new. The design of ADVANCED tier beamline and instrument control systems will use updated standard motion and IO components that maximize beamline performance capability. Programmable motion systems that enable coordination motion across components and field programmable FPGA based triggering and data acquisition systems will be the key strategic components of the ADVANCED tier beamlines.

ACSMotionControl motor controllers and drives have been selected as a standard APS-U motion solution. This motion system uses EtherCAT technology to coordinate motors across multiple devices. The MP4U 8-axis controller/drive solution will be preferred but when needed other ACS products will be deployed. A VME based motion system (OMS MAXv/Phytron) will be available when high density/low duty cycle motors need to be supported. These devices will be used for major beamline optical components, including monochromators, high heat load mirrors, and transfocators, and general motion control, including beamline devices such as slits, flags, etc.

New instruments, especially the nano- and micro-probe scanning instruments, require fast scanning and feedback capabilities. APS-U instrument fast fly scanning requirements will be met with an APS designed, user configurable, fast triggering/timing and data acquisition system, *softGlueZynq*. This system installs the EPICS framework on a commercial FPGA/ARM processor board, AVNET microZed. *softGlueZynq* provides pre-built, yet configurable, hardware circuits (gate/delay generators, frequency counters, multi-channel scaler) required for fast and precise experiments with APS-U Era instruments. The *softGlueZynq* focal spot tracking circuit, pixelTrigger, can generate data-acquisition triggers and record six interferometers and two additional channels (time tag and dwell time), at up to 400 kHz to meet APS-U microscope position accuracy requirements. See Figure 1-2 for an example of *softGlueZynq* applied to the APS-U InSitu Nanoprobe (ISN) Feature beamline.

A commercial FPGA DAQ appliance (ACQ2106) from D-TACQ Solutions Ltd. will be used to deploy *softGlueZynq* solutions customized for each APSU instrument requirements. The FPGA DAQ appliance provides FMC slots for FPGA I/O cards which will be selected to match the needs of each APSU instrument.

The hardware and software flexibility that the *softGlueZynq* system provides for developing APS-U Era instrument control and experiment solutions makes it the preferred platform over similar FPGA based solutions. The *softGlueZynq* system was presented at the 2019 APS Advanced Controls Workshop (sponsored by the APS Advanced Controls Working Group) and determined to be a sound solution for APS-U Era experiment needs.

Networked industrial IO devices will be used for lower performance beamline IO needs (analog, digital, relays, thermocouples). LabJack and Advantech ADAM series products are examples of preferred networked IO solutions.

EPICS is used as a layered control structure onto the beamline control systems. This layered approach enables specialized collaboration with instrument scientists and controls communities within the APS as well as at other DOE facilities and abroad. APS-U EPICS IOCs will support EPICS V7 PVAccess applications and clients as EPICS client/server solutions transition from Channel Access to PVAccess. Priority is placed on developing capabilities that capture and create economies of scale aligned with the priorities of XSD and the APS.

New high data-rate detectors can generate thousands of frames per second using tens of Gbps of bandwidth necessitating fast data handling capabilities. The newly developed Python-based *pvaPy* framework (https://github.com/epics-base/pvaPy/blob/master/documentation/streamingFramework.md) provides a streaming data framework for EPICS V7 that can combine multiple data sources, and process data at thousands of frames per second (see Figure 1-3.) The *pvaPy* framework will serve as the basis for fast data handling for APS-U beamlines.

In the past year, the APS-U Era Beamline Data Pipeline (BDP) Project was started to explore, identify, demonstrate, and deploy a portable data pipeline solution that addresses APS-U Era beamline data needs. This project will create a template for APS beamlines and support groups to follow when deploying new instruments or data pipelines addressing detector integration, data movement, network infrastructure, storage systems, multi-tiered computing, and cyber security. The template will be validated first in a laboratory setting using a testbed, and then by the successful application to the APS-U Feature Beamlines and APS-U Enhancement Projects. This project will also identify gaps in implementations and capabilities, and suggest action items needed to fill the identified gaps.

Each APS-U beamline project has been assigned a Controls Lead from the XSD Beamline Controls group. These leads are the primary contact for the APS-U beamline project lead and coordinate with the APS-U beamline project lead on installation and commissioning planning and execution. The XSD Beamline Controls group meets regularly to share detailed planning efforts on the various feature beamlines to help ensure that the beamline controls designs are as uniform as sensibly possible.

The high-level beamline controls planning and installation schedule in administered using project management best practices in accordance with APS-U project planning guidelines. Each planning and installation task has been assigned effort hours, duration hours, and labor resources required. Scheduling dependencies between tasks are tracked. Each major element of beamline controls (instrument control, motion systems, detectors, experimental software, i.e., *bluesky*, instrumentation network, system monitoring and control, and beam characterization) have a design, procurement, and installation phase that has been estimated and will be tracked. Each feature beamline controls work timeline has been determined separately based on the beamline enclose Beneficial Occupancy dates.

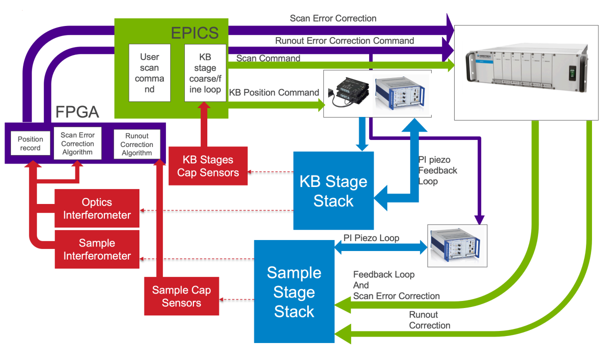

Figure 1-2 Schematic of fast scanning and interferometry for the APS-U InSitu Nanoprobe (ISN) Feature beamline.

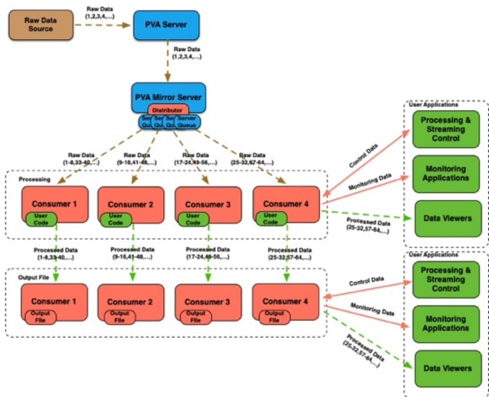

Figure 1-3 pvaPy streaming framework depicting multiple data processing consumers.

1.4 Data Management, Workflows, and Science Portals

The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, provides a data management, workflow, and storage system sufficient to retain experimental data in accordance with sponsor requirements.

The need for data management, workflow, and distribution tools, and data storage resources continues to grow. Currently the APS X-ray Science Division operates beamlines that collect on the order of 5 PB of raw data per year. Over the next decade, it is estimated that the data storage needs of the APS are anticipated to increase by at least two orders of magnitude to 100s of PBs of raw data per year (see Figure 1-4). Great strides have been made in this area over the past years. The APS will continue to deliver a multi-tiered data management and distribution system for all current and future APS beamlines.

During FY13 - FY15, the APS piloted facility-wide data management and distribution tools and resources with effort and funding from LDRDs. These activities provided R&D effort and seeded ongoing connections between the APS and the Argonne Leadership Computing Facility (ALCF), the Mathematics and Computer Science (MCS) division, the Data Science and Learning (DSL) division, and the Globus Services team at the University of Chicago.

Through APS operations funding, the APS Data Management System integrates with beamline data workflows, and large data storage systems. These tools automate the transfer of data between acquisition devices, computing resources, and data storage systems. Ownership and access permissions are granted to the users signed-up to perform a particular experiment. A metadata catalog allows beamline staff to populate experiment conditions and information for access via a web portal. Users can download data at their home institutions using Globus Transfer (globus.org) or SFTP. At present, approximately 53 APS beamlines (XSD and non-XSD) take advantage of this system.

Medium-term data storage is available within the APS; longer-term storage systems are provided by the Argonne Leadership Computing Facility (see Figure 1-5). Currently, the APS provides approximately 5.6 PB of central disk storage (easily expandable to 15 PB) for medium-term data retention, and several Data Transfer Nodes (DTNs) for reliable, high-speed data movement internally and externally (see Figure 1-6). The Argonne Leadership Computing Facility currently provides approximately 10 PB of tape storage (easily expandable to meet future APS needs) for longer-term data retention. The ALCF has recently deployed a 100 PB community file system (Eagle) and a 100 PB project file system (Grand) along with additional tape storage that is available for APS use. These resources are currently funded, and will continue to be funded, by APS and ALCF operations budgets. Both the National Energy Research Scientific Computing (NERSC) Center and the Oak Ridge Leadership Computing Facility (OLCF) are deploying similar systems.

The APS is working with Argonne's Data Science and Learning Division and the Globus Services team to develop a computational data fabric for end-to-end data lifecycle management. This fabric is named Gladier and connects and automates many stages of the data lifecycle from acquisition to processing to publication.

Science web portals will allow APS users to view and download their data and reprocess their data on ALCF and other large-scale computing resources using Globus Automate and FuncX. The Materials Data Facility (MDF) and the DOE Office of Scientific and Technical Information will serve as a DOI generating service for APS datasets. The APS and Globus team have prototyped a computational fabric for XPCS (see Figure 1-7) and serial crystallography, and are working to develop such workflows for ptychography (see Figure 1-8), High-Energy Diffraction Microscopy (HEDM) (see Figure 1-9), and Bragg Coherent Diffraction Imaging (BCDI) over the next years. These tools will be applied at more beamlines in the years after and will serve as the basis for enabling searchable data catalogs and adopting FAIR data practices.

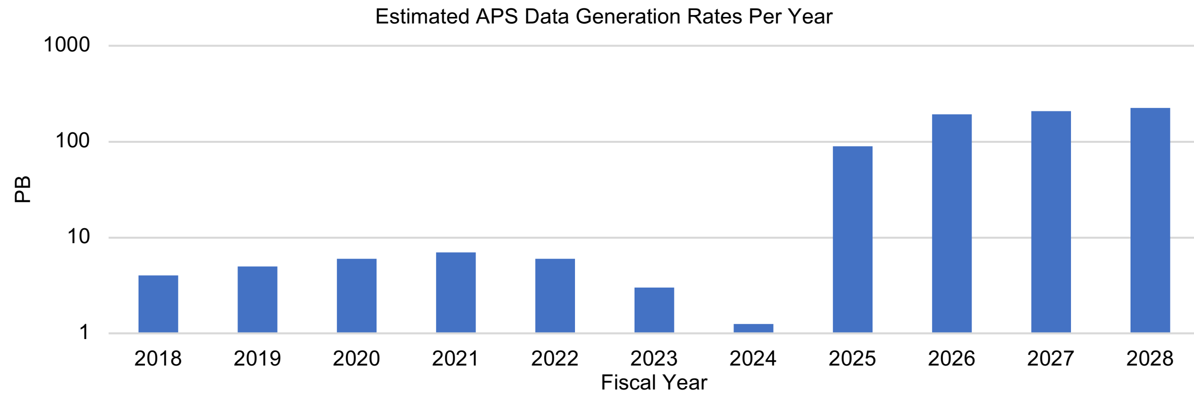

Figure 1-4 Log scale: Anticipated aggregate APS X-ray Science Division data generation per year. Data generation during FY23 and FY24 is estimated to be lower due to the storage ring replacement period followed by the storage ring and beamline commissioning periods.

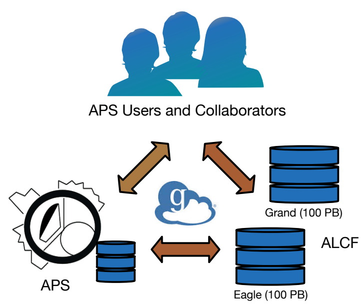

Figure 1-5 Storage available for APS beamlines. A multi-PB data storage system located at the APS serves medium-term needs. The Argonne Leadership Computing Facility (ALCF) provides multiple systems for long-term storage. Capacity will be expanded as needed to meet sponsor requirements.

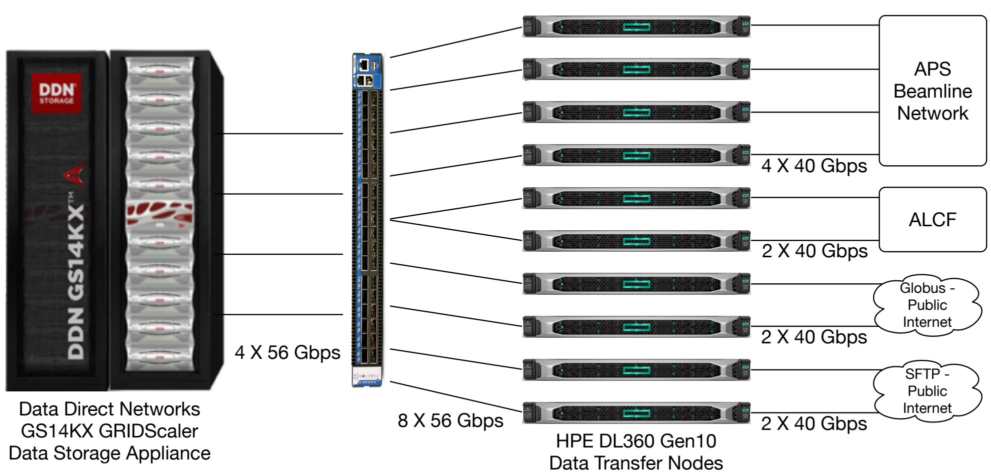

Figure 1-6 The APS Data Management System storage infrastructure. A Data Direct Networks storage appliance connects to an InfiniBand switch. Four data transfer nodes link the storage to the beamline network, two data transfer nodes connect the storage to the Argonne Leadership Computing Facility, two data transfer nodes provide links to the public Internet for Globus transfers, and two data transfer nodes provide links to the public Internet for SFTP transfers.

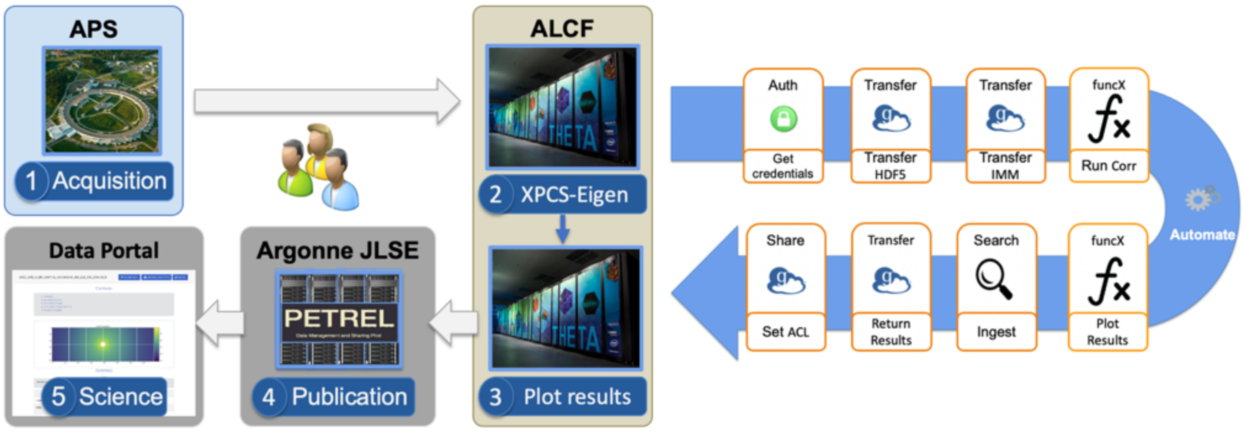

Figure 1-7 Automation used to perform on-demand analysis of XPCS data using computing resources at the Argonne Leadership Computing Facility (ALCF). Data are transferred to ALCF where compute nodes are provisioned to perform analysis, extract metadata, and plot results, which are then published to a Globus data portal for user analysis and reprocessing.

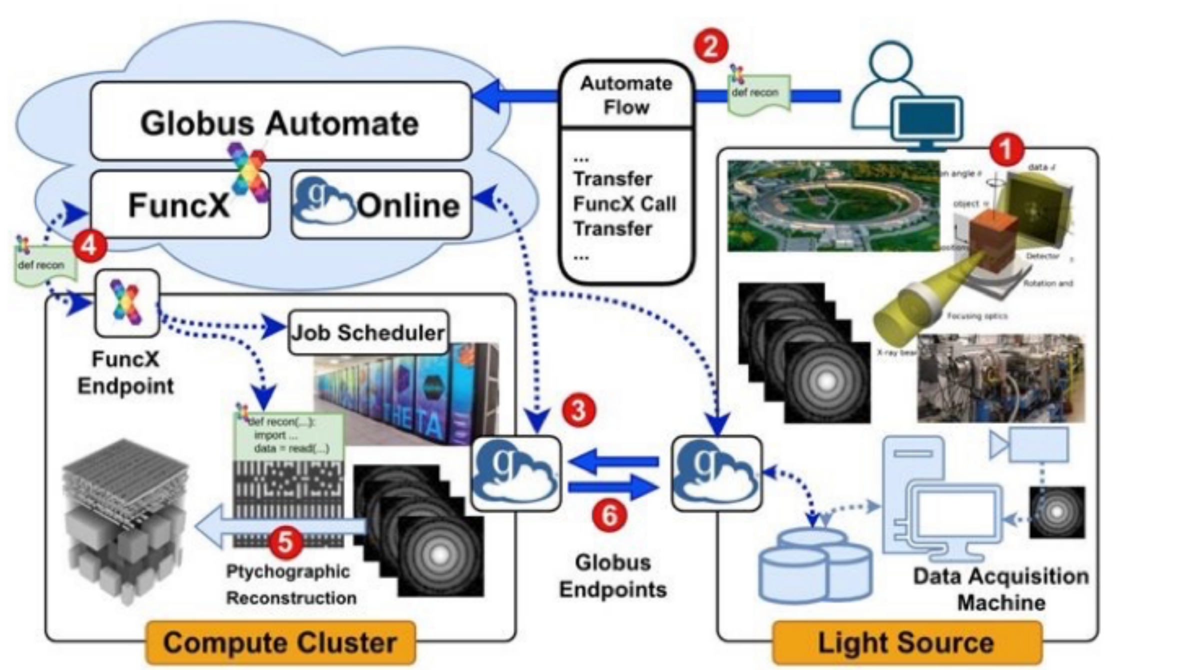

Figure 1-8 Automation used to perform on-demand analysis of ptychography data using computing resources at the Argonne Leadership Computing Facility (ALCF). (1) Diffraction patterns are collected at the APS. (2) A beamline scientist submits a ptychography workflow definition file to the Globus Automate service. (3) The Globus Automate service begins executing the workflow and transfers the data from the beamline to the ALCF compute resource. (4) Remote function calls are triggered that (5) run the ptychography reconstruction code. (6) Results are transferred back to the beamline.

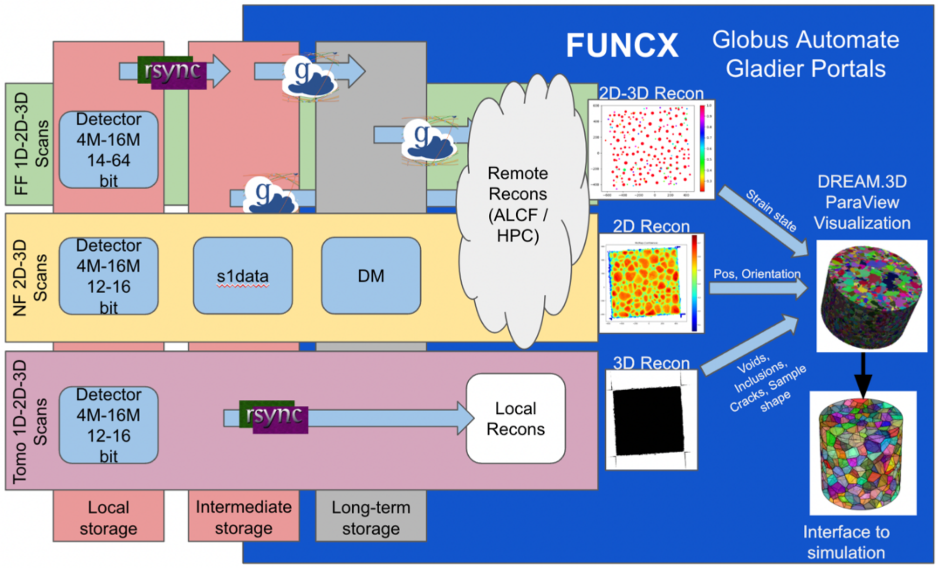

Figure 1-9 Automation used to perform on-demand analysis of HEDM data using computing resources at the Argonne Leadership Computing Facility (ALCF). Diffraction and tomography data are transferred to ALCF where compute nodes are provisioned to perform analysis.

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1.5 Computing Infrastructure

Demands for increased data processing capabilities in the APS-U era are driven by new scientific opportunities enabled by the upgraded facility. The increase in brightness and advances in detector data rates will generate multiple orders-of-magnitude more data than is generated today; this increase in data volume necessitates an increase in processing power to keep pace. The utilization of multi-modal data to answer new questions requires more complex and sophisticated data processing algorithms requiring increases in computing capabilities. Increases in computing power are needed by advanced algorithms for existing techniques that, for example, provide higher-fidelity results, and to train AI/ML models. The need for real-time analysis and feedback to make crucial experiment decisions and enable autonomous experiment steering also requires more computing cycles than have been traditionally utilized.

As with data storage, the computing resources required by the APS are anticipated to grow by at least two orders-of-magnitude. Prior to the APS-U, most data processing can be performed within the range of TFLOP/s of computing resources. In the APS-U era, first pass data processing at the APS will require on-demand access to tens of PFLOP/s of computing resources. There is wide variability in the computational requirements among techniques and processing approaches with those instruments and techniques that benefit most from high-energy, high-brightness, and coherent x-rays driving most requirements [1].

The APS-U project may provide funding for certain local computing resources at feature beamlines, however, the majority of resources and effort will be provided outside of APS-U project scope. To satisfy these needs, the APS adopts a graded approach to resource utilization. Small-scale resources, such as multi-core processors and GPUs, local to beamlines will be used when sufficient. For moderate computational needs, the APS maintains an on-site computing cluster, and ANL maintains computing resources as a part of the Laboratory Computing Resource Center (LCRC). For the most demanding computational problems, large-scale computing facilities must be used, including the Argonne Leadership Computing Facility (ALCF), the National Energy Research Scientific Computing (NERSC) Center, and the Oak Ridge Leadership Computing Facility (OLCF). To mitigate challenges surrounding processing and storing such large, anticipated data volumes, the APS is exploring the utilization of edge computing resources coupled closely to detectors and instruments, to run AI/ML data reduction algorithms. See Figure 1-10 for a list of computing resources available at Argonne.

Integrated ALCF Supercomputing Resources at the APS: A New Era of APS Computing

In the APS-U era, it will be impractical and unreasonable to support the scale of computing required with only local APS resources. The colocation of the APS and world-leading supercomputing infrastructure at the ALCF on Argonne's campus provides an unprecedented opportunity for collaboration. The APS and ALCF have partnered to deliver a new model of computing, tightly coupling APS experiment instruments with ALCF supercomputers, to accelerate scientific discovery. See Figure 1-11.

The ALCF has deployed a new computing system, Polaris, in 2022. Polaris is a combination commodity CPU/GPU system with performance of approximately 44 PFLOP/s. This system follows a new model for supercomputing systems, Instrument to Edge (I2E), to better enable use by experimental facilities. Up to 4 PFLOP/s of computing is prioritized to explore on-demand use of high-end computing resources by experimental and observational facilities, including the APS.

Work is underway to test preemptive scheduling queues to provide immediate, on-demand access for APS jobs. Gateway nodes on this system will provide the ability for the APS to stream data directly to Polaris from detectors, avoiding local file I/O. The APS is working with Argonne's Data Science and Learning Division and the Globus Services team to develop a computational data fabric for end-to-end data lifecycle management, Gladier (see 1.4 above). A combined team of APS and ALCF scientists and engineers are developing end-to-end workflow pipelines that will connect APS instruments to this new resource, focusing first on x-ray photon correlation spectroscopy (XPCS), ptychography, high-energy diffraction microscopy (HEDM), and AI/ML methods.

These new capabilities combined will provide the necessary coupling between the APS and the ALCF to more seamlessly utilize large computing resources to enable the data processing needed in the APS-U era. This model, once refined using Polaris, will be deployed on more computing resources at the ALCF and at Argonne. These capabilities will be deployed for many other APS techniques and beamlines for data processing during beam time and for post-processing by APS Users after allocated experiment time is over.

Designed in collaboration with Intel and Cray, the 11 PFLOPS Theta supercomputer serves as a stepping-stone to the ALCF's next leadership-class supercomputer, the Aurora exascale supercomputer, to become available in 2023. Aurora is designed to support numerical simulation, data analysis, and deep learning applications. To this end, it is architected with a mix of Intel CPUs and GPUs to deliver sustained performance of greater than one exaflop/s 10^{18} full-precision floating point operations per second, and substantially higher compute rates at reduced precision. It will have aggregate system memory of more than 10 petabytes. The APS will utilize this new class of supercomputer to couple the results of simulations and modeling with experiment data and train ML models in real-time.

The APS is developing software applications that run on the ALCF Theta (and ThetaGPU) supercomputer for high-energy diffraction microscopy (HEDM), ptychography, serial crystallography (SX), tomography, x-ray fluorescence microscopy (XRF) elemental mapping, and x-ray photon correlation spectroscopy (XPCS). These applications are being ported to run on GPUs and to scale for the upcoming Polaris system.

The APS has been involved in many activities aimed at using centralized and large-scale computing resources. Notable activities include:

- A team comprising of staff at the APS, ALCF, and DSL have successfully demonstrated the first use of the new ALCF Polaris supercomputer for processing XPCS data.
- ALCF researchers demonstrated the use of the Balsam resource and queue scheduler to run XPCS and serial crystallography (SX) processing jobs in an on-demand fashion [2].
- At SC'19, ALCF researchers demonstrated large-scale real-time reconstruction and visualization of tomography data. Data acquisition was simulated at the convention center and streamed to Theta at the ALCF for denoising and reconstruction. Data was visualized back on the show floor. This demonstration won the first annual SCinet Technology Challenge (TC) [3]. See Figure 1-12.
- Argonne scientists have demonstrated tomographic reconstructions of a fixed adult mouse brain specimen consisting of 10^{12} voxels in 2.5 minutes using 24,576 GPUs on the Summit Supercomputer reaching 65 PFLOPS throughput [4, 5]. This work won the SC'20 Best Paper Award.
- The APS has successfully utilized NERSC for high-energy diffraction microscopy (HEDM), tomography, and x-ray photon correlation spectroscopy (XPCS) data processing.
- The Argonne Leadership Computing Resource Center (LCRC) has been used routinely for high-energy diffraction microscopy (HEDM) reconstructions.

Edge computing offers the ability to process data quickly on or near detectors and experiment instrumentation without the need to first transfer all data to high-end computing resources. This is particularly promising for handling large data when coupled with machine-learning methods. Using only a subset of data, machine-learning models may be trained on supercomputers. The trained model is then run using edge computing devices to process newly acquired data, providing fast feedback for experiment steering. See Figure 1-13. For example, APS and Argonne researchers have developed deep neural networks that perform ptychography reconstructions 300 times faster than the conventional iterative approaches and require up to 5 times less data [6], and 200 times faster than the conventional pseudo-Voigt profiling to locate Bragg peak positions [7].

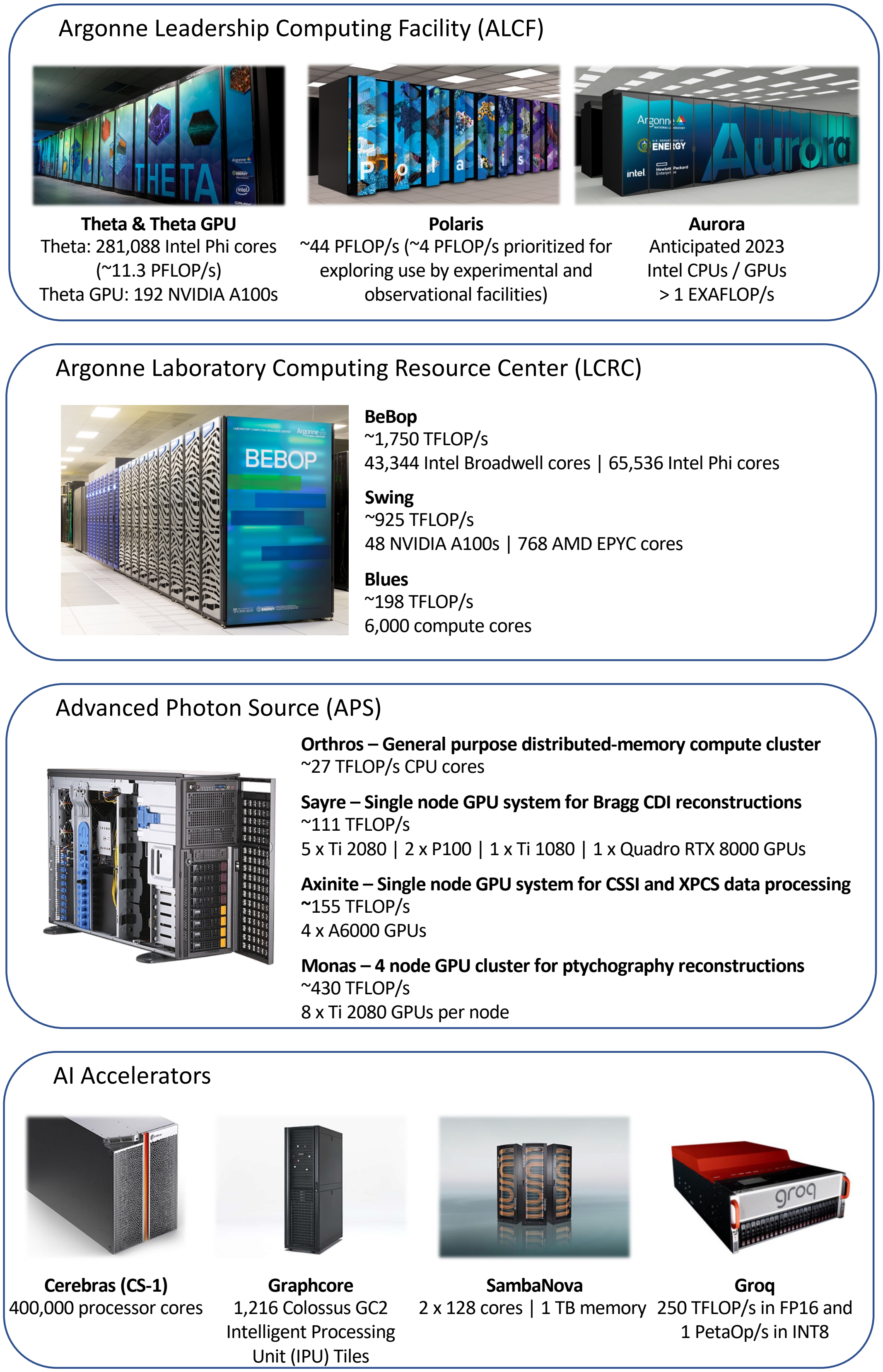

Figure 1-10 Computing resources and respective specifications and performance available for use by the APS at Argonne.

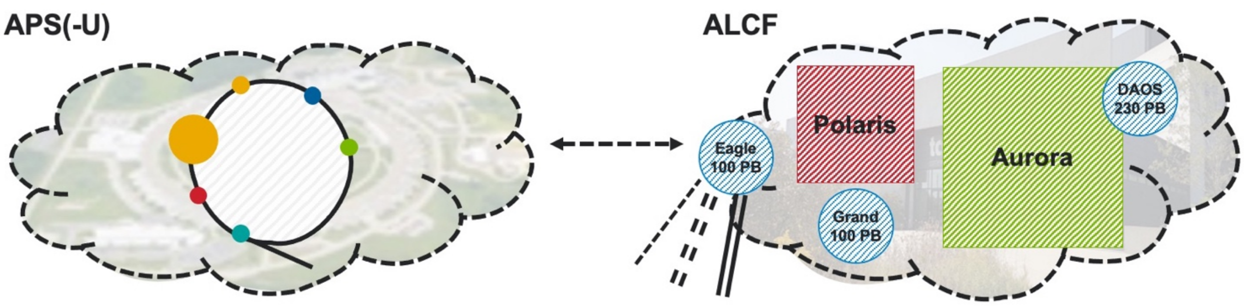

Figure 1-11 The APS and ALCF have partnered to deliver a new model of computing, tightly coupling APS experiment instruments with ALCF supercomputers and storage infrastructure, to accelerate scientific discovery.

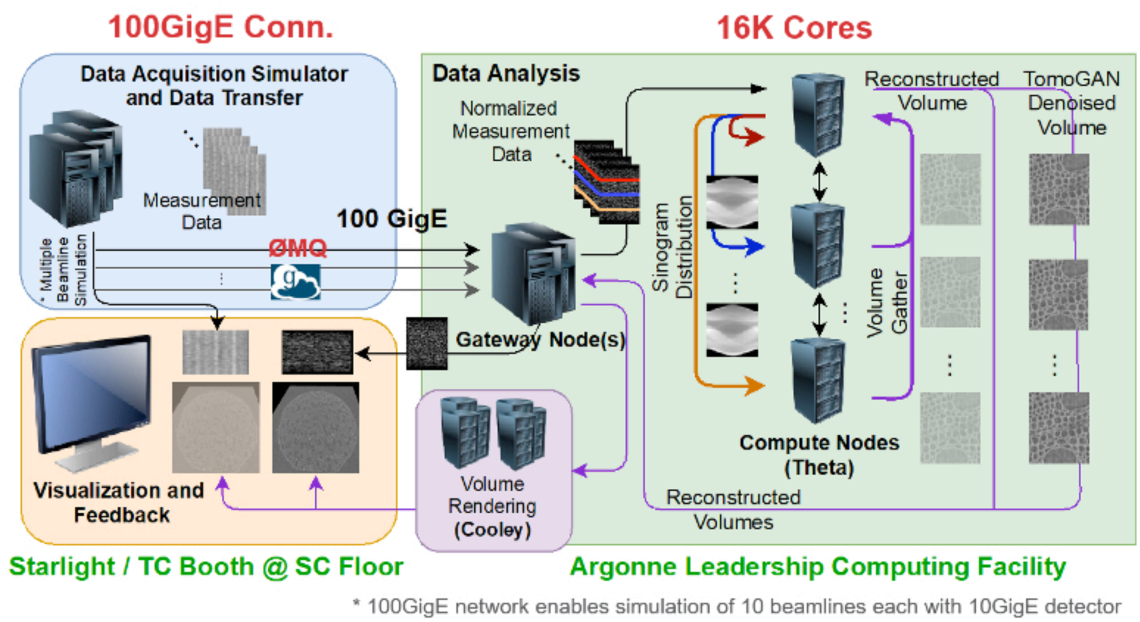

Figure 1-12 Demonstration setup for "Real-Time Analysis of Streaming Synchrotron Data" at SC'19.

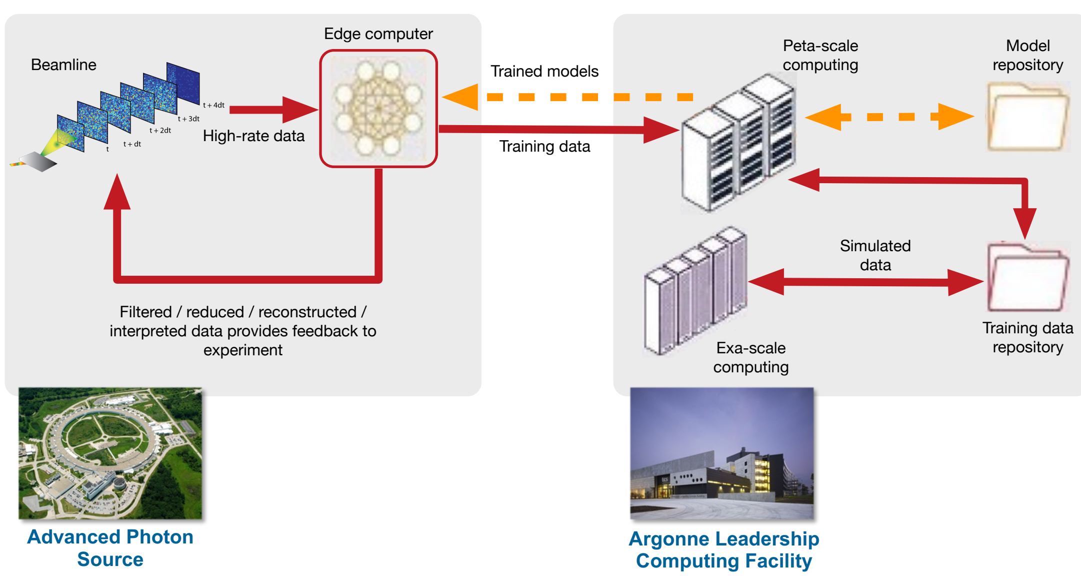

Figure 1-13 Edge computing architecture using machine-learning models trained on supercomputers.

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1.6 Data Reduction and Analysis

The APS is focusing data analysis algorithm and software development in the areas needed to answer the novel scientific inquiries enabled by the future APS and the APS-U project. 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, identify and classify features and patterns, and provide feedback to experiments dynamically using real-time reduction and novel AI/ML approaches. Detailed descriptions and plans for algorithm and software development for each APS-U feature beamline, including funding sources and collaborative efforts, may be found in each APS-U feature beamline’s area in section 2.

Coherence, imaging, high-energy, and multi-modal techniques are already the most computationally intensive techniques performed at the APS and throughput demands are expected to grow by as much as multiple orders of magnitude due to improved detectors and the upgraded source. Data reduction and analysis will rely heavily on the use of high-performance computing (HPC), utilizing appropriate technologies such as multi-threading, General Purpose Graphical Processing Units (GPUs), edge devices, and distributed computing environments to obtain results with near real-time completion, so that results enable user-driven or even automated steering of experiments.

Most software will be developed as open source and will be made available with user community code contributions encouraged. A graded approach according to impact and priority will be applied to development. Packaging and active support either as distributable applications or as Software-as-a-Service (SaaS) will be provided for software systems that have been deemed to be most important for the success of APS users. Beamlines not directly part of APS-U will also benefit from the reuse of tools developed for priority applications.

Key software developments have been made in this area over the past years including:

- *cohere:* Bragg Coherent Diffraction Imaging (BCDI) reconstruction tools
- *MIDAS:* Software for High-Energy Diffraction Microscopy (HEDM) microstructure analysis
- *RSMap3D:* High-performance software for rapid reciprocal-space mapping
- *Tike:* A comprehensive ptychography reconstruction package
- *TomoPy:* A comprehensive tomography reconstruction package
- *XPCS:* X-ray Photon Correlation Spectroscopy (XPCS) correlation software
- *XRF-Maps:* High-performance x-ray fluorescence mapping tools
- *GSAS-II/GSAS/EXPGUI:* Crystallography data analysis software receiving over 500 citations per year

Applications will continue to be developed for improved performance and algorithms. A complete list of software produced at the APS can be found at https://www.aps.anl.gov/Science/Scientific-Software and https://github.com/AdvancedPhotonSource.

New efforts are underway to address the development of new algorithms and HPC software for multi-modal analysis, including fluorescence tomography, fluorescence ptychography, tomography diffraction, and Bragg CDI and ptychography, and for a new approach to Laue diffraction reconstructions. Computer vision approaches are being developed to speed up beamline calibration and sample alignment. The MONA (Monitoring, Optimization, Navigation, Adaptation) project has prototyped data streaming coupled with real-time data analysis and automated feedback.

Artificial Intelligence / Machine Learning (AI/ML)

The development of new x-ray characterization techniques has notably relied on the co-invention of algorithms and mathematical models for the analysis and interpretation of the data produced by each technique. In fact, several synchrotron imaging techniques are only made possible because of the existence of an underlying algorithm or computational solver (for example, computational imaging methods, such as ptychography and tomography). Numerical algorithms have enabled transformational science at synchrotron sources, but next-generation light sources provide an enormous computational challenge for many existing algorithmic approaches. APS-U Era data rates are expected to be so large that traditional algorithms may not be able to keep up with acquired data. Artificial intelligence / machine learning (AI/ML) advances have shown promise in not only speeding up but also expanding the potential robustness of x-ray data analysis methods and is poised to play an increasing role in the APS-U Era.

Key AI/ML advances have been made over the past few years. Some examples are:

- *A.I. C.D.I. – AI-enabled real-time Bragg Coherent Diffraction Imaging:* A deep convolutional neural network (CDINN) can reconstruct high-quality images from CDI data quickly by skipping the phase-recovery step. Such real-time image reconstruction has the potential to dramatically improve the various advanced imaging modalities that rely on phase-retrieval algorithms. [1]
- *Intelligent Ptychography Scans via Diffraction-Based Machine Learning:* An unsupervised clustering framework to identify the region of interest of a sample purely based on diffraction patterns, so that the overall computational cost is reduced by only focusing on the “important” data. The methodology is further extended to guide the scanning pattern to only focusing on the region of interest instead of using a traditional raster scan pattern. [2]
- *ML-assisted Oversampling in Ptychography:* An ML based approach to complement sparsely acquired or under sampled data with data sampled from a deep generative network to satisfy the oversampling requirement in ptychography. Because the deep generative network is pre-trained and its output can be computed as data is collected, the experimental data and the time to acquire the data can be reduced. [3]
- *Compressive Ptychography with Semi-Supervised Priors:* An ML based image reconstruction technique that combines unsupervised ML models with supervised ML models. The unsupervised approach optimizes a deep generative neural network to create a solution for a given dataset. We complement our approach with a prior acquired from a previously trained discriminator network to avoid a possible divergence from the desired output caused by the noise in the measurements. [4]

- *Combining Physics and ML Models for Limited-angle CT:* A generative ML model to effectively constrain the solution of a standard physics-based approach. Our approach is self-training that can iteratively learn the nonlinear mapping from partial projections to the scanned object. Because our approach combines the data likelihood and image prior terms into a single deep network, it is computationally tractable and improves performance through end-to-end training. [5]
- *Plug-and-Play Deep Priors for Joint Reconstruction of Ptychography and Tomography Data:* An alternating method of multipliers (ADMM) algorithm with plug-and-play denoisers to recover refractive index of a 3D material through diffraction data by replacing the regularization subproblem with a general denoising operator based on machine learning. [6]
- *Sinogram Inpainting with Supervised ML Models:* A effective GAN-based inpainting method to restore the missing sinogram data for limited-angle CT. To estimate the missing data, we design the generator and discriminator of the patch-GAN and train the network to learn the data distribution of the sinogram. [7]
- *Low-Dose CT with CNNs:* A deep convolutional neural network (CNN) method that increases the acquired X-ray tomographic signal by at least a factor of 10 during low-dose fast acquisition by improving the quality of recorded projections. [8]
- *Supervised ML for Digital CT Calibration:* A machine learning approach based on a convolutional neural network architecture to calibrate the center-of-rotation for X-ray tomography. [9]
- *CNNs for 3D Volume Segmentation of CT Data:* An approach for automated segmentation of large 3D tomography datasets using a Convolutional Neural Network (CNN) architecture based on a deep learning approach. [10]
- *Automatic Differentiation for beyond Depth of Focus:* As Argonne's APS Upgrade enables higher-resolution imaging, researchers must account for diffractive blurring in the image of the thick samples that x-rays will be able to image. This method computes the gradient values using automatic differentiation (AD). Because AD is used for neural network training, it is part of many AI toolkits that are already built for large-scale data handling on supercomputers. A detailed comparison of the forward model approaches (Fresnel multislice versus finite-difference methods) shows that the AD-based approach can be used to recover beyond-DOF objects. [11]
- *BraggNN:* BraggNN is a deep-learning-based method that can determine Bragg peak positions much more rapidly than conventional pseudo-Voigt peak fitting. BraggNN runs more than 200 times faster than a conventional method on a GPU card with out-of-the-box software. The speedup is important for high-resolution, high-throughput, and latency-sensitive applications, moving the field closer to realizing real-time analysis and experiment steering for materials exploration and discovery. [12]
- *Low-Dose X-ray Tomography with Self-supervised Learning*: A neural network that learns through optimization of the differences between a few low-dose/high-dose pairs. Using this map, convolutional neural network (CNN) can enhance the remaining low-dose projections, thereby allowing the imaging of dose-sensitive materials at the nanoscale. [13]
- *ML Interatomic Potentials from X-ray Diffraction Data:* A new machine learning scheme uses experimental high energy x-ray diffraction data to drive an active learning algorithm that tests *ab initio* molecular dynamics simulations using a Gaussian Approximation Potential approach. The interatomic potential developed reproduces the measured structural phases and predicts dynamic and physical properties of the system. [14]
- *ML Potentials for Molten Salts from X-ray PDF data:* A machine learning approach driven by x-ray pair distribution function data uses an active learning algorithm to test *ab initio* molecular dynamics simulations using a Gaussian Approximation Potential. The ML potential developed reproduces the temperature-dependent molten salt structure and predicts the density, self-diffusion coefficients and ionic conductivity of the liquid. [15]
- *PtychoNN – AI-enabled scanning coherent diffraction imaging:* PtychoNN is a deep convolutional neural network that learns to solve the image reconstruction problem in Ptychographic x-ray imaging. PtychoNN learns a direct mapping from measured diffraction data to sample amplitude and phase, eliminating the need for iterative phase retrieval entirely. PtychoNN is 100s of times faster than current methods that use phase retrieval algorithms, and it can reconstruct sample images with up to 25x less data than that required by current methods. [16]

- *TomoGAN – Low-Dose Synchrotron X-Ray Tomography with Generative Adversarial Networks*: A denoising technique based on generative adversarial networks, for improving the quality of reconstructed images for low-dose imaging conditions. Evaluation with both simulated and experimental datasets shows that this approach can significantly reduce noise in reconstructed images, improving the structural similarity score of simulation and experimental data. [17]
- *AutoPhaseNN - Unsupervised Physics-aware Deep Learning of 3D Nanoscale Bragg Coherent Diffraction Imaging:* A neural network that uses known physics and learns to invert 3D Bragg CDI data completely unsupervised, i.e., without ever being shown sample images during training, that is more than 10x faster than traditional methods while also being more accurate. [18]

Work continues to develop and apply new AI/ML methods. With recent funding from the DOE for Artificial Intelligence and Machine Learning at DOE Scientific User Facilities (see 1.7), the APS is collaborating on AI/ML tools for spectroscopy data analysis, a digital twin for in silico time-resolved experiments, high-energy diffraction microscopy data reduction, accelerator tuning and optimization, and sharing and cataloging ML models and data. See https://www.anl.gov/ai for a full list of AI/ML developments.

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1.7 Effort, Funding, and Collaborations

Effort

The majority of effort required under this strategy will be carried out by the core groups under the X-ray Science Technologies (XST) umbrella within the X-ray Science Division (XSD). The XSD Beamline Controls (BC) group is responsible for beamline data acquisition, through control and operations systems and software. The XSD Computational X-ray Science (CXS) group is mainly responsible for the development of theory, mathematical models, and algorithms and software for interpreting x-ray measurements. The XSD Scientific Software Engineering & Data Management (SDM) group is responsible for software engineering for data analysis applications and data management tools, enabling high-performance computing (HPC). Effort for the management and support of information technology resources within the APS is handled by the APS Engineering Support (AES) division Information Technology (IT) and Information Solutions (IS) groups. APS Operations funding supports most of the effort in these groups.

Funding

The APS-U project provides funding for networking infrastructure within the APS-U feature beamlines. Controls systems for the APS-U feature beamlines are also supported by the APS-U project. The APS-U project may provide funding for certain local computing resources at APS-U feature beamlines but the majority of resources and effort are outside of APS-U project scope.

One way Argonne National Laboratory supports computational efforts at the APS is via Laboratory Directed Research & Development Funding (LDRD) funding. Beginning in FY11, the *Tao of Fusion* LDRD helped seed the *TomoPy* application and the APS Data Management System; likewise, the FY13 *Next Generation Data Exploration: Intelligence in Data Analysis, Visualization and Mining* LDRD was aimed at multi-modal analysis. Other previously funded LDRDs include *Visualization and Mining, Modeling, Analysis, and Ultrafast Imaging (MAUI)*, *Multimodal Imaging of Materials for Energy Storage (MIMES)*, *Enabling Nanometer-scale X-ray Fluorescence Tomography*, and *Coherent Surface Scattering Imaging*.

Recently funded LDRDs of direct benefit to the APS in the computing space include:

- FY17 *Integrated Imaging*
- FY17 *A Universal Data Analytics Platform for Science*
- FY17 *COHED: Coherence for High-Energy Diffraction*
- FY17 *Developing Advanced Coherent Surface Scattering Reconstruction Method Incorporating Dynamical Scattering Theory*
- FY17 *Enabling Multidimensional X-ray Nano-Tomography*
- FY17 *The Perfect Thermodynamics of Imperfect Materials*

- FY18 *A.I. C.D.I.: Atomistically Informed Coherent Diffraction Imaging*
- FY18 *Integrated Approach to Unravel Four Dimensional Spatiotemporal Correlation in Highly Transient Phenomena: Ultrafast X-ray Imaging and High-Performance Computing*
- FY18 *Novel Capabilities for Ultra-fast and Ultra-low-dose 3D Scanning Hard X-ray Microscopy*
- FY19 *Enabling Automatic Learning of Atmospheric Particles through APS-U*
- FY19 *Finding Critical Processes of Deformation in Structural Materials with Artificial Intelligence*
- FY19 *Learning and Differentiating: Using Artificial Intelligence to Image Beyond the X-ray Depth of Focus Limit*
- FY19 *Machine Learning Enabled Advanced X-ray Spectroscopy in the APS-U Era*
- FY20 *Machine Learning Methods for Spectral Data from X-ray Transition Edge Sensor Arrays*
- FY20 *Tomographic Data Analysis Accelerated by Deep Learning*
- FY20 *Self-supervised deep learning for x-ray imaging without reference data*
- FY20 *Coded Apertures for Depth Resolved Diffraction*
- FY20 *Intelligent Ptychography Scan via Diffraction-Based Machine Learning*
- FY20 *AI-steer: AI-driven online steering of light source experiments*
- FY20 *AI patterns for executable end-to-end biological programming experiments*
- FY20 Innovate *High-Energy X-ray Diffraction and Machine Learning Driven Molecular Dynamics Simulation Study of Molten Chloride Salts*
- FY21 *AutoPtycho: Autonomous, Sparse-sampled Ptychographic Imaging*
- FY21 *Scalable DL-based 3D X-ray nanoscale imaging enabled by AI accelerators*
- FY21 ALCF Expedition *Scalable DL-based 3D X-ray Nanoscale Imaging Enabled by AI Accelerators*
- FY21 *High Pressure Material Characterization in 3-Dimensions Using X-Ray Diffraction Contrast Computed Tomography*
- FY22 *Intelligent Analysis of Scattering and Spectroscopic Signatures of Quantum Materials*
- FY22 *Development of 3D dichroic ptychography at the APS*
- FY22 *High Energy X-Ray Imaging for Non-Destructive and Rapid Nuclear Forensics*
- FY22 *Intermittent Dynamics in Hard and Soft Materials enabled by APS-U*
- FY 22 ALCF Expedition *Deep Learning Accelerated X-ray Data Analysis for Experiment Steering*
- FY 22 ALCF Expedition *Machine earning at the edge for real-time analysis in X-ray ptychography enabled by hardware AI accelerators*
- FY 22 ALCF Expedition *AI accelerator for scalable DL-based 3D X-ray nanoscale imaging*
- FY 22 ALCF Expedition *Exploring Groq as a Real-time AI Inference Accelerator for Scientific Instruments*
- FY 22 ALCF Expedition *Scalability Study of AI-based Surrogate for Ptychographic Image Reconstruction on Graphcore*
- FY23 *AI/ML accelerated high-performance image analysis using supercomputers*
- FY23 *Three-dimensional multiscale diffraction imaging of nanoscale defect kinetics during corrosion and mechanical deformation*
- FY23 *Developing Point-Focus High-Energy Diffraction Microscopy to Reveal Battery Material Degradation*

The APS has received funding and personnel support from the Argonne Leadership Computing Facility (ALCF) Data Sciences Program (ADSP):

- *Large-Scale Computing and Visualization on the Connectomes of the Brain*
- *Developing High-Fidelity Dynamic and Ultrafast X-ray Imaging Tools for APS-Upgrade*
- *X-ray Microscopy of Extended 3D Objects: Scaling Towards the Future, and Dynamic Compressed Sensing for Real-Time Tomographic Reconstruction*
- *Dynamic Compressed Sensing for Real-Time Tomographic Reconstruction*

The NERSC Exascale Science Applications Program supported the APS on the *Optimization of data-intensive tomography workflows at light sources* project.

The APS receives funding for AI/ML efforts in part from collaborative awards from the DOE for Artificial Intelligence and Machine Learning at DOE Scientific User Facilities**,** Lab 20-2261:

- *A Collaborative Machine Learning Platform for Scientific Discovery*, Principal Investigator (PI) - Alex Hexemer (Advanced Light Source, Lawrence Berkeley National Laboratory [LBNL]), Subramanian Sankaranarayanan (CNM-Argonne), Nicholas Schwarz (APS-Argonne)
- *A Digital Twin for In Silico Time-resolved Experiments*, PI - Subramanian Sankaranarayanan (CNM-Argonne), Maria Chan (CNM-Argonne), Mathew Cherukara (APS-Argonne), Pierre Darancet (CNM-Argonne), Ross Harder (APS-Argonne), Haidan Wen (APS-Argonne), Jianguo Wen (CNM-Argonne)
- *Actionable Information from Sensor to Data Center*, PI - Jana Thayer (Linac Coherent Light Source, SLAC National Accelerator Laboratory), Ian Foster, Zhengchun Liu (DSL-Argonne), Peter Kenesei, Antonino Miceli, Nicholas Schwarz (APS-Argonne)
- *Machine Learning for Autonomous Control of Accelerators*, PI - Daniel Ratner (SLAC National Accelerator Laboratory), Xiaobiao Huang (APS-Argonne)
- *Integrated Platform for Multimodal Data Capture, Exploration and Discovery Driven by AI Tools*, PI - Eli Stavitski (National Synchrotron Light Source-II, Brookhaven National Laboratory) Chengjun Sun, Steve Heald, Nicholas Schwarz (APS-Argonne) Maria Chan (CNM-Argonne)

Additionally, the APS receives funding from other DOE awards:

- *Randomized algorithms for optimal data acquisition in Bayesian inverse Problems*, PI - Youseff Marzouk (MIT), Zichao Wendy Di (MCS/XSD-Argonne)
- *Privacy-Preserving Federated Learning on Multimodal Data*, PI - Kibaek Kim (ANL/MCS), Zichao Wendy Di (MCS/XSD-Argonne)

Collaborations

Collaborations play a key role in the computing strategy for the APS. The APS actively collaborates with other facilities and organizations, and members of the APS User community to develop data analysis algorithms and software. As examples, most Argonne-funded LDRDs in this area involve collaborators from Argonne's Mathematics and Computer Science Division, Computational Science Division, or Data Science and Learning Division. Select APS User groups have contributed greatly to analysis algorithms and software.

The Center for Advanced Mathematics for Energy Research Applications (CAMERA) at Lawrence Berkeley National Laboratory aids in the development of software, modeling, and mathematics. For example, CAMERA helped develop GISAXS algorithms and tools, and the *SHARP* ptychographic reconstruction package. Most recently CAMERA has been involved in the development of the *XPCS-Eigen* correlation application for XPCS and in the application of the Multi-Tiered Iterative Phasing (M-TIP) algorithm for the reconstruction of Coherent Surface Scattering Imaging (CSSI) data. APS staff and researchers participate regularly in annual workshops for tomography, ptychography, and XPCS organized by CAMERA.

Innovative APS applications, improved Globus-based data management and transfer capabilities, and the Gladier software has benefited, and continues to benefit, from ASCR support to Argonne research projects, such as RAMSES: Robust Analytical Models for Science at Extreme Scales and Braid: Data Flow Automation for Scalable and FAIR Science. Effort for CDI ptychography was initially funded by ASCR and now via the Intelligence Advanced Research Projects Activity (IARPA) and Northwestern University. Early efforts for the *MIDAS* software for High-Energy Diffraction Microscopy (HEDM) data processing were funded by APS industrial partners. The APS and the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL) have developed a comprehensive computing collaboration plan so as to best utilize our scare resources, especially related to expanding *bluesky* use at the APS. Work on support for multi- and distributed-GPU N-dimensional complex FFTs is supported by NVIDIA and the Argonne Leadership Computing Facility (ALCF).

The APS has been involved in the NOBUGS conference community and maintains active participation in the series of hack-a-thons organized by the Experimental Facilities Computing (ExFaC) Working Group.

Researchers at the APS and Argonne's Data Science and Learning Division co-organize the annual Workshops on Large-scale Experiment-in-the-Loop Computing (XLOOP) at SC. This workshop focuses on the intersection of large-scale experimental science from user facilities, such as the APS, with high-performance computing. A peer review process led by the workshop's program committee selects manuscripts for presentation. Accepted manuscripts are published by the IEEE Computer Society Technical Consortium on High Performance Computing (TCHPC). The program committee selects the recipient of the best paper award, and the workshop attendees selects the recipient of the best presentation award. The novel work presented during at this workshop will help the APS develop solutions critical to handling massive amounts of data generated during the APS-U era.

APS and Argonne scientists co-chair and serve on the program committees of conferences that cover a wide range of large-scale imaging and data science problems relevant to the APS, including, the Parallel and Distributed Algorithms for Data Science track at the IEEE International Parallel and Distributed Processing Symposium (IPDPS'23), IEEE Conference on Image Processing (ICIP), IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), Computational Imaging (COIMG), Machine Learning for Scientific Imaging (MLSI), High Performance Computing for Imaging (HPCI'22) at Electronic Imaging, and the Denver X-ray Conference (DXC). Additionally, APS and Argonne scientists have organized AI/ML workshops and symposia at the annual Materials Science and Technology (MS&T) meeting, the International Materials Research Congress (IMRC) meeting, The Minerals, Metals and Materials (TMS) annual meeting, and meetings of the American Crystallographic Association (ACA).

The APS and the computing divisions within Argonne's Computing, Environment, and Life Sciences (CELS) directorate hosted a series of town hall meetings in December 2020. Over 150 attendees participated from across Argonne. The goal is to develop a common vision for the future of APS computing within Argonne. Breakout sessions focused on new algorithm, math, and AI/ML, scalable software tools, workflow and orchestration, computing architecture, sustainable and discoverable data repositories, and networking.

The X-ray Science Division has organized the APS Scientific Computation Seminar Series since 2015. This seminar series focuses on scientific computation for APS experiments. The series focuses on advanced software and computing infrastructure for analysis, reduction, reconstruction, and simulation. It provides an opportunity to learn about state-of-the-art computational techniques and tools and how they are being applied to science at the APS.

In 2017, the directors of the 5 BES funded light sources chartered the Light Source Data & Computing Steering Committee (previously the Data Working Group). The role of the committee is to develop and maintain, with input from the directors of the BES light sources, a strategic plan in computing and data. This is defined to include data acquisition, analysis, visualization and management, and the associated hardware and software infrastructure. The committee also advises and assists the directors in the coordination and execution of work in this area, consistent with that strategic plan, and is responsible for reporting and responding to charges, achieving consensus on paths forward, coordinating proposal submissions, and tracking funded activities.

The Light Source Data & Computing Steering Committee has developed a common vision for computing across the light sources, the Distributed Infrastructure for Scientific Computing for User Science (DISCUS), and a decade long roadmap to achieve the vision. This vision proposes a transformative computational fabric that covers the full lifecycle of data generated at the BES Light Sources to accelerate discovery and insight. See Figure 1-14.

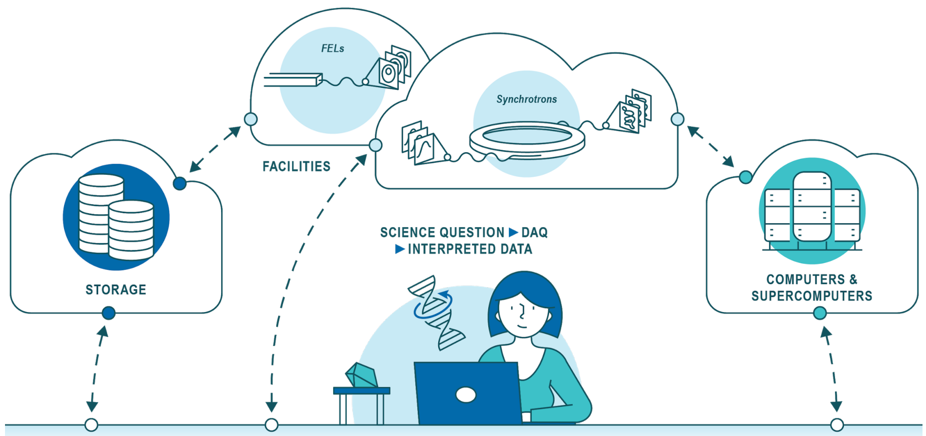


Figure 1-14 The Distributed Infrastructure for Scientific Computing for User Science (DISCUS) vision for computing at the light sources.

In 2019, the directors of the five BES funded light sources and the directors of the 4 ASCR computing and networking facilities charted the BES Light Source and ASCR Computing Facilities Directors' Data Working Group tasked with identifying how the ASCR facilities can help meet the needs of the BES facilities regarding data and computing. Membership is from the US DOE light sources and the US DOE supercomputing and networking facilities, and observers from the US neutron sources and Nano Science Research Centers (NSRCs) (ALS, APS, LCLS, MF, NSLS-II, SNS, SSRL, ALCF, ESnet, NERSC, and OLCF). The working group has formulated a plan for the desired data management architecture across the facilities, identified gaps in current planning, suggested a balance of responsibilities among the facilities, suggested next steps, and has undertaken pilot activities to utilize ASCR computing and networking facilities for processing and storing light source data. See Figure 1-15.

Figure 1-15 The BES-ASCR Facilities Information Exchange held at Lawrence Berkeley National Laboratory on June 12, 2019 established a working group across the BES light sources and the ASCR facilities.

The BES Data Solutions Task Force Pilot Project (see Figure 1-16) is a 2-year pilot project to develop common software for data acquisition, management, and analysis across the five BES light sources (ALS, APS, LCLS, NSLS-II, SSRL). The project aims at creating a synergistic approach to software where the five light sources work as a team to deliver common solutions across the facilities. This is being achieved by leveraging tools and expertise from all the BES light sources and integrating complementary components, including *bluesky* from NSLS-II, *Xi-Cam* from CAMERA and ALS, and *XPCS-Eigen* and *TomoPy*, high-performance data processing software, from the APS. The project is focusing on X-ray Photon Correlation

Spectroscopy (XPCS), ptychography, and tomography beamlines across the facilities. At the APS, *bluesky* and *Xi-Cam* were successfully deployed at the 8-ID XPCS beamline.

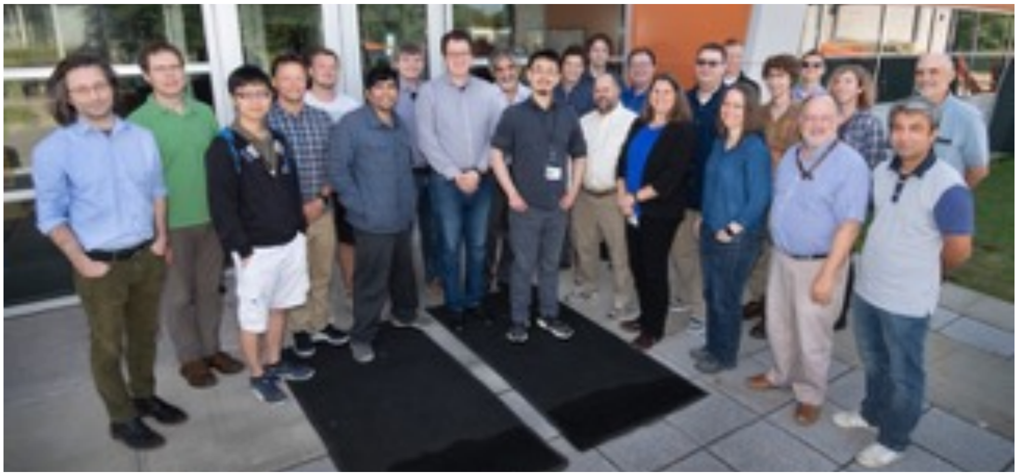


Figure 1-16 BES Data Solutions Task Force Pilot Project kick-off meeting held August 8-9, 2019 at NSLS-II/BNL.

Beginning in 2021, members of the APS and the other five BES light sources have participated in the DOE SC Integrated Research Infrastructure Architecture Blueprint Activity (IRI ABA). This activity aims to produce the reference conceptual foundations to inform a coordinated whole-of-SC strategy for an integrative research ecosystem. The overarching motivation is to achieve a more seamlessly composable, interoperable, and extensible ecosystem of SC experimental and observational user facilities with SC advanced computing, data, and networking infrastructure. This ecosystem approach is critical to accomplishing many envisaged SC, DOE, and national R&D priorities such as AI for Science, Advanced Computing Ecosystem, National AI Research Resource, Future of Advanced Computing Ecosystem, Earthshots, and other initiatives and priorities. Participants worked to gather insight from across SC programs and design cross-cutting blueprints addressing SC needs.

Most recently, APS scientists have begun collaborating with Diamond Light Source on software for tomography reconstructions and AI/ML applications.

2 APS-U Feature Beamlines

Table 2-1 Summary of APS-U feature beamlines.

Feature Beamline	Synopsis
ATOMIC	Uses the enhanced coherence of the APS-U x-ray beam for high-resolution studies of the structural, chemical, and physical properties exhibited by advanced functional materials by acquiring atomistic structural information across many length scales in full three-dimensional detail.
Coherent High-Energy X-rays (CHEX)	Use coherent x-ray techniques to advance the frontier for in situ, real-time studies of advanced materials synthesis and chemical transformations in natural operating environments, employing condensed-matter physics and environmental science.
Coherent Surface-Scattering Imaging (CSSI)	Combines a surface X-ray probe using novel coherent scattering methods with state-of-the-art X-ray optics and detectors to study a range of materials surface and interface phenomena.
High-Energy X-ray Microscope (HEXM)	Investigates structure and evolution within bulk materials, often in extreme environments, with the established high-energy X-ray scattering techniques and novel coherence-based techniques enabled by APS-U.
In Situ Nanoprobe (ISN)	An x-ray nanoprobe designed to have a relatively large optical working distance enabling investigation of complex functional materials and materials systems such as catalysts, batteries, photovoltaic systems, and nanoscale Earth and environmental samples, during synthesis, operation, and under actual environmental conditions.
Polarization Modulation Spectroscopy (Polar)	Generates photon beams with highly tunable and modulated polarization states for imaging electronic and magnetic inhomogeneity in quantum materials with ~ 50 nm resolution as well as discovery of novel electronic states of matter at extreme pressure conditions (P < 7 Mbar).
PtychoProbe	Realizes the highest possible spatial-resolution X-ray microscopy both for structural and chemical information, with the goals of focusing an X-ray beam to a 5-nanometer spot and ultra-fast scanning of the beam across the sample being studied.
X-ray Photon Correlation Spectroscopy	Advances studies in physics and materials science and engineering including dynamic heterogeneity, structural dynamics in super-cooled liquids, and fluctuations associated with competing mesoscale interactions in emergent materials.
3D Micro and Nano (3DMN) Diffraction	Addresses a wide range of problems in materials science, physics, and geoscience by providing small, intense X-ray spots (between 50 and 200 nanometers) to investigate spatial variations and correlations of strain and structure that define a wide range of scientifically and technologically important materials.

2.1 ATOMIC APS-U Feature Beamline

2.1.1 Summary

The ATOMIC APS-U feature beamline will be dedicated to coherent x-ray diffraction imaging experiments for a diverse scientific community; experiments will exploit the brilliance of the upgraded source to study fundamental materials structures.

In the APS-U era, the ATOMIC APS-U feature beamline will perform Bragg CDI acquisitions in two modes: fast and high-resolution. Table 2-2 shows estimated data generation rates at the ATOMIC APS-U feature beamline, and current data rates at the 34-ID-C instrument, for comparison. The ATOMIC APS-U feature beamline is anticipated to collect approximately 250 to 300 TB of raw data per year, in comparison to approximately 0.65 TB of data collected today at the 34-ID-C Bragg CDI instrument. This represents a nearly 400x increase in data. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-2 Data generation rates today at the 34-ID-C Bragg CDI instrument (for comparison) and estimated data generation rates at the ATOMIC APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Written Frame Rate (Hz)	Written Data Rate (MB/s)*	Daily Utilization (%)**	Data Set Size (MB)+	Data Per Day (GB)**	Annual Utilization (%)++	Data Per Year (TB)++

Today	Bragg CDI	ASI Si Timepix, ASI GaAs Timepix+++	0.25	0.2	0.05	80	60	3.38	90	0.65
APS-U Era++++	Fast Bragg CDI	TBD	1.00	20.0	20.00	80	500	1,350.00	80	220
	High-Resolution CDI	TBD	61.22	0.2	12.24	80	> 6,000	826.47	20	35

* The collection rate is high, but the frames are combined and written at a lower rate.
** Based on 1,440 minutes in one day.
+ The data set sizes are approximate and representative of typical experiments, as this value varies.
++ Based on 210 days of beam time per fiscal year.
+++ The number of pixels for ASI Si Timepix is 65,536 and ASI GaAs Timepix is 262,144, however the frame size is typically cropped.
++++ The APS-U project has descoped certain parts of the ATOMIC Feature beamline, including detector purchases. Although the detectors listed in the table may not be purchased as a part of the APS-U project, this table represents the desired long-term potential capabilities intended for this beamline.

2.1.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.1.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.1.4 Data Management, Workflows, and Science Portals

The APS-U ATOMIC feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the ATOMIC APS-U feature beamline, workflows will provide a pipeline to automatically run tools to remove artifacts from data, reconstruct Bragg CDI data set, and view results.

2.1.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.1.6 Data Reduction and Analysis

The preliminary step is finding diffraction peaks from a crystal sample. This is accomplished by using the micro-diffraction technique and analyzing the captured data with the *LaueGo* software package. The data collected during this phase is only used to find the coordinates to guide the sample stage during data acquisition and is not retained.

The APS develops and supports the *cohere* software package for Bragg CDI data. The software is available as an open-source package (https://github.com/AdvancedPhotonSource/cohere). The package performs routine data correction, formatting, reconstruction, and visualization for Bragg CDI data. *cohere* currently implements conventional phase retrieval algorithms. It is written in Python and uses the ArrayFire package for data processing on CPUs and GPUs. Work is underway to add additional backend library choices so that ArrayFire can be replaced with CuPy or NumPy for easier distribution and deployment at computing centers.

The current feature set and performance of *cohere* is adequate for most of today's needs. However, the estimated approximate 400-fold increase in overall data that will be generated at the ATOMIC APS-U feature beamline, and the increase in size of individual datasets necessitates improvements and advances in software and algorithms.

The APS is currently developing higher-performance implementations of conventional phase retrieval algorithms and exploring novel AI/ML methods that may replace computationally complex phase retrieval methods. Table 2-3summarizes Bragg CDI data reduction needs, approaches, and status for the ATOMIC APS-U feature beamline.

AutoPhaseNN - Unsupervised Physics-aware Deep Learning of 3D Nanoscale Bragg Coherent Diffraction Imaging: A neural network that uses known physics and learns to invert 3D Bragg CDI data completely unsupervised, i.e., without ever being shown sample images during training, that is more than 10x faster than traditional methods, enabling real-time analysis, while also being more accurate. AutoPhaseNN has been integrated in to *cohere*, providing users the option of starting phase retrieval from an initial guess provided by AutoPhaseNN (see Figure 2-1).

The APS is optimizing implementations of conventional phase retrieval algorithms in *cohere* for better performance. In order to process data quickly in the APS-U era using conventional phase retrieval approaches, the APS is developing distributed-memory CPU and multi-GPU implementations of presently utilized algorithm. N-dimensional complex FFTs are at the core of conventional phase retrieval (and many ML) algorithms. The anticipated size of high-resolution Bragg CDI datasets and intermediate results will be too large to fit in the memory of a single GPU. The APS is working with the Argonne Leadership Computing Facility (ALCF) and a team at NVIDIA to realize better, optimized multi- and distributed-GPU support for N-dimensional complex FFTs.

Argonne researchers are exploring the use of AI and Automatic Differentiation (AD) as a high-performance alternative to conventional phase retrieval algorithms for Bragg CDI. This new workflow leverages a library of pre-computed, large-scale Molecular Dynamics (MD) simulations to provide on-the-fly, best guess structure to measured diffraction data through a trained deep convolutional neural network. Predictions are displayed in real-time at the instrument and are also used as the initial guess for iterative refinement through AD. This two-step approach will enable real-time feedback to an experiment and provide the highest possible fidelity in image reconstruction. A recently funded ALCF Expedition LDRD is focusing on using AI accelerators, such as SambaNova for Bragg CDI calculations.

Table 2-3 Summary of Bragg CDI data reduction needs, approaches, and status for the ATOMIC APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
Conventional Phase Retrieval Reconstructions	CPU and GPU software for Bragg CDI reconstructions	Done – APS Operations
Faster Conventional Phase Retrieval Reconstructions	Scalable distributed-memory CPU and GPU implementation of conventional phase retrieval algorithms	In Progress – APS Operations
High-Resolution Conventional Phase Retrieval Reconstructions	Support for multi- and distributed-GPU N-dimensional complex FFTs	In Progress – APS Operations working with the Argonne Leadership Computing Facility (ALCF) and NVIDIA
AI / Automatic Differentiation (AD) Methods	A deep learning (DL) approach to structure and strain prediction from raw X-ray diffraction data without the use of phase retrieval algorithms	Demonstrated at low resolution – LDRD
	A CNN training set generator and a trained CNN for the study of metals; this can grow to other advanced materials without changes to the underlying workflow	Demonstrated – LDRD
	Physics based image generation workflow installed at the CDI instrument to analyze coherent diffraction data in real-time	In Progress – LDRD
	Network optimization and combining deep learning with automatic differentiation to enable highest possible image reconstruction accuracy	Demonstrated – LDRD
	Scale to TB dataset sizes	To do – APS Operations

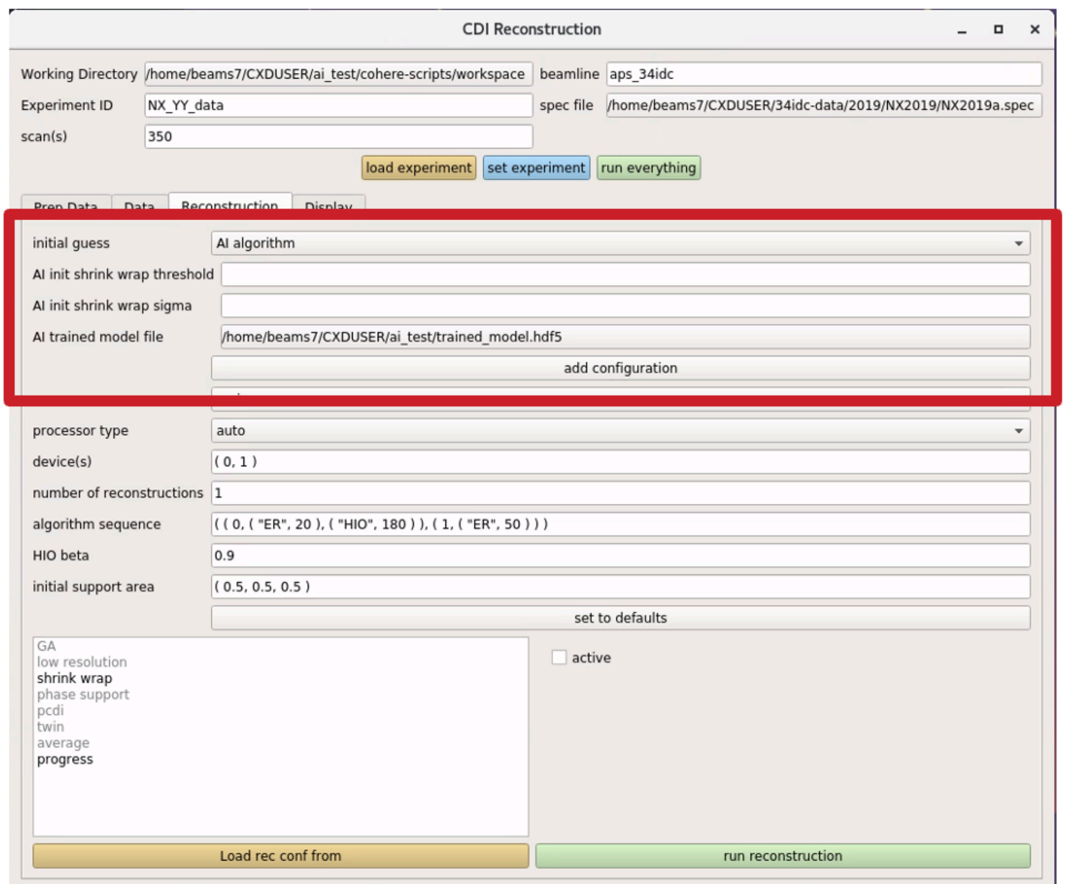
2.1.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the ATOMIC APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the ATOMIC APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1 FTE per year for Bragg CDI software development from APS Operations funding.

Work on support for multi- and distributed-GPU N-dimensional complex FFTs is supported by NVIDIA and the Argonne Leadership Computing Facility (ALCF).

The following LDRD funding was awarded to support these efforts:

- *A.I. C.D.I.: Atomistically Informed Coherent Diffraction Imaging* (FY18)
- *Finding Critical Processes of Deformation in Structural Materials with Artificial Intelligence* (FY19)
- *Scalable DL-based 3D X-ray Nanoscale Imaging Enabled by AI Accelerators* (ALCF Expedition LDRD - FY21)



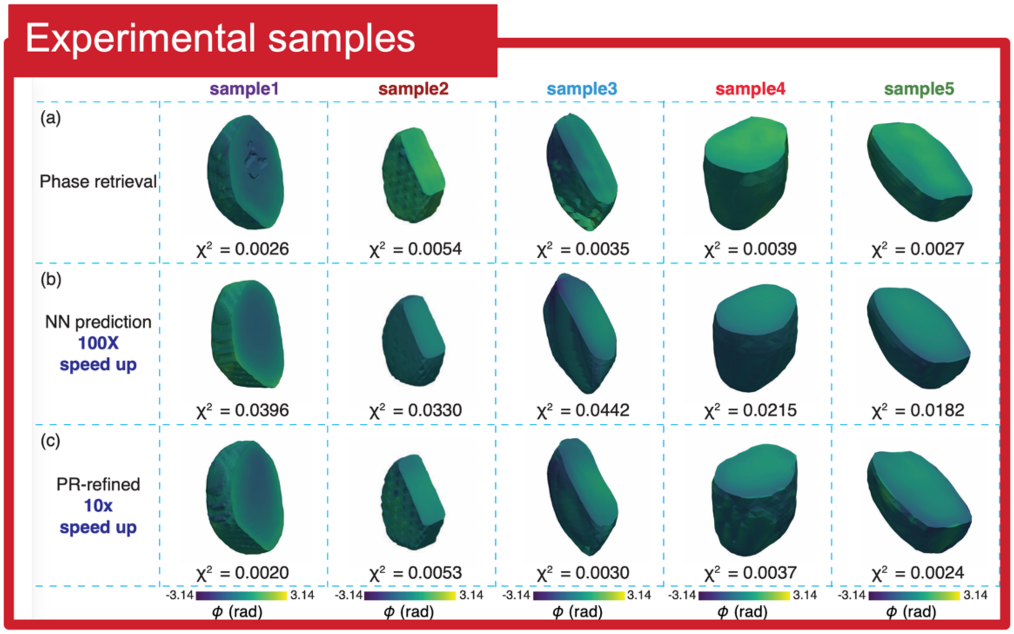


Figure 2-1 AutoPhaseNN within cohere - AutoPhaseNN provides an initial guess for iterative phase retrieval run through cohere. Results are obtained faster and are more accurate than conventional iterative phase retrieval methods.

2.2 Coherent High-Energy X-rays (CHEX) APS-U Feature Beamline

2.2.1 Summary

The Coherent High Energy X-rays (CHEX) APS-U feature sector will advance the frontier for in situ, real time studies of materials synthesis and chemical transformations in natural operating environments, using the unprecedented coherence of the high energy X-ray beams that will be provided by the upgrade. State-of-the-art experimental techniques that will be used, include, but are not limited to, Bragg coherent diffraction imaging (BCDI), Bragg ptychography, coherent Bragg rod analysis (COBRA), dark field X-ray microscopy (DFXM), and X-ray photon correlation spectroscopy (XPCS). These approaches will be used to provide transformative insight into materials structure, heterogeneity and disorder, chemical and long-range interactions, atomic-level dynamics, and structural, chemical, and morphological evolution under challenging environmental conditions and a wide range of time frames.

When fully built out, the CHEX sector will consist of four branch lines, with each line having two experimental stations. Two canted undulators will be used to operate one of the branches at tunable energies from 5-60 keV, while the other three branch lines will operate at fixed selectable energies of 15, 25, or 35 keV (D/E and F hutches) or 45, 75, or 105 keV (G hutch). The multiplexed nature of the design will allow up to four separate experiments to be performed simultaneously (one per branch line). The in-situ studies that will be performed at these stations are often data-intensive, due to desired frequent periodic monitoring of processes over long times, e.g., millisecond resolution over seconds, or second resolution over thousands of seconds. The current plans are to primarily use pixel array detectors with small (55-75 μm) pixel sizes, e.g., Lambda 750K or Eiger 1M. Under these conditions, a preliminary conservative estimate is that on the order of 1.5 TB of data can be generated per 24 hours of operation. As faster detectors with smaller pixel sizes become available, this data generation rate will increase correspondingly.

2.2.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2

2.2.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.2.4 Data Management, Workflows, and Science Portals

The CHEX APS-U feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the CHEX APS-U feature beamline, workflows will provide a pipeline to automatically run data processing software for preliminary analysis of coherent imaging and XPCS data, with a goal of providing near-real-time feedback useful in planning and modifying experiments.

2.2.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.2.6 Data Reduction and Analysis

The experimental techniques that will be used at CHEX, include, but are not limited to, Bragg coherent diffraction imaging (BCDI), Bragg ptychography, coherent Bragg rod analysis (COBRA), dark field X-ray microscopy (DFXM), and X-ray photon correlation spectroscopy (XPCS). Since it is anticipated that there will be at least an order-of-magnitude increase in data rates and volumes at the APS over the next decade, combined with continual rapid developments in these coherent imaging and spectroscopy, there is a great need for there to be a concomitant emphasis on the development of advanced data analysis approaches that will enable realization of the full potential of the CHEX beamlines to elucidate materials behavior. APS is currently devoting significant effort to developing data analysis packages relevant to experimental techniques of interest to the CHEX sector. For example:

- The *cohere* software package is being developed to provide tools for reconstruction of images from data obtained using Bragg Coherent Diffraction Imaging techniques
- The *MIDAS* software package is being developed to enable users to non-destructively image the microstructure of crystalline materials in 3D
- Development of the *tike* toolbox is enabling tomographic reconstruction of 3D objects from ptychography data

Implementations of the above software packages will be of great value to CHEX users. It is anticipated, however, that many planned experiments at CHEX will have specific, unique data analysis requirements that will require significant refinements/extensions of the above-mentioned packages and/or developments of new analysis approaches. Experiments with these unique needs will form the foundation of many of the initial science campaigns at CHEX and will serve as a backbone for future science at CHEX. For example, several planned early experiments at CHEX will have specific data analysis needs that due to unique experimental requirements at CHEX that require additional algorithm and software development, including:

- High-energy BCDI capabilities for imaging experiments via phase retrieval with high-energy coherent focused beams, possibly implemented in *cohere* or *MIDAS*

- High-q pixel mapping and two-time and higher-order correlation function incorporation into XPCS analysis packages requires significant new development, especially for experiments planned at CHEX that will target very weakly scattering surface-sensitive regions of q-space
- Support, in *tike*, for example, for ptychography in the Bragg geometry, and optimization for studies of the epitaxial films of interest to thin film synthesis programs that are planned at CHEX
- Software for COBRA and DFXM analyses are required as both of these techniques are anticipated to be employed in key roles in planned in-situ synthesis and materials processing experiments at CHEX.

2.2.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the CHEX APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the CHEX APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5.

To accelerate progress in the development of the advanced data analysis tools to support state-of-the-art science at CHEX, a joint scientific staff appointment between the APS and MSD has been proposed, requesting 50% funding by APS Operations funds. Through this collaboration, a co-located staff member will both adopt the computational data science approaches of currently supported APS software packages to meet the specific needs of a broad range of CHEX users and be involved in the planning and execution of pioneering coherent imaging and XPCS materials science experiments at CHEX that will be carried out by the MSD Synchrotron Studies of Materials Group. Creation of this joint appointment will ensure a healthy data analysis ecosystem at CHEX and will simultaneously improve the breadth and impact of the suite of ongoing software package design by addressing and eliminating current key blind spots in software packages used for analysis of BCDI, XPCS, Bragg geometry ptychography, COBRA, and DFXM data.

2.3 Coherent Surface-Scattering Imaging (CSSI) APS-U Feature Beamline

2.3.1 Summary

The Coherent Surface-Scattering Imaging (CSSI) APS-U feature beamline will take advantage of the MBA lattice's dramatically improved x-ray beam coherence for probing and understanding mesoscopic structures and dynamics at surfaces and interfaces.

In the APS-U era, the CSSI APS-U feature beamline will employ two primary operation modes: Coherent Surface Scattering Imaging (CSSI) and Grazing-Incidence X-ray Scattering (GIXS). The latter includes Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS), GIWAXS with XPCS, Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), and GISAXS with XPCS. In addition, to characterize fast kinetics across a broad range of length scales, a fast data acquisition mode will be provided where both GIWAXS and GISAXS detectors are operated at high frame rates for short periods. Table 2-4 shows estimated data generation rates at the CSSI APS-U feature beamline. The CSSI APS-U feature beamline is anticipated to collect approximately 17 PB raw data per year. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-4 Estimated data generation rates at the CSSI APS-U feature beamline.

	Technique	**Detector**	**Frame Size (MB)**	**Frames Per Dataset**	**Compression Factor***	**Compressed Dataset Size (GB)**	**Daily Utilization (%)****	**Data Per Day (TB)****	**Annual Utilization (%)*****	**Data Per Year (PB)*****
	GIWAXS+	Eiger 9M	33.750	40	1	1.3	13	3.5	38	0.27

APS-U Era	GIWAXS-XPCS+	Eiger 9M	33.750	120,000	10	197.8	25	69.5		5.42
	GISAXS+	Eiger 16M	61.035	40	1	2.4	13	6.3		0.49
	GISAXS-XPCS+	Eiger 16M (4M XPCS mode)	15.26	135,000	10	201.2	25	70.7		5.51
	Fast GIXS ++	Eiger 9M	33.750	30,000	1	988.8	14	38.9	8	0.64
		Eiger 16M	61.035	30,000	1	1788.1	14	70.4		1.16
	CSSI+++	Eiger 16M	61.035	60,000	10	357.6	80	40.2	46	3.80

* A compression factor of 1.0 represents no compression.
** Based on 1,440 minutes in one day. Routine GIXS: 2 min data out of 20 min/sample = 10%. Spin GIXS: 5 min data out of 40 min/sample = 12/5%.
*** Based on 210 days of beam time per fiscal year.
+ GIXS: Static simultaneous GIWAXS and GISAXS for 1 dataset, followed by 1 dataset simultaneous GIWAXS/GISAXS surface XPCS, assuming 5 min alignment.
++ Fast GIXS: Simultaneous GIWAXS/GISAXS for 5 minutes, assuming 30 minutes required to set up sample.
+++ CSSI: 20% of each day required for alignment and sample motions during scan.

2.3.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2

2.3.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.3.4 Data Management, Workflows, and Science Portals

The APS-U CSSI feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended.

All operation modes of the APS-U CSSI feature beamline will generate data at high rates. The APS Data Management System will coordinate data transfer, data backup, preprocessing, and analysis, and provide visualization of analysis results to users.

2.3.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources may be provided for on-the-fly data processing and experiment steering. The anticipated high data rate and large data volume generated by the CSSI beamline makes processing data likely beyond the capability of local workstations. Computing capacity for these data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). To develop performant codes suitable for ALCF, a local workstation with four GPUs has been commissioned as a test bed. The APS Data Management System and Globus tools will be used to integrate these resources.

2.3.6 Data Reduction and Analysis

Coherent Surface-Scattering Imaging (CSSI) Data Processing

CSSI is a coherent imaging technique for creating quantitative 3D high resolution images of surface and interface structures. The method combines ideas from scanning coherent diffractive imaging (ptychography) and computed laminography to create very large diffraction datasets. The process here is done in two steps: the datasets for each laminographic rotation angle must fed into ptychographic reconstruction algorithms to create various 2D projection images of the overall 3D sample structure. These 2D projection images will then be combined in a computed laminography algorithm to synthesize the final 3D sample image.

Conventional transmission-based ptychography and laminography algorithms for data inversion must be modified to account for CSSI's geometry and the multiple-scattering effects that are significant at low incidence angles. One particular laminography challenge here is due to the very shallow incident angle encountered in CSSI, the "missing cone" problem can be quite severe. Novel variations of iterative constrained laminography must be developed using multiple GPUs due to the large 3D sample arrays used in CSSI (which are too large for a single GPU to contain). Additionally, we can also vary the incident angle and perform further laminography data collection, but this obviously further greatly increases the data volume that must be computationally processed.

For the ptychography step, one must fundamentally change the forward model to account for non-kinematical scattering. Recent investigations have determined that a multislice Fresnel propagation approach is the most accurate model here. One challenge encountered with attempting to simply extend existing ptychography inversion algorithms like rPIE is that the number of slices in the multislice approach cannot be too large otherwise multiplicative error propagation becomes too dominant. We can somewhat "ignore" the multiple-scattering effects with careful selection of appropriate regions of the diffraction measurements, but this ultimately amounts to only reconstructing lower resolution 2D projection images; to achieve the best possible spatial resolution other ptychographic multislice methods are necessary.

Another option here is to move beyond this "two-step" ptychography-laminography process and combine both into a single unified "one-step" 3D ptychographic phase retrieval problem. In this way, the Fresnel multislice model (which inherently represents a complex valued probing wavefield interacting with and propagating through a 3D sample volume) will be used in a 3D ptychography algorithm where the laminographic rotation is treated as a type of "rotational" diversity which is used as a constraint alongside the usual 2D translational diversity. The mathematics of the numerical nonlinear optimization problem have already been established and demonstrated on small dimensionality problems to establish proof of principle; the work that must be done here is to scale this algorithm up for realistic CSSI problem sizes for computation on multiple GPUs.

Additionally, a Multi-Tiered Iterative Phasing (M-TIP) approach to decompose the larger problem into smaller solvable parts is being developed in collaboration with CAMERA.

GIXS and GIXS-XPCS Data Processing

Today, GIXS data analysis is performed with the APS developed and supported MATLAB package, GIXSGUI, and the CAMERA developed Python-based package, Xi-CAM, for long sequences of time-resolved measurements. The integration of GIXSGUI with the APS Data Management System to automate data reduction and analysis at the 8-ID-E beamline is underway. High-performance algorithms for near real-time GIXS data processing will be implemented.

At CSSI, the data production rate will be many orders-of-magnitude higher. Multiple-detector collection modes will be routine, adding further complexity for data processing. These challenges necessitate large volume and multiple-dimension real-time data visualization. The APS Data Management System will accommodate increased data volumes. Work will be undertaken to replace the current MATLAB-based tools with a new higher-performance and scalable Python-based toolkit. Thin-film structure peak indexing capabilities will also be improved.

For XPCS data reduction and analysis, CSSI will leverage the resources and tools available and being developed for the XPCS beamline.

Table 2-5 Summary CSSI APS-U feature beamline data reduction and processing capabilities and needs.

Capability	Algorithm / Software Requirement	Status
Data Visualization and Preprocessing	Single image	Done – *GIXSGUI* – APS Operations
	Multiple images	Done – *Xi-Cam* – CAMERA
	Support for scattering vector q	To do – APS Operations
	New Python-based software package	To do – APS Operations
	Near real-time processing	To do – APS Operations
Thin-film Structure Indexing	Basic implementation of space groups and indexing	Done – APS Operations developed *GIXSGUI,* CAMERA developed *Xi-Cam,* and SSRL developed a thin-film structural indexing package *SIIRkit*.

	New scalable Python-based software package that integrates surface scattering (Distorted Wave Born Approximation)	To do – APS Operations
Coherent Surface Scattering Imaging (CSSI)	Image reconstruction algorithms	Done – APS Operations & DOE Early Career Award developed an algorithm to reconstruct CSSI ptychography data
		In Progress – CAMERA is developing an M-TIP based CSSI reconstruction algorithm
	Scalable CPU and GPU software	In Progress – APS Operations & DOE Early Career Award is developing a multi-GPU CSSI ptychography reconstruction software package
Surface XPCS	XPCS correlation algorithms and software	In Progress – APS Operations work is underway as part of effort for the XPCS APS-U feature beamline

2.3.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the CSSI APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the CSSI APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1.5 FTE per year for CSSI related algorithm and software development from APS Operations funding.

CAMERA provides effort in support of CSSI algorithm development.

The following awards support these efforts:

- *Unraveling Mesoscale Spatial-temporal Correlations in Materials Using Coherent X-ray Probes* (FY15 LDRD)
- *Developing Advanced Coherent Surface Scattering Reconstruction Method Incorporating Dynamical Scattering Theory* (FY17 LDRD)
- *Development of Coherent Surface Scattering Imaging with Nanometer Resolution for Revealing 3D Mesoscaled Structures* (DOE Early Career Award)

2.4 High-Energy X-ray Microscope (HEXM) APS-U Feature Beamline

2.4.1 Summary

The High-Energy X-ray Microscope (HEXM) APS-U feature beamline is designed to investigate structure and evolution within bulk materials, often in extreme environments, with established high-energy x-ray scattering techniques and novel coherence-based techniques enabled by the APS-U.

Table 2-6 shows estimated data generation rates at the HEXM APS-U feature beamline. The HEXM instrument will perform near- and far-field, diffraction tomography, and imaging tomography measurements. The HEXM APS-U feature beamline is anticipated to collect approximately 20 PB of raw data per year and 5 PB of compressed raw data per year in comparison to approximately 4 PB of raw data and approximately 1 PB of compressed raw data collected today at the 1-ID High-Energy Diffraction Microscopy (HEDM) instrument. Both uncompressed and compressed data sizes are given because uncompressed data is often required for data processing. This represents an approximately 4x increase in data. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-6 Data generation rates today at the 1-ID High-Energy Diffraction Microscopy (HEDM) instrument (for comparison) and estimated data generation rates at the HEXM APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Average Frame Rate (Hz)	Peak Data Rate (MB/s)	Raw Data set Size (GB)	Compression Factor *	Daily Utilization (%)**	Raw Data Per Day (TB)**	Compressed Raw Data Per Day (TB)**	Annual Utilization (%)***	Raw Data Per Year (TB)***	Compressed Raw Data Per Year (TB)***
Today	Near-Field	Qimaging Retiga 4000DC (4MP, CCD, 12-bit)	8	3.3	26	11	4	54	1	0.25	25	62	15
	Far-Field	Varex 4343CT (8MP, 14-16-bit)	16	15	237	22	4	63	12	3	25	647	162
	Far-Field	GE RT41 (4MP, 14-bit)	8	7	56	11	2	63	3	1.5	25	153	76
	Far-Field	Hydra 4x GE RT41 (16MP, 14-bit)	32	7	224	45	2	63	12	6	15	366	183
	Far-Field	Pilatus 2M CdTe (20-bit)	7	250	1,771	10	4	63	92	23	15	2,896	724
	Diffraction Tomography	GE RT41 (4MP, 14-bit)	8	2	16	281	2	72	1	0.5	5	10	5
	Diffraction Tomography	Hydra 4x GE RT41 (16MP, 14-bit)	32	2	64	1,125	2	72	4	2	5	40	20
	Diffraction Tomography	GE RT41 (4MP, 14-bit)	8	7	56	2,250	2	72	3	1.66	5	35	17
	Diffraction Tomography	Hydra 4x GE RT41 (16MP, 14-bit)	32	7	224	9,000	2	72	13	6.5	5	140	70
	Imaging Tomography	PointGrey CMOS (2.3MP, 12-bit)	4	5	22	15	1	54	1	1	20	41	41
APS-U Era	Near-Field	FLIR Oryx (5MP, 12-bit)	10	40	383	13	4	54	17	4	25	894	223
	Far-Field	Dectris Pilatus 6M (20-bit)	18	125	2,226	25	4	63	116	29	40	9,706	2,426
	Diffraction Tomography	Dectris Pilatus 2M CdTe (20-bit)	7	50	354	249	4	72	21	5	10	441	110
	Diffraction Tomography	Dectris Eiger 16M CdTe (12-bit)	52	50	2,595	1,825	4	72	154	39	10	3,233	808
	Diffraction Tomography	Sydor SMM-PAD CdTe (22-bit)	0.75	50	38	26.37	4	72	2.22	0.56	10	47	12
	Diffraction Tomography	Dectris Pilatus 2M CdTe (20-bit)	7	250	1,771	1,993	4	72	105	26	5	1,103	276
	Diffraction Tomography	Dectris Eiger 16M CdTe (12-bit)	52	133	6,902	14,596	4	72	410	102	5	4,300	1,075
	Diffraction Tomography	Sydor SMM-PAD CdTe (22-bit)	0.75	1,000	750	211	4	72	45	11	5	467	117
	Imaging Tomography	FLIR Oryx 5MP (12-bit)	10	10	96	34	1	54	4	4	15	134	134
	Fast Imaging Tomography	FLIR Oryx 5MP (12-bit)	10	100	956	34	1	12	10	10	5	99	99

* A compression factor of 1.0 represents no compression.
** Based on 1,440 minutes in one day. Utilization reflects the overhead associated with detector duty cycles and motion, as well as related setup time for alignment, calibration, sample changes and sample alignment, in situ environment modification, etc.
*** Based on 210 days of beam time per fiscal year.

2.4.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.4.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.4.4 Data Management, Workflows, and Science Portals

The HEXM APS-U feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the HEXM APS-U feature beamline, workflows will provide a pipeline to automatically run data processing software for near- and far-field, diffraction tomography, and imaging tomography data reconstructions, and to view results.

2.4.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.4.6 Data Reduction and Analysis

The HEXM APS-U feature beamline requires data processing algorithms and software for near- and far-field, diffraction tomography, and imaging tomography measurements. Descriptions of current efforts and plans in each of these areas follow. Table 2-7 summarizes capabilities for each of these modes, respectively.

Near- and Far-Field Diffraction Microscopy

The APS develops and supports the *Microstructural Imaging using Diffraction Analysis Software (MIDAS)* software package for near- and far-field diffraction microscopy data processing. The software is available as an open-source package (https://github.com/marinerhemant/MIDAS). *MIDAS* is written in C and uses Python for scripting. Distributed-memory parallelization is achieved using the SWIFT parallel execution framework. Time-critical parts of the code have been ported to run on GPUs with CUDA. *MIDAS* has been demonstrated to scale to tens-of-thousands of cores on supercomputers at the Argonne Leadership Computing Facility (ALCF) and at the National Energy Research Scientific Computing Center (NERSC). An average size data set today is typically processed within a few minutes. The APS will continue to develop *MIDAS* by enabling the processing of data taken with 3D scans, implementing intensity fitting, closely integrating with tomographic reconstruction algorithms and software, and scaling and optimizing performance to support APS-U Era data rates and sizes.

In addition to APS developed software, *IceNine* supports processing near-field diffraction data, and *Fable* and *HEXRD* support far-field data processing.

Diffraction Tomography

APS staff in the Materials Physics & Engineering group have developed prototype software in MATLAB to reconstruct diffraction tomography data. This prototype MATLAB software serves as a proof-of-principle for algorithm quality. The APS will develop production ready, higher-performance software for diffraction tomography reconstructions, for APS-U Era data. Algorithmic work will continue to integrate more advanced algorithms uses for imaging tomography, such as Algebraic Reconstruction Technique (ART) based reconstruction methods.

As part of the *High Pressure Material Characterization in 3-Dimensions Using X-ray Diffraction Contrast Computed Tomography* LDRD, modules have been added in MIDAS for rapid and automated analysis of diffraction tomography data. These include rapid correction and transformation of diffraction data, extraction of peak properties and tomographic inversion.

Imaging Tomography

The APS develops and supports the *TomoPy* tomographic reconstruction library. *TomoPy* is available as an open-source library (https://github.com/tomopy/tomopy). *TomoPy* is primarily written in Python and has integrated MPI-based and GPU-based routines for performance. Reconstruction algorithms in TomoPy have been scaled to run on supercomputers at the Argonne Leadership Computing Facility (ALCF), the National Energy Research Scientific Computing Center (NERSC), and the Oak Ridge Leadership Computing Facility. In the APS-U Era, close integration of tomography reconstruction algorithms with *MIDAS* will improve performance and add convenience for users.

AI/ML Developments for the HEXM APS-U Feature Beamline

Researchers at the APS and from Argonne's Data Science & Learning (DSL) division have developed a deep neural network called BraggNN. This method enables extraction of precise Bragg peak locations from far-field High-Energy Diffraction Microscopy (HEDM) data. The model runs more than 200 times faster than the conventional pseudo-Voigt profiling to locate Bragg peak position (see Figure 2-2).

The APS is researching Point Focused High-Energy Diffraction Microscopy (PF-HEDM) as a technique that pushes the limits of HEDM techniques to smaller grains to obtain sub-granular information. Preliminary algorithms developed using tomography-like reconstructions are promising. Researchers are developing inversion tools using AI/ML to improve the quality of reconstructions and obtain higher-quality answers. These developments may provide an alternative to conventional diffraction tomography methods. The *Developing Point-Focus High-Energy Diffraction Microscopy to Reveal Battery Material Degradation* LDRD has been funded in FY23 for development of the PF-HEDM technique and leverage the beam capabilities of the APS-U era.

Table 2-7 Summary of near- and far field-diffraction, diffraction tomography, and imaging tomography data processing needs and status for the HEXM APS-U feature beamline.

Science Driver	Capability	Algorithm / Software Requirement	Status
Smaller grains Greater dispersity Higher deformation	Near-Field Diffraction	Scalable distributed-memory CPU and GPU implementation	Done – APS Operations – *MIDAS*
		Intensity fitting	To do – APS Operations
Smaller grains Greater dispersity Higher deformation	Far-Field Diffraction	Scalable distributed-memory CPU and GPU implementation	Done – APS Operations – *MIDAS*
		Multi-panel support	Done – APS Operations – *MIDAS*
		3D scanning support	To do – APS Operations
Nano-grains Amorphous materials	Diffraction (Scattering) Tomography	Prototype implementation	Done – APS Operations - MATLAB
		Scalable distributed-memory CPU and GPU implementation	Done – LDRD – *MIDAS*
		Integrate more advanced tomographic reconstruction algorithms, e.g., ART	To do – If needed – APS Operations
Faster processes (sub-second)	Imaging Tomography	Scalable distributed-memory CPU and GPU implementation	Done – APS Operations – *TomoPy*
		Integration with *MIDAS*	To do – APS Operations

2.4.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the HEXM APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the HEXM APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1 FTE per year for HEDM software development and approximately 1 FTE per year for *TomoPy* development from APS Operations funding.

In addition to APS Operations funding, the APS benefits from long-term collaborations with the Air Force Research Laboratory (AFRL), Carnegie Mellon University (CMU), in particular an NSF-MRI grant to CMU supported the development of a new APS High-Throughput High-Energy Diffraction Microscopy (HEDM) beamline at 6-ID-D, and past and future industrial partnerships with GE and Pratt & Whitney.

AI/ML BraggNN work is funded by *Information from Sensor to Data Center* (PI: Jana Thayer, SLAC National Accelerator Laboratory, LAB 20-2261).

The following LDRD funding was awarded to support these efforts:

- *Finding Critical Processes of Deformation in Structural Materials with Artificial Intelligence* (FY19)
- *AI-steer: AI-driven Online Steering of Light Source Experiments* (FY20)
- *High Pressure Material Characterization in 3-Dimensions Using X-ray Diffraction Contrast Computed Tomography (FY21)*
- *Developing Point-Focus High-Energy Diffraction Microscopy to Reveal Battery Material Degradation (FY23)*

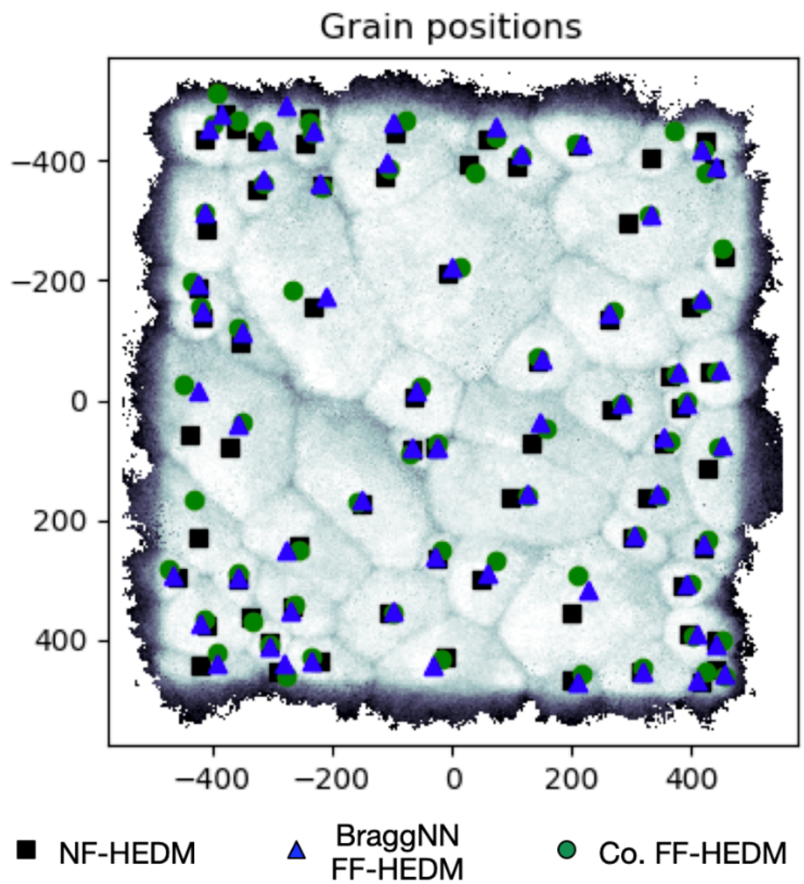


Figure 2-2 BraggNN: Grain center positions in microns determined by three methods, with a full high-resolution grain map from Near-Field HEDM superimposed in background. The Near-Field HEDM results provide the highest accuracy against which the grain-averaged Far-Field HEDM results can be compared. On average BraggNN provided slightly smaller position error than the conventional method.

2.5 In Situ Nanoprobe (ISN) APS-U Feature Beamline

2.5.1 Summary

The In Situ Nanoprobe (ISN) APS-U feature beamline is designed to study advanced materials during fabrication and operation. Its large working distance enables broad in situ environments, including heating, cooling, flow of process gases and fluids, and application of electric fields. The ISN beamline takes advantage of the upgraded source and is ideally suited for applications requiring diffraction-limited focusing. The ISN instrument will be a scanning nanoprobe, with x-ray fluorescence (XRF) detection and ptychography as major contrast modes. A secondary area detector will collect diffracted x-rays and provide some capability to identify local crystalline states.

Table 2-8 shows estimated data generation rates at the ISN APS-U feature beamline, and current data rates at the 2-ID-D ptychography, 2-ID-E XRF, and Bio Nano-Probe (BNP) XRF instruments for comparison. The ISN APS-U feature beamline is anticipated to collect approximately 10 PB of raw data per year and 1 PB of compressed raw data per year, in comparison to approximately 730 TB of raw data and approximately 73 TB of compressed raw data collected today across the 2-ID-D ptychography, 2-ID-E XRF, and Bio Nano-Probe (BNP) XRF instruments. Both uncompressed and compressed data sizes are given because uncompressed data is often required for data processing. This represents a nearly 15x increase in data. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-8 Data generation rates today at the 2-ID-D ptychography and diffraction, 2-ID-E XRF, and Bio Nano-Probe (BNP) XRF instruments (for comparison) and estimated data generation rates at the ISN APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Average Frame Rate (Hz)	Data Rate (MB/s)	Raw Data set Size (GB)	Compression Factor *	Daily Utilization (%)**	Raw Data Per Day (GB)**	Compressed Raw Data Per Day (GB)**	Annual Utilization (%)***	Raw Data Per Year (TB)***	Compressed Raw Data Per Year (TB)***
Today	2-ID-D Ptychography	Dectris Eiger 500K	1.010	100	100	40	10	80	6,912	691	50	726	72.6
	2-ID-E XRF	Vortex ME4	0.008	20	0.15	1.91	5	100	13.18	2.64	80	2.16	0.43
	BNP XRF	Vortex ME4	0.008	20	0.15	0.69	15	100	13.18	0.88	80	2.16	0.14
APS-U Era	ISN XRF	2 X Vortex ME7	0.1484375	1,000	144.95	579.83	5	80	1,956	116	80	329	65
	ISN Ptychography	Dectris Eiger 1M	2.092	3,000	5,000	204,322	10	35	185,362	18,536	20	7,603	760
	ISN Diffraction	Dectris Eiger 1M	2.092	3,000	5,000	40.86	10	10	52,960	5,296	20	3,528	326

* A compression factor of 1.0 represents no compression.
** Based on 1,440 minutes in one day.
*** Based on 210 days of beam time per fiscal year.

2.5.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.5.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.5.4 Data Management, Workflows, and Science Portals

The ISN APS-U feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the ISN APS-U feature beamline, workflows will provide a pipeline to automatically run tools to remove artifacts from data, reconstruct the XRF, Ptychography, and Diffraction data set, and view results.

2.5.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.5.6 Data Reduction and Analysis

The ISN APS-U feature beamline requires three modes of data processing: elemental fitting for XRF microscopy data, ptychography data reconstruction, and space-mapping for diffraction data. Descriptions of current efforts and plans in each of these areas follow. Table 2-9, Table 2-10, and Table 2-11 summarize capabilities for each of these three modes, respectively. Many of the data processing requirements for the ISN APS-U feature beamline are like those of the PtychoProbe APS-U feature beamline described in 2.7.

Elemental Fitting for XRF Microscopy Data

The APS develops and supports the *XRF-Maps and uProbeX* software packages for XRF microscopy data processing and visualization (see Figure 2-3). This software is available as open-source packages (https://github.com/AdvancedPhotonSource/XRF-Maps and https://github.com/AdvancedPhotonSource/uProbeX). The *XRF-Maps* package performs elemental map fitting and the *uProbeX* application is a GUI for visualizing *XRF-Maps* results. *XRF-Maps* and *uProbeX* are both written in C++. *XRF-Maps* supports multi-core data processing in a shared-memory CPU environment and has a Python wrapper which allows all the functionality to be called from a Python environment.

APS-U enhancements will allow for larger scan areas resulting in larger datasets. These larger datasets may not be able to fit in system memory. To accommodate this *XRF-Maps* implements a streaming architecture that allows processing a dataset spectra by spectra without having to load the entire dataset. Only a limited number of spectra are loaded based on memory limits, processed, and saved to an HDF5 file until the whole dataset is processed. As data sizes increase, it may be become necessary to develop GPU-based and distributed-memory CPU- and GPU-based elemental fitting software.

The higher intensity x-ray beam generated by the APS-U storage ring necessitates the use of self-absorption correction when generating elemental maps. APS researchers and instrument staff are working on developing new self-absorption correction algorithms in collaboration with staff at the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL). These algorithms are being implemented and tested in the *XRF-Maps* software.

Table 2-9 Summary of XRF microscopy elemental mapping data processing needs and status for the ISN APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
XRF Elemental Map Fitting	Algorithms for elemental map fitting	Done
	Multi-core shared-memory CPU implementation	Done – APS Operations
	Streaming data processing / operate on out-of-core data	Done – APS Operations
	Distributed-memory CPU and GPU implementation	To do – If required
XRF Self-Absorption Correction	Self-absorption correction algorithm development	In Progress – APS Operations and collaborations with NSLS-II

	Self-absorption correction implementation in *XRF-Maps*	In Progress – APS Operations

Ptychography Reconstruction

Ptychography has emerged as a powerful technique at synchrotron light sources. It will play a central role in answering many emerging scientific questions that the upgraded APS will help solve. Advanced ptychographic reconstruction algorithms and software are critical to take advantage of this new and innovative technique.

Multiple ptychographic reconstruction algorithms are required to achieve reasonable reconstruction quality to best analyze ptychography data collected for different domains and of varying sample characteristics. The APS has implemented the extended Ptychographic Iterative Engine (ePIE), regularized Ptychographic Iterative Engine (rPIE), conjugate gradient, Difference Map (DM), and iterative Least-SQuares solver for generalized Maximum-Likelihood (LSQ-ML) methods. Algorithms to help improve reconstruction quality, such as position and probe variation correction, and affine position regularization, are being developed and implemented.

Due to the computationally complex nature of ptychographic reconstruction algorithms and due to the anticipated increase in data rates and sizes in the APS-U Era, distributed high-performance implementations of ptychography reconstruction software are required. The APS with collaborators in Argonne's Mathematics & Computer Science (MCS) division developed *PtychoLib*, a distributed-memory GPU implementation of the extended Ptychographic Iterative Engine (ePIE) in 2014 and integrated Difference Map (DM) algorithms in 2018. *PtychoLib* was written in C++ and uses MPI and CUDA. The software was shown to scale on up to 256 GPUs on the Argonne Leadership Computing Facility's Cooley GPU cluster. This software has been supported and extended since then and has been the main tool used for high-performance ptychography reconstructions at APS beamlines. *PtychoLib* has been the main tool used for high-performance ptychography reconstructions at APS beamlines for the past decade. *PtychoPy* (https://github.com/kyuepublic/ptychopy) was developed as a Python wrapper and GUI for *PtychoLib*. Since then, the APS has consolidated ptychography development into the *tike* (https://github.com/AdvancedPhotonSource/tike) toolkit in order to make installing and developing new ptychography features and algorithms easier. This toolkit is written in Python and uses CuPy as the underlying GPU framework. All the reconstruction features of *PtychoLib* have been reimplemented in the tike toolkit including MPI and thread-based parallelism. *Ptychodus*, is a new pyQT-based GUI/workflow manager for ptychography reconstruction workflows has also been created in order to provide live reconstruction visualization and analysis.

Table 2-10 Summary of ptychography reconstruction needs and status for the ISN APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
Conventional Reconstruction	GPU implementation of extended Ptychographic Iterative Engine (ePIE) method	Done – APS Operations
	GPU implementation of Difference Map (DM) method	Done – APS Operations
	GPU implementation of the iterative Least-SQuares solver for generalized Maximum-Likelihood (LSQ-ML) method	Done – APS Operations
Improved Reconstruction Quality	Position correction	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Probe variation correction	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Multi-probe retrieval	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Mini-batches	In Progress – Implemented and currently being tested – APS Operations
	Multi-wavelength	In Progress – APS Operations
	Arbitrary fly-scan	To do – APS Operations
	Multi-slice ptychography	To do – APS Operations
	Integration with CNN denoising and priors (regularization)	In Progress – APS Operations
	Affine position regularization	In Progress – APS Operations

High-Performance Implementations	Scalable distributed-memory GPU implementation of extended Ptychographic Iterative Engine (ePIE) method	Done – APS Operations and ASCR funding
	Scalable distributed-memory GPU implementation of Difference Map (DM) method	Done – APS Operations and ASCR funding
	Scalable distributed-memory GPU implementation of iterative least-squares solver for generalized maximum-likelihood (LSQ-ML) method	Done – APS Operations
	Ptychographic reconstruction using AI/ML	In Progress – APS Operations & LDRD

APS-U Era data rates are expected to be so large that traditional algorithms may not be able to keep up with acquired data. These data rates are so large, and the scientific problems that APS-U Era capabilities can enable are so great, that porting and scaling current models and algorithmic approaches may not realize the full promise of next-generation light sources. Using AI techniques, APS researchers have developed an approach to improve the performance of ptychographic reconstructions. A deep neural network model is trained to predict and reconstruct ptychographic x-ray data. This approach, PytchoNN, can then perform reconstructions up to 300 times faster than conventional iterative approaches and uses up to 5 times less data, speeding up both data acquisition and data reconstruction (see Figure 2-4).

Space-Mapping for Diffraction Data

The APS develops and supports the *RSMap3D* tool for diffraction space-mapping (see Figure 2-5). This software is available as an open-source package (https://github.com/AdvancedPhotonSource/rsMap3D). The tool allows users to examine the volume of collected data and select portions on which to apply transformations that convert detector pixel locations from diffractometer geometry to reciprocal-space units, and then map pixel data onto a 3D reciprocal-space grid. This application uses diffractometer angles, the energy of the scan and sample to detector distances to calculate either q-vector component values or HKL values. These values are calculated for each detector pixel and scan position. The calculated q/HKL value and pixel intensity is then binned in a 3D grid based on the selected q/HKL values. The core routines utilize OpenMP to parallelize operations across multiple cores on a shared-memory CPU. Data too big to fit entirely into memory at one time are processed in smaller chunks and reassembled to form the final output volume, allowing users to process arbitrarily large input datasets. It will be straightforward to extend this application to operate in a distributed-memory CPU environment if needed. These parallel and out-of-core computational techniques will be critical to handle larger data rates expected in the APS-U Era.

Table 2-11 Summary of diffraction space-mapping data processing needs and status for the ISN APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
RSM for Diffraction Data	Multi-core shared-memory CPU implementation	Done – APS Operations in collaboration with DESY
	Operate on out-of-core data	Done – APS Operations
	Distributed-memory CPU and GPU implementation	To do – If required

Spectroscopy Tools

An additional need for ISN is a spectroscopy tool. The relevant data acquisition mode is 2D or (possibly 3D) spatial scans with a full spectrum XANES spectrum at each pixel. Software should display spectra at each pixel. Related is a tool that allows PCA analysis of the data within an interactive feature that that allows display of the local spectra for each major component. For example, PCA would identify uniform/crystalline areas of a multicrystalline sample and grain boundaries, and extraction of the spectra for the relevant principal components would enable direct visualization of the spectral differences between uniform/crystalline areas and grain boundaries.

2.5.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the ISN APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the ISN APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1 FTE per year for XRF elemental mapping and diffraction space-mapping software development from APS Operations funding.

The following LDRD funding was awarded to support these efforts:

- *Novel Capabilities for Ultra-fast and Ultra-low-dose 3D Scanning Hard X-ray Microscopy* (FY18)
- *Enabling Automatic Learning of Atmospheric Particles through APS-U* (FY19)
- *Learning and Differentiating: Using Artificial Intelligence to Image Beyond the X-ray Depth of Focus Limit* (FY19)
- *Intelligent Ptychography Scan via Diffraction-Based Machine Learning* (FY20)
- *AutoPtycho: Autonomous, Sparse-sampled Ptychographic Imaging* (FY21)
- *AI Accelerator for 3D X-ray Phase Retrieval with Automatic Differentiation* (FY21)

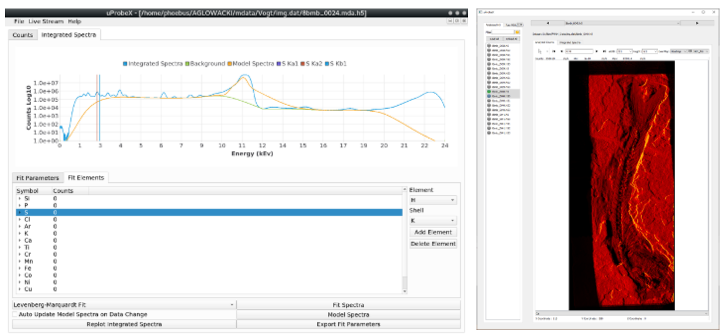


Figure 2-3 Left: uProbeX displaying integrated spectra from a dataset in blue, background subtraction in green, modeled spectra in orange, and elemental lines for element S. Right: uProbeX displaying Calcium quantities of an analyzed fish fossil. Elemental maps are generated with XRF-Maps.

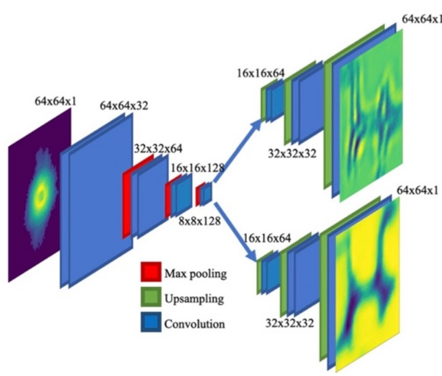


Figure 2-4 Architecture of PtychoNN, a deep convolutional neural network that can predict real-space amplitude and phase from input diffraction data alone.

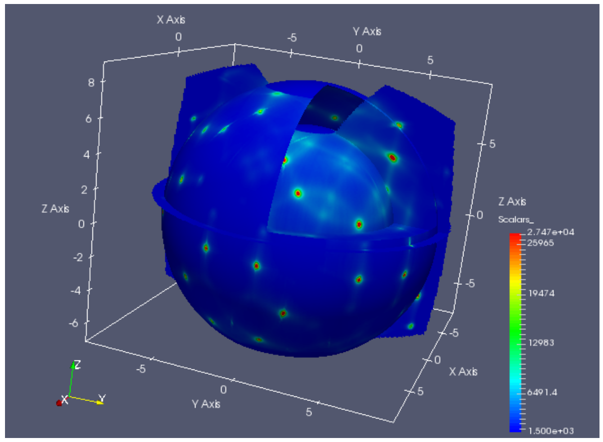


Figure 2-5 Visualization of a dataset from a pixel from a Silicon analyzer crystal processed with RSMap3D. This data shows a combination of diffraction (bright spots) and thermal diffuse scattering (broad lines connecting diffraction spots). This data was taken on the High Energy Resolution Inelastic X-Ray Spectrometer (HERIX) at APS Sector 30.

2.6 Polarization Modulation Spectroscopy (Polar) APS-U Feature Beamline

2.6.1 Summary

The Polarization Modulation Spectroscopy (Polar) APS-U feature beamline will use the polarization dependence of resonant absorption and scattering to study emergent quantum states in novel electronic and magnetic materials. Emphasis is placed on tuning/controlling competing ground states and electronic inhomogeneity with a combination of extreme high-pressures, low temperature, and high magnetic fields. Brilliant beams with tunable circular-and linear-polarization states will allow reaching extreme pressures as well as mapping electronic inhomogeneity in both real and reciprocal space.

In the APS-U era, the Polar APS-U feature beamline will continue to support techniques relying on x-ray polarization control but will augment its capabilities by leveraging the enhanced brilliance and coherence of APS-U beams, coupled with extreme sample environments. A future installation of a pair of polarizing undulators that leverage use of round insertion device vacuum chambers made possible in APS-U will provide exquisite polarization control (circular, elliptical, arbitrary linear) and extend the energy range of polarization modulated spectroscopies to high energy resonances up to 27 keV. Dichroic techniques currently supported include X-ray Magnetic Circular Dichroism (XMCD), X-ray linear dichroism (XLD), and Resonant Magnetic Scattering/Reflectivity. New techniques in Polar that require software development, and entail significant increases in data volumes, are: (1) Dichroic Ptychography, including fly scanning/interferometry and tomographic modes, for imaging of electronic/magnetic domains in reciprocal space with ~ 10 nm resolution; (2) Scanning dichroic x-ray absorption imaging, including fly scanning/interferometry and tomographic modes, for imaging of electronic/magnetic domains in real space with ~ 200 nm resolution. New sample environments such as a 3-axis 9-1-1 T magnet also enable expansion of dichroic technique modalities to include X-ray Magnetic Linear Dichroism (XMLD) and Dichroic emission spectroscopy (RXES-MCD). The new dichroic imaging techniques are implemented in combination with extreme conditions of ultra-high pressure, low temperature, and high magnetic field. The data volume estimates for these techniques form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-12 shows the estimated data generation rates at the Polar APS-U feature beamline. The Polar APS-U feature beamline is anticipated to collect approximately 84 TB of compressed raw data per year. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-12 Estimated data generation rates at the Polar APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Data Rate (MB/s)	Raw Data set Size (MB)	Daily Utilization (%)*	Annual Utilization (%)**	Raw Data Per Year (GB)**
Today	4-ID-D XAS/XMCD/XLD	Si Drift Multi-Element, photodiodes	2.73	0.0014	547	90	15	3
	4-ID-D Dichroic Resonant Scattering/Reflectivity	Scintilator (NaI) / Avalanche Photodiode	0.38	7.6E-7	0.3815	90	10	0.0012
APS-U Era	4-ID-G Dichroic Ptychography imaging 2D/3D modes (fly scans, interferometry)	Dectris EIGER2 X 1M	4.16	208	21,000	90	20	76,000
	4-ID-G Dichroic Resonant Scattering imaging (200 nm)	Dectris EIGER 2 X 1M	4.16	41.6	4,000	90	10	7,500
	4-ID-G Dichroic Absorption Tomography (200 nm)	Photodiodes	0.38	7.6E-7	0.3815	90	10	0.0012
	4-ID-H Dichroic Absorption XAS/ XMCD/XMLD (mapping 300 nm, high-pressure 7 Mbar)	Si Drift 7-Element Photodiodes	1.302	0.33	1172	70	25	51
	4-ID-H Dichroic X-ray emission (RXES-MCD)	Lambda 250k	1	1	20	90	10	1

* Based on 1,440 minutes in one day.
** Based on 210 days of beam time per fiscal year.

2.6.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.6.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs). Dichroic Ptychography in 2D and 3D (tomographic) modes will make use of interferometry to inform on actual sample and beam position during fly scans, information to be used for image alignment before reconstructions. Integration of interferometry with beamline controls will be done with FPGA-based *softGlueZynq*.

2.6.4 Data Management, Workflows, and Science Portals

The APS-U Polar feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the Polar APS-U feature beamline, workflows will provide a pipeline to automatically run analysis and reconstruction tools.

2.6.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Under the scope of LDRD project 2022-0008, *Development of 3D Dichroic Ptychography at APS*, a 2 x A100 80GB GPU server was purchased in FY22 to provide a dedicated platform for reconstruction of ptychography data at 4-ID-D. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.6.6 Data Reduction and Analysis

The processing and analysis of dichroic data currently collected at 4-ID-D leverages a variety of in-house scripting tools and open-source software, such as *GenX* code for Dichroic Resonant Reflectivity data (https://aglavic.github.io/genx), and *polartools* for python-based processing of dichroic and resonant diffraction data (https://github.com/APS-4ID-POLAR/polartools).

Reconstruction algorithms for processing Dichroic Ptychography data, including tomographic mode, are currently being developed with funding from LDRD 2022-0008, *Development of 3D Dichroic Ptychography at APS*. The APS will leverage the *tike* ptychography toolkit as a framework for implementing algorithms in this area. If required, the APS will develop scalable distributed-memory CPU and GPU implementations for processing the large volumes of Dichroic Ptychography data generated by the Polar APS-U feature beamline, especially for fly-scan implementations.

Reconstruction algorithms for scanning Dichroic Tomography are not yet defined. The APS is currently performing preliminary R&D in this area under LDRD 2022-0008. The APS will leverage the *TomoPy* toolkit as a framework for implementing algorithms in this area. If required, the APS will develop scalable distributed-memory CPU and GPU implementations for processing the large volumes of Tomographic CDI data generated by the Polar APS-U feature beamline.

Table 2-13 Summary of data reduction needs, approaches, and status for the Polar APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
Dichroic Resonant Absorption and Scattering	Algorithm development	Done – APS Operations
	Single CPU software implementation	Done – APS Operations – *polartools* Open Source - *GenX*, etc
	Scalable distributed-memory CPU and GPU implementation	In progress – LDRD, APS operations
Dichroic Ptychography	Algorithm development	In progress – LDRD
	Single CPU software implementation	In progress – LDRD
	Scalable distributed-memory CPU and GPU implementation	In progress – LDRD, APS operations
Dichroic Tomography	Algorithm development	In progress – APS Operations
	Single CPU software implementation	In progress – APS Operations – Leverage *TomoPy* tools for tomographic reconstruction
	Scalable distributed-memory CPU and GPU implementation	In progress – LDRD, APS operations

2.6.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the Polar APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the Polar APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. LDRD 2022-0008, *Development of 3D Dichroic Ptychography at APS* is providing effort to develop reconstruction algorithms for dichroic ptychography data (2D and 3D), and resources to augment local computing infrastructure.

The following LDRD funding was awarded to support these efforts:

- *Development of 3D Dichroic Ptychography at APS* (FY22)

2.7 PtychoProbe APS-U Feature Beamline

2.7.1 Summary

The PtychoProbe APS-U feature beamline (Ptychography + Nanoprobe) is designed to realize the highest possible spatial resolution X-ray microscopy both for structural and chemical information. The unprecedented brightness of the APS MBA lattice will be exploited to produce a nm-beam of focused hard X-rays to achieve the highest possible sensitivity to trace elements, and ptychography will be used to further improve the spatial resolution for structural components to its ultimate limit. The proposed beamline will enable high resolution two- and three-dimensional imaging of thick objects and bridge the resolution gap between contemporary X-ray and electron microscopy. Extending X-ray microscopy into the nanoscale is crucial for understanding complex hierarchical systems on length scales from atomic up to meso and macroscales, and time scales down to the microsecond level, and is applicable to scientific questions ranging from biology to earth and environmental materials science, to electrochemistry, catalysis and corrosion, and beyond.

Table 2-14 shows estimated data generation rates at the PtychoProbe APS-U feature beamline. The PtychoProbe APS-U feature beamline is anticipated to collect approximately 48.8 PB of raw data per year and 4.8 PB of compressed raw data per year, in comparison to approximately 730 TB of raw data and approximately 73 TB of compressed raw data collected today across the 2-ID-D ptychography, 2-ID-E XRF, and Bio Nano-Probe (BNP) XRF instruments. Both uncompressed and compressed data sizes are given because uncompressed data is often required for data processing. This represents an approximately 100x increase in data. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-14 Data generation rates today at the 2-ID-D ptychography, 2-ID-E XRF, and Bio Nano-Probe (BNP) XRF instruments (for comparison) and estimated data generation rates at the PtychoProbe APS-U feature beamline.

	Technique	**Detector**	**Frame Size (MB)**	**Average Frame Rate (Hz)**	**Data Rate (MB/s)**	**Raw Data set Size (GB)**	**Compression Factor** *	**Daily Utilization (%)** **	**Raw Data Per Day (GB)** **	**Compressed Raw Data Per Day (GB)** **	**Annual Utilization (%)** ***	**Raw Data Per Year (TB)** ***	**Compressed Raw Data Per Year (TB)** ***
Today	2-ID-D Ptychography	Dectris Eiger 500K	1.010	100	100	40	10	80	6,912	691	50	726	72.6
	2-ID-E XRF	Vortex ME4	0.008	20	0.15	1.91	5	100	13.18	2.64	80	2.16	0.43
	BNP XRF	Vortex ME4	0.008	20	0.15	0.69	15	100	13.18	0.88	80	2.16	0.14
APS-U Era	PtychoProbe XRF	Vortex ME7	0.054	1,000	53	214	5	80	631	42.7	80	106	21
	PtychoProbe Ptychography – Slow	Dectris Eiger 2XE 1.5M	3	2,000	6,000	120	10	80	414,720	41,472	40	34,836	3,483.6
	PtychoProbe Ptychography – Fast	TBD – Small fast detector (200x200)	0.08	30,000	2,400	3.2	10	80	165,888	16,589	40	13,934	1,393.4

* A compression factor of 1.0 represents no compression.
** Based on 1,440 minutes in one day.
*** Based on 210 days of beam time per fiscal year.

2.7.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.7.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.7.4 Data Management, Workflows, and Science Portals

The PtychoProbe APS-U feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the PtychoProbe APS-U feature beamline, workflows will provide a pipeline to automatically run tools to remove artifacts from data, reconstruct the XRF and Ptychography data set, and view results.

2.7.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.7.6 Data Reduction and Analysis

The PtychoProbe APS-U feature beamline requires two modes of data processing: elemental fitting for XRF microscopy data and ptychography data reconstruction. Descriptions of current efforts and plans in each of these areas follow. Table 2-15 and Table 2-16 summarize capabilities for each of these two modes, respectively. Many of the data processing requirements for the PtychoProbe APS-U feature beamline are like those of the ISN APS-U feature beamline described in 2.5.

Elemental Fitting for XRF Microscopy Data

The APS develops and supports the *XRF-Maps and uProbeX* software packages for XRF microscopy data processing and visualization (see Figure 2-6). This software is available as open-source packages (https://github.com/AdvancedPhotonSource/XRF-Maps and https://github.com/AdvancedPhotonSource/uProbeX). The *XRF-Maps* package performs elemental map fitting and the *uProbeX* application is a GUI for visualizing *XRF-Maps* results. *XRF-Maps* and *uProbeX* are both written in C++. *XRF-Maps* supports multi-core data processing in a shared-memory CPU environment and has a Python wrapper which allows all the functionality to be called from a Python environment.

APS-U enhancements will allow for larger scan areas and/or finer pixel sizes resulting in larger datasets. These larger datasets may not be able to fit in system memory. To accommodate this *XRF-Maps* implements a streaming architecture that allows processing a dataset spectra by spectra without having to load the entire dataset. Only a limited number of spectra are loaded based on memory limits, processed, and saved to an HDF5 file until the whole dataset is processed. As data sizes increase, it may be become necessary to develop GPU-based and distributed-memory CPU- and GPU-based elemental fitting software.

The higher intensity x-ray beam generated by the APS-U storage ring necessitates the utilization of self-absorption correction when generating elemental maps. APS researchers and instrument staff are working on developing new self-absorption correction algorithms in collaboration with staff at the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory (BNL). These algorithms are being implemented and tested in the *XRF-Maps* software.

Table 2-15 Summary of XRF microscopy elemental mapping data processing needs and status for the ISN APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
XRF Elemental Map Fitting	Algorithms for elemental map fitting	Done
	Multi-core shared-memory CPU implementation	Done – APS Operations
	Streaming data processing / operate on out-of-core data	Done – APS Operations
	Distributed-memory CPU and GPU implementation	To do – If required
XRF Self-Absorption Correction	Self-absorption correction algorithm development	In Progress – APS Operations and collaborations with NSLS-II
	Self-absorption correction implementation in *XRF-Maps*	In Progress – APS Operations

Ptychography Reconstruction

Ptychography has emerged as a powerful technique at synchrotron light sources. It will play a central role in answering many emerging scientific questions that the upgraded APS will help solve. Advanced ptychographic reconstruction algorithms and software are critical to take advantage of this new and innovative technique.

Multiple ptychographic reconstruction algorithms are required to achieve reasonable reconstruction quality to best analyze ptychography data collected for different domains and of varying sample characteristics. The APS has implemented the extended Ptychographic Iterative Engine (ePIE), regularized Ptychographic Iterative Engine (rPIE), conjugate gradient, Difference Map (DM), and iterative Least-SQuares solver for generalized Maximum-Likelihood (LSQ-ML) methods. Algorithms to help improve reconstruction quality, such as position and probe variation correction, and affine position regularization, are being developed and implemented.

Due to the computationally complex nature of ptychographic reconstruction algorithms and due to the anticipated increase in data rates and sizes in the APS-U Era, distributed high-performance implementations of ptychography reconstruction software are required. The APS with collaborators in Argonne's Mathematics & Computer Science (MCS) division developed *PtychoLib*, a distributed-memory GPU implementation of the extended Ptychographic Iterative Engine (ePIE) in 2014 and integrated Difference Map (DM) algorithms in 2018. *PtychoLib* was written in C++ and uses MPI and CUDA. The software was shown to scale on up to 256 GPUs on the Argonne Leadership Computing Facility's Cooley GPU cluster. This software has been supported and extended since then and has been the main tool used for high-performance ptychography reconstructions at APS beamlines. *PtychoLib* has been the main tool used for high-performance ptychography reconstructions at APS beamlines for the past decade. *PtychoPy* (https://github.com/kyuepublic/ptychopy) was developed as a Python wrapper and GUI for *PtychoLib*. Since then, the APS has consolidated ptychography development into the *tike* (https://github.com/AdvancedPhotonSource/tike) toolkit in order to make installing and developing new ptychography features and algorithms easier. This toolkit is written in Python and uses CuPy as the underlying GPU framework. All the reconstruction features of *PtychoLib* have been reimplemented in the tike toolkit including MPI and thread-based parallelism. *Ptychodus*, is a new pyQT-based GUI/workflow manager for ptychography reconstruction workflows has also been created in order to provide live reconstruction visualization and analysis.

Table 2-16 Summary of ptychography reconstruction needs and status for the PtychoProbe APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
Conventional Reconstruction	GPU implementation of extended Ptychographic Iterative Engine (ePIE) method	Done – APS Operations
	GPU implementation of Difference Map (DM) method	Done – APS Operations
	GPU implementation of the iterative Least-SQuares solver for generalized Maximum-Likelihood (LSQ-ML) method	Done – APS Operations
Improved Reconstruction Quality	Position correction	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Probe variation correction	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Multi-probe retrieval	In Progress – Implemented in *tike* and currently being tested – APS Operations
	Mini-batches	In Progress – Implemented and currently being tested – APS Operations
	Multi-wavelength	In Progress – APS Operations
	Arbitrary fly-scan	To do – APS Operations
	Multi-slice ptychography	To do – APS Operations
	Integration with CNN denoising and priors (regularization)	In Progress – APS Operations
	Affine position regularization	In Progress – APS Operations
High-Performance Implementations	Scalable distributed-memory GPU implementation of extended Ptychographic Iterative Engine (ePIE) method	Done – APS Operations and ASCR funding
	Scalable distributed-memory GPU implementation of Difference Map (DM) method	Done – APS Operations and ASCR funding

	Scalable distributed-memory GPU implementation of iterative least-squares solver for generalized maximum-likelihood (LSQ-ML) method	Done – APS Operations
	Ptychographic reconstruction using AI/ML	In Progress – APS Operations & LDRD

APS-U Era data rates are expected to be so large that traditional algorithms may not be able to keep up with acquired data. These data rates are so large, and the scientific problems that APS-U Era capabilities can enable are so great, that porting and scaling current models and algorithmic approaches may not realize the full promise of next-generation light sources. Using AI techniques, APS researchers have developed an approach to improve the performance of ptychographic reconstructions. A deep neural network model is trained to predict and reconstruct ptychographic x-ray data. This approach, PytchoNN, can then perform reconstructions up to 300 times faster than conventional iterative approaches and uses up to 5 times less data, speeding up both data acquisition and data reconstruction (see Figure 2-7).

2.7.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the PtychoProbe APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the PtychoProbe APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1 FTE per year for XRF elemental mapping and diffraction space-mapping software development from APS Operations funding.

The following LDRD funding was awarded to support these efforts:

- *Novel Capabilities for Ultra-fast and Ultra-low-dose 3D Scanning Hard X-ray Microscopy* (FY18)
- *Enabling Automatic Learning of Atmospheric Particles through APS-U* (FY19)
- *Learning and Differentiating: Using Artificial Intelligence to Image Beyond the X-ray Depth of Focus Limit* (FY19)
- *Intelligent Ptychography Scan via Diffraction-Based Machine Learning* (FY20)
- *AutoPtycho: Autonomous, Sparse-sampled Ptychographic Imaging* (FY21)
- *AI Accelerator for 3D X-ray Phase Retrieval with Automatic Differentiation* (FY21)

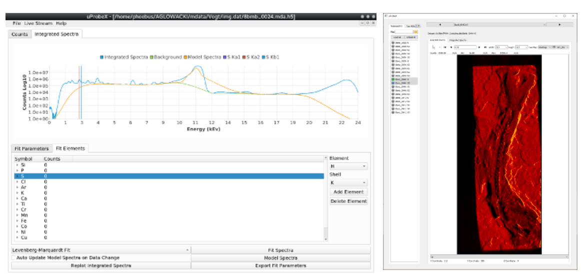


Figure 2-6 Left: uProbeX displaying integrated spectra from a dataset in blue, background subtraction in green, modeled spectra in orange, and elemental lines for element S. Right: uProbeX displaying Calcium quantities of an analyzed fish fossil. Elemental maps are generated with XRF-Maps.

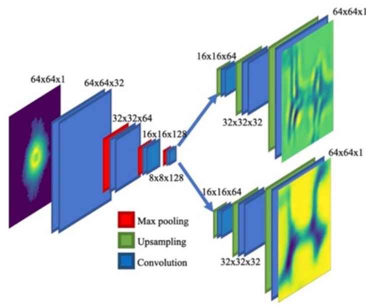


Figure 2-7 Architecture of PtychoNN, a deep convolutional neural network that can predict real-space amplitude and phase from input diffraction data alone.

2.8 X-ray Photon Correlation Spectroscopy (XPCS) APS-U Feature Beamline

2.8.1 Summary

The X-ray Photon Correlation Spectroscopy (XPCS) APS-U feature beamline will be dedicated to time-resolved coherent x-ray scattering experiments for a diverse scientific community; experiments will exploit the brilliance of the upgraded source to study fundamental materials structures. Since the signal to noise for XPCS scales as the square of the brilliance which will increase 500x in the APS-U era, it will be possible to measure faster dynamics and weaker scattering systems. The small- and wide-angle instruments will probe dynamics in soft and hard matter respectively.

In the APS-U era, the XPCS APS-U feature beamline will operate in modes that vary between collecting time series of area detector frames at very high frame rates (up to 100 kHz) and at moderate frame rates (a few kHz to Hz). The XPCS APS-U feature beamline is anticipated to collect up to approximately 20 PB of raw data per year, in comparison to approximately 0.1 PB of data collected today at the 8-ID beamline. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning. Table 2-17summarizes the data rates and total data accumulation for the anticipated experimental configuration at the XPCS APS-U feature beamline.

Table 2-17 Estimated data generation rates at the XPCS APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Detector Rate (Hz)	Data Rate (GB/s)*	Raw Dataset Size (GB)	Daily Utilization (%)**	Data Per Day (TB)**	Annual Utilization (%)***	Data Per Year (TB)***
Today	XPCS	LAMBDA 750K	1.5	500	0.74	14.84	25	1.57	25	82
APS-U Era	XPCS – Fast	UHSS 500K	0.5	56,000	27.34	48.83	5	2.31	5	20
	XPCS – Fast	Eiger 4M	4.0	4,000	15.63	390.63	20	65.92	20	2,765
	XPCS – Fast	UHSS 3M	3.0	56,000	164.06	292.97	15	207.64	20	8,725
	XPCS – Average	Eiger 4M	16.0	1,000	15.63	468.75	15	65.92	20	2,765
	XPCS – Average	UHSS 3M	6.0	8,500	49.80	351.56	20	168.09	20	7,055

* Raw uncompressed data rate.
** Based on 1,440 minutes in one day.
*** Based on 210 days of beam time per fiscal year.

2.8.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.8.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.8.4 Data Management, Workflows, and Science Portals

The APS-U XPCS feature beamline will leverage the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the XPCS APS-U feature beamline, workflows will provide a pipeline to automatically transfer data to computing resources for processing, launch processing jobs, and save results for visualization. A streaming data pipeline will be developed so that the data is processed in near real-time.

2.8.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources may be provided for on-the-fly data processing and experiment steering. Computing capacity for these data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.8.6 Data Reduction and Analysis

The main technique used for analyzing XPCS data involves auto-correlating time-resolved signals. Table 2-18 shows algorithm requirements based on science drivers, along with current algorithm development status. The Multi-Tau and Two-Time correlation algorithms are most used when processing data that studies equilibrium and non-equilibrium dynamics, respectively. These algorithms are already well developed and in common use. Higher-order time correlations are required to study spatial and temporal heterogeneity, intermittent dynamics, and avalanches. The study of speckle metrology, nanoscale flow, and velocimetry require the use of spatial-temporal cross-correlations. Development of these latter two classes of algorithms is underway at the APS and with APS Users and collaborators, including collaborators at CAMERA.

Table 2-18 Summary of algorithm requirements for the XPCS APS-U feature beamline.

Science Driver	Algorithm Requirement	Status
Equilibrium Dynamics	Multi-Tau Correlation	Done
Non-Equilibrium Dynamics	Two-Time Correlation	Done
Spatial and temporal heterogeneity, intermittent dynamics, avalanches	Higher-Order Time Correlations	In Progress – APS Operations, APS User group collaborations, and CAMERA
Speckle metrology, nanoscale flow, and velocimetry	Spatial-Temporal Cross-Correlations	In Progress – APS Operations, APS User group collaborations, and CAMERA

The APS develops and maintains the high-performance *boost-corr* auto-correlation software package for processing XPCS data. This tool utilizes multiple CPU cores and a single GPU in a shared-memory environment to quickly produce auto-correlations of XPCS data using the Multi-Tau and Two-Time algorithms. The *pyXpcsViewer* tool (https://github.com/AdvancedPhotonSource/pyXpcsViewer) helps users visualize and analyze correlation results generated from *boost-corr* (see Figure 2-8). A GPU implementation of the Multi-Tau algorithm has been developed that shows significant performance improvements over the current CPU implementation.

The current feature sets and performance today's software is adequate for today's needs. However, the estimated increase in overall data that will be generated at the XPCS APS-U feature beamline necessitates improvements and advances in software. The APS is planning to develop implementations of higher-order time correlation and spatial-temporal cross-correlation algorithms and develop higher-performance distributed-memory CPU and GPU software applications. Table 2-19 summarizes XPCS software capabilities and current development statuses for the XPCS APS-U feature beamline.

Table 2-19 Summary XPCS APS-U feature beamline data reduction and processing software capabilities and needs.

Capability	Software Requirement	Status
Multi-Tau Correlation	Shared-memory CPU implementation	Done – APS Operations
	Distributed-memory CPU implementation	To do – APS Operations
	Single GPU implementation	Done – APS Operations
	Multiple GPU implementation	To do – APS Operations
Two-Time Correlation	Shared-memory CPU implementation	Done – APS Operations
	Distributed-memory CPU implementation	To do – APS Operations
	Single GPU implementation	Done – APS Operations
	Multiple GPU implementation	To do – APS Operations
Higher-Order Time Correlations	CPU implementation	To do – APS Operations – pending algorithm development
	GPU implementation	To do – APS Operations – pending algorithm development
Spatial-Temporal Cross-Correlations	CPU implementation	To do – APS Operations – pending algorithm development
	GPU implementation	To do – APS Operations – pending algorithm development

Physics-Informed Machine Learning from Speckle Patterns

While fitting measured correlation functions to approximate models is often used to extract physical insights from raw speckle patterns, there are potential benefits to learning physics directly from the data. To this end, we outline and test a proof of concept for recovering physical equations from measured speckle patterns based on neural Ordinary Differential Equations (ODEs). In contrast to a traditional neural ODE workflow, the real-space dynamics of the system probed by coherent scattering are considered inaccessible apart from the initial condition. Instead, a neural network model of the ODE is trained by minimizing a loss function of the predicted and true sequence of speckle patterns. Using the trained model, we can then not only accurately predict future dynamics but also extract the model's dependence on the system variables to recover quantitative information about the governing equations. The extension of this framework to more complex systems and more realistic simulations is ongoing and will seek answers to additional questions, particularly the suitable balance between model flexibility and interpretability.

Automated Classification of Experimental Data

Recent work by APS scientists has applied unsupervised machine learning to automate the processing of XPCS Two-Time correlations. While algorithms exist for calculating these correlations from scattering data, methods for interpretation and quantification of Two-time correlations are still needed for studying non-equilibrium dynamics. A deep neural network was trained to recognize and reproduce spatial patterns in two-time correlations and encode these features into a low-dimensional representation. After using this neural network to encode entire datasets, clustering was performed to classify experimental data without requiring any input or physical knowledge form the user. In a similar manner, this automated method can be used to suggest similar two-time correlations based on a user-specified feature of interest, drastically reducing the analysis time required to comb through large XPCS datasets and identify interesting results. Future work aims to again use unsupervised machine learning to detect anomalous events and changes in the dynamic behavior of evolving systems to enable on-line data analysis at the beamline.

2.8.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the XPCS APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the XPCS APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. The APS dedicates approximately 1.0 FTE per year for XPCS related algorithm and software development from APS Operations funding.

CAMERA provides effort in support of XPCS algorithm development. An Argonne MGM Fellow provides effort related to physics-informed machine learning.

The following LDRD funding was awarded to support this effort:

- *Intermittent Dynamics in Hard and Soft Materials enabled by APS-U* (FY22)

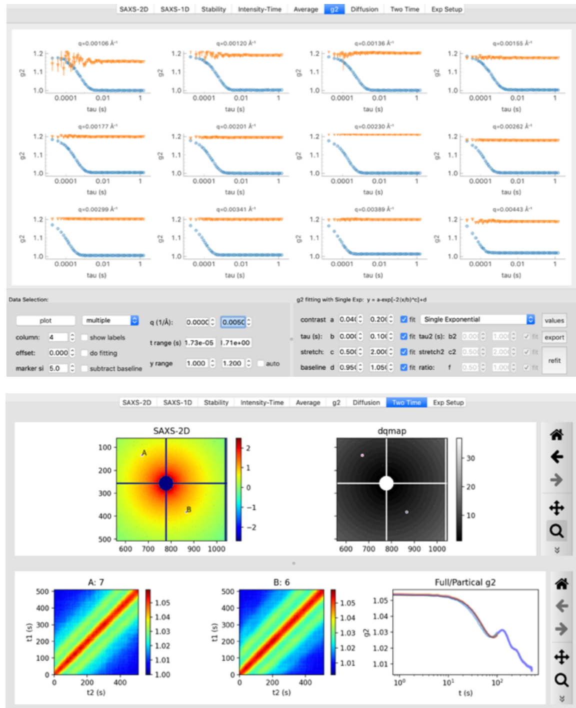


Figure 2-8 Top: g2 plots of the multi-tau correlation results. Users have many options to visualize data. Bottom: Visualization of a two-time correlation of a rubber sample. Users can select the region of interest by clicking the mouse.

2.9 3D Micro and Nano (3DMN) Diffraction APS-U Feature Beamline

2.9.1 Summary

The 3D Micro and Nano Diffraction (3DMN) APS-U feature beamline is designed to address a wide range of spatially inhomogeneous materials problems at the mesoscopic scale. These problems range over many areas of science where previous x-ray diffraction techniques are insufficient due to the short length scale of the inhomogeneities in the materials. 3DMN proposes to overcome current difficulties by using the bright MBA source to provide small intense x-ray spots (50-200nm) to investigate the important spatial variations of strain and structure that define this wide range of scientifically and technologically important materials.

In the APS-U era, the 3DMN feature beamline will perform Laue depth reconstruction diffraction scans. 3DMN will be able to operate in a mode like the current wire or knife-edge scan mode. This should allow analysis to work with some adjustments for data volume. 3DMN's updated detectors will lead to an increase in the size of acquired data from 6 megapixels (from 3 detectors) to 10 megapixels per collection point. To optimize use of updated beam parameters, it will be necessary to further decrease the size of the steps in a scan thus increasing the data volume. A new more efficient data collection mode is proposed that uses scans with a mask in place of a wire. Instead of blocking off one row with a wire in the scattered beam, a mask is used which passes only the previously blanked row. This new method allows for processing a larger data volume at each point by holding the number of scanned points close to the current wire scan. This will keep data volumes per dataset lower but requires implementing a new algorithm that is currently being developed. The new mode will allow more datasets of equal quality to be collected in the same amount of time as compared to the current wire scan method.

Table 2-20 shows the estimated data generation rates at the 3DMN APS-U feature beamline, and current data rates at the 34-ID-E instrument, for comparison. The 3DMN APS-U feature beamline is anticipated to collect approximately 2.8 PB of raw compressed data per year, in comparison to approximately 400 TB of data collected today at the 34-ID-E instrument. This represents slightly less than a one-order-of-magnitude increase in data. Note that in the APS-U era, it is anticipated that the 3DMN instrument will likely use the mask scan mode instead of the wire scan mode, assuming sufficient algorithmic developments. Although the overall amount of data generated by the two modes is the same in Table 2-20, the mask scan mode estimates represent a much larger amount of individual sample scans, and thus more final data. These data generation estimates form the basis for networking infrastructure, controls, data management, and data processing planning.

Table 2-20 Data generation rates today at the 34-ID-E Laue diffraction instrument (for comparison) and estimated data generation rates at the 3DMN APS-U feature beamline.

	Technique	Detector	Frame Size (MB)	Detector Rate (Hz)	Data Rate (GB/s)	Frames Per Dataset	Raw Dataset Size (GB)	Compression Factor*	Compressed Dataset Size (GB)	Dataset Collection Time (min)	Daily Utilization (%)**	Data Per Day (TB)**	Annual Utilization (%)***	Data Per Year (TB)***
Today	Wire Scan	PE XRD 1620 AN	8	4	0.03	500	3.91	1	3.91	2.08	50	1.32	45	125
		PE XRD 1620 AN + 2 x PE XRD 0820 AN	12	4	0.05	500	5.86	1	5.86	2.08	50	1.98	5	21
		PE XRD 1620 AN	8	8	0.06	500	3.91	1	3.91	1.04	50	2.64	45	249
		PE XRD 1620 AN + 2 x PE XRD 0820 AN	12	8	0.09	500	5.86	1	5.86	1.04	50	3.96	5	42
APS-U Era[++]	Wire Scan – Fast[+]	Pilatus 6M	24	100	2.34	1000	23.44	3.5	6.7	0.17	50	28.25	20	1,187
		Pilatus 6M + 2 x 2 MP Detectors	40	100	3.91	1000	39.06	3.5	11.16	0.17	50	47.08	5	494
	Wire Scan – Average[+]	Pilatus 6M	24	25	0.59	1000	23.44	3.5	6.7	0.67	50	7.06	70	1,038
		Pilatus 6M + 2 x 2 MP Detectors	40	25	0.98	1000	39.06	3.5	11.16	0.67	50	11.77	5	124
	Mask Scan – Fast[+]	Pilatus 6M	24	100	2.34	200	4.69	3.5	1.34	0.03	50	28.25	20	1,187
		Pilatus 6M + 2 x 2 MP Detectors	40	100	3.91	200	7.81	3.5	2.23	0.03	50	47.08	5	494
	Mask Scan – Average[+]	Pilatus 6M	24	25	0.59	200	4.69	3.5	1.34	0.13	50	7.06	70	1,038
		Pilatus 6M + 2 x 2 MP Detectors	40	25	0.98	200	7.81	3.5	2.23	0.13	50	11.77	5	124

[*] A compression factor of 1.0 represents no compression.
[**] Based on 1,440 minutes in one day.
[***] Based on 210 days of beam time per fiscal year.
[+] It is anticipated that the 3DMN instrument will likely use the mask scan mode instead of the wire scan mode, assuming sufficient algorithmic developments. Although the overall amount of data generated by the two modes is the same, the mask scan mode estimates represent a much larger amount of individual sample scans.
[++] The APS-U project has descoped certain parts of the 3DMN Feature beamline, including detector purchases. Although the detectors listed in the table may not be purchased as a part of the APS-U project, this table represents the desired long-term potential capabilities intended for this beamline.

2.9.2 Network Architecture and Infrastructure

Network infrastructure needs will be addressed by the facility plan described in 1.2.

2.9.3 Controls, Data Acquisition, and Detector Integration

Controls, data acquisition, and detector integration needs will be addressed by the facility plan described in 1.3. Detailed plans and schedules are described in respective APS-U beamline controls documents, Equipment Specification Documents (ESDs), and Instrument Specification Documents (ISDs).

2.9.4 Data Management, Workflows, and Science Portals

The APS-U 3DMN feature beamline will use the data management, workflow, and science portal efforts described in 1.4. The APS Data Management System, the facility-wide software and hardware system for managing data and workflows, will integrate data collection and processing workflows, manage user permissions based on experiment groups, and enable user access to data. Globus tools will provide a science portal for viewing and accessing data and automating the re-processing of data after the allotted experiment time has ended. For the 3DMN APS-U feature beamline, workflows will provide a pipeline to automatically run the wire or mask scan Laue depth reconstruction processing software and view results.

2.9.5 Computing Infrastructure

Computing infrastructure needs will be addressed by the facility plan described in 1.5. Some local computing resources will be provided for on-the-fly data processing and experiment steering. Computing capacity for larger data processing tasks and for post-experiment processing and analysis will be provided by computing centers, including the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC). The APS Data Management System and Globus tools will be used to seamlessly integrate these resources.

2.9.6 Data Reduction and Analysis

Processing Laue micro- and nano-diffraction microscopy data generally consists of three main steps in the following order: depth reconstruction, peak searching and indexing, and q-space histogram generation. The depth reconstruction process generates new images corresponding to the scattering observed from a single depth. Peak searching and indexing finds all the peaks and indexes them to get the crystal orientation of a Laue pattern. With energy scans, a 1D or 3D histogram of intensity in q-space may also be generated.

The APS develops and maintains the *LaueGo* software for Laue depth reconstructions of wire scan mode data. The software is available as an open-source package (https://github.com/34IDE/LaueGo). It performs peak searching and indexing, depth reconstruction, and q-space histogram generation for wire scan data. Versions are available in both Igor and C. A CUDA GPU implementation is available to improve performance on GPU equipped workstations.

The current feature set and performance of *LaueGo* and the corresponding GPU implementation is adequate for today's needs. However, the estimated increase in overall data that will be generated at the 3DMN APS-U feature beamline necessitates improvements and advances in software and algorithms.

In order to improve data collection time in the APS-U era, the APS is developing coded-aperture scans that may replace the current wire-scans for obtaining depth reconstructions. Along with higher-performance implementations of the contemporary wire scan mode data, high-performance implementations of coded-aperture reconstruction methods are being developed. Table 2-21 summarizes Laue depth reconstruction data reduction needs, approaches, and status for the 3DMN APS-U feature beamline.

Table 2-21 Summary of Laue depth reconstruction data reduction needs, approaches, and status for the 3DMN APS-U feature beamline.

Capability	Algorithm / Software Requirement	Status
Reconstruct Laue microscopy wire scan data	Algorithms for Laue microscopy wire scan reconstruction	Done – APS Operations
	CPU and GPU software for Laue microscopy wire scan reconstructions	Done – APS Operations
	Parallel distributed-memory CPU and GPU software for APS-U era wire scan data	To do – APS Operations

Reconstruct Laue microscopy mask scan data	Algorithms for Laue microscopy coded-aperture reconstruction	In Progress – Past LDRD, APS Operations
	CPU and GPU software for Laue microscopy wire scan reconstructions	In Progress – APS Operations
	Parallel distributed-memory CPU and GPU software for APS-U era mask scan data	In Progress – APS Operations

2.9.7 Effort, Funding, and Collaborations

Network infrastructure to the edge of the 3DMN APS-U feature beamline will be provided by APS-U funding. All other network infrastructure is funded by APS Operations funding as described in 1.2. Facility-wide data management, workflows, and science portal effort is funded by APS Operations (approximately 2.5 FTE per year) and the Globus Services team as described in 1.4. Some local computing resources dedicated to the 3DMN APS-U feature beamline for on-the-fly processing and experiment steering will be provided from APS-U funding. Large-scale computing resources are provided by APS Operations funding, Argonne Leadership Computing Facility (ALCF) funding, and Argonne Laboratory Computing Resource Center (LCRC) funding as described in 1.5. A postdoc is dedicated to development of the new mask scan algorithm. The APS will dedicate appropriate software development effort from APS Operations funding.

The following LDRD funding was awarded to support this effort:

- *Coded Apertures for Depth Resolved Diffraction* (FY20)

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