Scientific Software Engineering & Data Management
X-ray Science Division (XSD), Advanced Photon Source
Effort Plan for FY22 and FY23

The APS Scientific Software Engineering & Data Management group provides leadership and scientific software engineering expertise in the areas of data analysis, data management, high-performance computing, visualization, mobile applications, and workflow and orchestration applications in support of world-class photon sciences at the APS. This mission is realized through the creation of a core software application portfolio in prioritized areas, including coherence, imaging, and high-energy techniques, as well with software tools for data access and management, and data streaming for real-time feedback. Effort is aligned with facility priorities and strategies, which at this time include scientific software and data management tools critical to the techniques enabled by the APS-U, and is used in a transparent, flexible, and well-documented manner.

SDM believes it can uniquely enable great science (and x-ray synchrotron techniques) by creating great scientific and data management software. This is a key component in the creation of beamlines of the future, and is critical to the success of the APS-U project. Well-formed collaborative teams of software engineers, computer scientists, algorithm developers, beamline staff, users, peer groups, and other facilities and institutions develop the SDM group's software portfolio. The group works closely with the APS-CXS group, the CELS-DSL and CELS-MCS divisions, other facilities, and CAMERA to implement new algorithms and mathematical methods, and with the XSD-BC group and engineers at other facilities to integrate data analysis with beamline data acquisition systems, and with the APS-IT group, the CELS-DSL division, the Globus team, and other facilities to develop data management solutions. This document will be reviewed and updated at least once a year.

Five-year Goals

The SDM group's goals are directed at creating and deploying software tools enabling the full benefit of the portfolio of anticipated future beamlines, including the APS-U beamlines.

1. Creation and deployment of a robust set of high-performance computing (HPC) enabled software tools that address cross-cutting critical technique domain areas needed by future beamlines. This includes software in the areas of coherence, imaging, high-energy, and multi-modal techniques.
2. Deployment of a standard set of data management and distribution tools at XSD beamlines.
3. Integration of general-purpose data streaming, feedback, and verification tools with beamline control software and HPC data analysis software.

Goals and Action Plan for FY22 & FY23

High-level goals for FY22 & FY23 are:

- Continue to support HPC-enabled tools aligned with APS strategy for techniques such as XPCS, XRF, and ptychography by completing highest-priority goals in each area below.
- Meet FY22 and FY23 goals for the AI/ML for SUFs awards.
- In collaboration with the Globus team, deliver science data portals and workflow automation tools at select APS beamlines.
- Continue deployment and support of the APS Data Management System at APS beamlines.
- Continue development and support of remote access tools for APS beamlines.

Project	Summary	FY22 SDM FTE	FY23 SDM FTE
Remote Experiment Access Control	Continue support for and development of a web application for managing remote access to beamline computers for remote experiments.	0.50	0.50
A Collaborative Machine Learning Platform for Scientific Discovery	Support AI/ML for SUFs award, A Collaborative Machine Learning Platform for Scientific Discovery.	1.00 (postdoc)	(1.00 postdoc)
Globus Science Data Portals	Develop and support data science portals for select APS beamlines and techniques.	0.50	0.50
Workflow & Data Management Tools	Continue application of analysis workflow, web portals, and data management and distribution tools at APS beamlines.	2.50	2.50
A workflow combining the use of cryo-nanoprobe and cryo-focused ion beam for high resolution 3D imaging	Support LDRD, A workflow combining the use of cryo-nanoprobe and cryo-focused ion beam for high resolution 3D imaging.	0.10	0.10
Bragg Coherent Diffraction Imaging (CDI) Software	Provide distribution package and documentation, ongoing support for the Bragg CDI reconstruction tools. Optimize for size and speed and add a multi-phasing feature.	0.80	0.80
Coherent Surface Scattering Imaging (CSSI) Software	Implementation of high-performance CSSI and GISAXS software applications.	0.50	0.50
Correlation Toolkit	Develop a real-time HPC-enabled set of tools for time-based correlation data analysis.	1.00	1.00
General-Purpose Reciprocal-Space Mapping (RSM) Tools	Continue development and support for high-performance RSM tools.	0.10	0.10
Ptychography Software	Continue development of HPC ptychography reconstruction software.	1.00	1.00
X-ray Fluorescence Mapping (XFM) Software	Develop HPC-enabled fitting library and tools for fast elemental mapping.	0.70	0.70
Multi-modal XRF/Ptychography Tomography Alignment	Develop robust near real-time software for XRF/Ptychography tomographic alignment.	0.10	0.10
Laue Diffraction	Assist in the development of a high-performance computing tool kit for the new Laue depth reconstruction algorithm.	0.20	0.20
X-ray Emission Spectroscopy	Develop and support X-ray Emission Spectroscopy (XES) calibration, processing, and analysis tools.	0.10	0.10

In-operando AC scattering software	Continue development of software for in-operando AC scattering experiments.	0.10	0.10
Visualization Tools	Application and/or development of advanced visualization tools for APS beamline data analysis and experiment feedback.	0.10	0.10
Real-time Feedback & Data Acquisition System for APS-U Accelerator	Software framework and tools for the collection of data used for controls, statistics and diagnostics of technical systems for the MBA accelerator.	0.75*	0.75*
Multi-modal Diffraction Tomography	Develop robust near real-time software for diffraction tomography once algorithm development is complete	0.00**	0.00**
Multi-modal XRF Ptychography	Develop robust near real-time software for XRF ptychography once algorithm development is complete	0.00**	0.00**

* APS-U Funded – Pending FY22 ERA

** Additional funding/effort levels will enable the XSD-SDM group to take on additional projects and add further capabilities at the APS.

SWOT Analysis for Scientific Software

Strengths	Weaknesses
• World-leading software efforts in several scientific areas. • World-class beamline staff and user groups contribute new algorithms and software that expand the scientific productivity of the APS. • Highly productive internal group of professional scientific software engineers. • Close collaborations with APS users and staff, and the XSD-CXS group to provide algorithms and with the XSD-BC group to provide integration with beamline workflows.	• Current funding situation does not allow for the APS to meet its entire mission-critical data analysis software needs. • Most current generation data analysis tools are not suited to stream data in HPC environments needed to keep up with anticipated data rates. • Many scientist-developed packages lack professional software engineering needed to make them more productive • Lower facility productivity due to lack of data analysis tools.
Opportunities	**Threats**
• Collaborations with ANL expertise will help bring state-of-the-art HPC applications to the APS. • Collaborations with DOE facilities and resources could amplify development efforts and provide needed software in a cost-effective manner for the entire DOE complex. • The APS Upgrade-enabled techniques may be fully realized, answering new scientific questions; the APS maintains its position as the most productive light source.	• Without further investment and collaboration in this area, the APS will not fully realize the scientific potential of the APS Upgrade. • User groups may seek to perform cutting-edge experiments at other light sources where better software support is available. • Other domestic and international light sources have considerably larger and more active software and algorithm development programs that can leapfrog APS leadership.

SWOT Analysis for Data Management & Distribution

Strengths	Weaknesses
• World-leading expertise at ANL in data sciences, data management and transfer (e.g. Globus Services team). • APS is one of the DOE's largest data collecting user facility, producing a wealth of scientifically valuable data. • Collaborative efforts continue to form between the APS and expertise elsewhere at ANL.	• Preponderance of existing unique solutions at beamlines involving manual, inefficient management steps; no common user experience. • Current manual methods cannot keep pace with increasing data rates. • Lowered productivity due to time taken away from staff and users to address tasks that may be automated.
Opportunities	**Threats**
• Leverage expertise from CLS, UoC, and the Globus Services team. • Reduce cost by leveraging outside software resources and expertise. • Consistent data management user experience. • Increase scientific productivity through automation of data management tasks.	• The full potential of the APS Upgrade cannot be realized without managed data workflows. • Lowered scientific productivity due to an inability to keep up with increases in data. • International light sources that have invested heavily in data management software may overtake the APS in terms of scientific productivity.

Appendix - Project Details

Remote Experiment Access Control

Summary: Continue support for and development of a web application for managing remote access to beamline computers for remote experiments.

Team: John Hammonds (SDM), Arthur Glowacki (SDM), Faisal Khan (SDM), AES-IT, et al.

FY22 SDM Effort: 0.50 FTE
FY23 SDM Effort: 0.50 FTE
Out Years: TBD

Goals for FY22 and FY23 include:
1. Continue to provide support and development.
2. Implement scheme to automatically add/remove remote users to specific beamline computers. Enforce automatically removing user access after a set period.
3. Explore multi-factor authentication mechanisms.
4. Add end-of-run reporting.

A Collaborative Machine Learning Platform for Scientific Discovery

Summary: Support AI/ML for SUFs award, A Collaborative Machine Learning Platform for Scientific Discovery.

Team: Howard Yanxon (SDM), Nicholas Schwarz (SDM), et al.

FY22 SDM Effort: 1.00 postdoc
FY23 SDM Effort: 1.00 postdoc

Due to the tremendous increase in data generated by the scientific user facilities, building a software ecosystem that utilizes the power of machine learning technology is a logical step moving forward. The goals of the platform includes, but not limited to, data labeling to automatically extract features, build inferences with experiments through similarities/differences, developed search capabilities to help users navigate through their experiments, etc. The platform will be equipped with ML algorithms, trained ML models, and standard tagged/labeled data by the world domain experts to aid users with low barriers of entry across all the DOE SUF facilities.

In building the software ecosystem, it involves collaborative contributions from beamline scientists (Christopher Tassone (SLAC), Apurva Mehta (SLAC)), materials scientists (Alexander Hexemer and Edward Barnard (LBNL)), applied mathematicians (Sergei Kalinin (ORNL)), theorists (Subramanian Sankaranarayanan (ANL)), computer scientists (Harinarayan Krishnan (LBNL), Daniela Ushizima (LBNL), Nicholas Schwarz (ANL), and Stuart Campbell (BNL)), to software engineers (Ronald J. Pandolfi (LBNL)).

Goals for FY22 and FY23 include:
1. Develop classification capabilities for distinguishing different types of data. For example, transmission and reflection data can be distinguishable in scattering experiments.
2. Develop feature extraction from multi-dimensional data.
3. Constructed a foundational platform carrying the capabilities mentioned in 1 and 2, enabling low barrier of entry to access by users. In the platform, users can use the pre-trained models, make contribution to the platform, and provide feedback regarding the model or data integrities.

Globus Science Data Portals

Summary: Develop and support data science portals for select APS beamlines and techniques.

Team: Ian Foster (CELS-DSL), Rachana Ananthakrishnan (Globus), Ryan Chard (Globus), Ben Blaiszik (CELS-DSL), Nick Saint (CELS-DSL), Nicholas Schwarz (SDM), Junjing Deng (MIC), Olga Antipova (MIC), Si Chen (MIC), Lu Xi Li (MIC), Barry Lai (MIC), Peter Kenesei (MPE), Arthur Glowacki (SDM), Miaoqi Chu (SDM), Faisal Khan (SDM), Suresh Narayanan (DYS), Jun-Sang Park (MPE), Hemant Sharma (CXS), et al.

FY22 SDM Effort: 0.50 FTE
FY23 SDM Effort: 0.50 FTE

Goals for FY22 and FY23 include:
1. Meet goals in the A Smart Data and Computational Fabric Pilot for the APS and APS-U award.

Workflow & Data Management Tools

Summary: Continue application of analysis workflow, and data management and distribution tools at APS beamlines.

Team: John Hammonds (SDM), Steven Henke (SDM), Hannah Parraga (SDM), Sinisa Veseli (SDM), APS-IT, et al.

FY22 SDM Effort: 2.50 FTE
FY23 SDM Effort: 2.50 FTE
Out Years: TBD

As data rates and volumes increase due to a combination of advances in detector technologies, increased use of multi-modal acquisition techniques, and the planning benefits of the APS-U project, current manual data workflow and management mechanism will not be sufficient. The APS has a need for tools and infrastructure that automate analysis pipelines, maintain and track data ownership, catalog metadata, provides data distribution endpoints and Software as a Service (SaaS) web interfaces for data analysis, etc.

The APS team will place great emphasis on leveraging best-in-class tools, rather than on developing new systems. For example, they will continue to work closely with the Globus Services team in order to not duplicate effort and best leverage DOE and ANL resources. Open source tools will be used in order to best meet the needs of the APS in an efficient and cost-effective manner.

Goals for FY22 and FY23 include:
1. Continue support for existing beamlines.
2. Deploy system at additional beamlines.
3. Streamline deployment process with deployment tools and instructional materials.
4. Increase data confidentiality.
5. Interface with Argonne Leadership Computing Facility (ALCF) tape-based storage.
6. Develop web portal and a graphical user interface for workflow and data processing job management.
7. Interface with Globus automation tools where appropriate.

A workflow combining the use of cryo-nanoprobe and cryo-focused ion beam for high resolution 3D imaging

Summary: Support LDRD, A workflow combining the use of cryo-nanoprobe and cryo-focused ion beam for high resolution 3D imaging.

Team: Arthur Glowacki (SDM), Si Chen (MIC), et al.

FY22 SDM Effort: 0.10 FTE
FY23 SDM Effort: 0.10 FTE
Out Years: TBD

Bragg Coherence Diffraction Imaging (CDI) Software

Summary: Provide distribution package and documentation, ongoing support for the Bragg CDI reconstruction tools. Optimize for size and speed and add a multi-phasing feature.

Team: Barbara Frosik (SDM), Ross Harder (MIC), et al.
FY22 SDM Effort: 0.80 FTE
FY23 SDM Effort: 0.80 FTE
Out Years: TBD

Attaining a robust image of a sample in a computation time nearer the data acquisition time will allow nearer real-time feedback into the experimental parameters. The experimenter may begin to do guided, carefully executed experiments. Currently, most Bragg CDI users will benefit from semi-real-time phase retrieval for their data. It will also open the instrument up to far less sophisticated CDI users. This technique will be critical to one or more APS-U beamlines.

The cohere tool is a high-performance package that can complete phase retrieval of a typical image in about 1 minute. With different cases this may vary, as data sizes may be large, or users may use different features based on data the reconstruction may benefit from, such as the genetic algorithm, or multiple reconstructions. The tools provide a user-friendly GUI that is used for configuration and to control the reconstruction process. The tools can be installed with Anaconda. The tools run on both CPUs and GPUs. With greater resolution detectors the data size is growing. There is a need to optimize the software so the GPU can fit the reconstruction process. This will be the main goal for the next release of the tools.

Goals for FY22 and FY23 include:
1. Provide full Python version of cohere tools.
2. Provide access to code and scheme to easily add new functionality and document the process.
3. Offer choice of libraries that can be utilized to run tools.
4. Provide easy installation tools.
5. Provide and maintain documentation.
6. Optimize for size and speed, considering APS-U era needs.
7. Collaborate with ALCF resources to enable running the tools on ALCF supercomputers.
8. Investigate feasibility of the software platform to add multi-phasing feature, and if possible, enhance these tools.

Coherent Surface Scattering Imaging (CSSI) Software

Summary: Implementation of high-performance CSSI and GISAXS software applications.

Team: Miaoqi Chu (SDM), Ashish Tripathi (DYS), Zhang Jiang (DYS), Jin Wang (TRR), et al.

FY22 SDM Effort: 0.50 FTE
FY23 SDM Effort: 0.50 FTE
Out Years: TBD

CSSI is a coherent X-ray technique that can non-destructively probe 3D surface structures with very high resolution. A featured beamline for CSSI will be built under the APS-U project. Due to the unique geometry of CSSI experiments (reflection at grazing incident angles), the scattering process involves strong dynamical scattering effects that are absent in the traditional transmission-type coherent diffractive imaging/ptychography. A collaboration of teams with physics, applied mathematics, and computer science backgrounds is underway to identify the best algorithms to reconstruct CSSI data. Software support is required to implement the algorithms with high efficiency and maintainability.

Goals for FY22 and FY23 include:
1. Explore the physical nature that distinguishes between the CSSI's surface scattering and transmission type scattering.
2. Develop physics-based forward simulation packages to generate high quality data to test and benchmark reconstruction algorithms.
3. Implement reconstruction algorithms that account for the surface scattering geometry that can yield high fidelity CSSI reconstructions.
4. Optimize the algorithms on HPC to enable reconstruction on large input datasets.

Correlation Toolkit

Summary: Develop a real-time HPC-enabled set of tools for time-based correlation data analysis.

Team: Miaoqi Chu (SDM), Faisal Khan (SDM), Qingteng Zhang (DYS), Suresh Narayanan (DYS), et al.
FY22 SDM Effort: 1.00 FTE
FY23 SDM Effort: 1.00 FTE
Out Years: TBD

Time-based correlations are an important analysis tool used to study the dynamic nature of complex materials. The recent development and application of higher-frequency detectors allows the investigation of faster dynamic processes enabling novel science in a wide range of areas resulting in the creation of greater amounts of image data that must be processed within the time it takes to collect the next data set to guide data collection. The increased brightness afforded by the APS-U project will compound this data processing challenge by producing data with higher count rates.

Goals for FY22 and FY23 include:
1. Continue supporting the current tool and adding new features.
2. Develop a python interface that is more suitable for deployments at collaborating facilities.
3. Incorporate analysis from other light sources based on ongoing discussions.
4. Continue developing the new XPCS GUI, to incorporating functions and requirements from beamline staff and the XPCS user communities.
5. Develop a web-based XPCS visualization tool to provide a highly flexible tool for users to quickly assess XPCS data.
6. Begin planning and implementing a new version that can address APS-U era data rates.
7. Test and deploy the prototype GPU-based correlation algorithm we developed in FY21. Develop and benchmark the code with APS-U datasets.

General-Purpose Reciprocal-Space Mapping (RSM) Tools

Summary: Continue development and deployment of high-performance RSM tools.

Team: John Hammonds (SDM), Henry Smith (SDM), Jonathan Tischler (SSM), Zhan Zhang (SSM), et al.
FY22 SDM Effort: 0.10 FTE (staff), 1 Research Aide Technical
FY23 SDM Effort: 0.10 FTE (staff), 1 Research Aide Technical
Out Years: TBD

This project aims to continue development of a general-purpose tool for reciprocal-space mapping at the APS. The tool allows users to examine a volume of 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 on to a 3D reciprocal-space grid. It can map data acquired using 4- and 6-circle diffractometers, and with scans taken over angles or energy, and can operate via a graphical user interface, or in batch processing mode. Data too big to fit entirely into memory at one time is processed in smaller chunks and reassembled to form the final output volume, allowing users to process arbitrarily large input datasets.

This tool has the potential to serve an even larger number of APS beamlines, and will be critical to a number of APS-U beamlines and high-energy diffraction experiments. It is currently in regular use for scattering and diffraction experiments at the 33-BM and 33-ID beamlines, for micro-diffraction analysis at 34-ID, and for time-resolved diffraction work at 7-ID. Development is underway for WA-XPCS analysis at 8-ID, and for data exploration with inelastic x-ray measurements at 30-ID. Fast tools for reciprocal-space mapping using distributed computing resources are needed to make nearer real-time decisions regarding the next set of data that is collected. This work will leverage effort related to workflow and management tools, and data streaming and analysis tools for real-time analysis.

Goals for FY22 and FY23 include:
1. Continue supporting the current tool and adding new features as requested.
2. Continue GUI development.

Ptychography Software

Summary: Continue development of HPC ptychography reconstruction software.

Team: Ke Yue (SDM), Tekin Bicer (DSL/CXS), Daniel Ching (CXS), Mathew Cherukara (CXS), Yudong Yao (CXS), Junjing Deng (MIC), Stefan Vogt (XSD-ADMIN), et al.

FY22 SDM Effort: 1.00
FY23 SDM Effort: 1.00
Out Years: TBD

Ptychography is one of the exemplar APS-U enabled techniques, and will be one of the largest data producing techniques post APS-U. Proper support and development of existing tools, complementary use with other APS-U planned techniques, such as fluorescence ptychography, and integration with data streaming infrastructures mentioned in the description of other projects in this document is needed. Provide support and new feature development for the tike ptychography code base.

Goals for FY22 and FY23 include:
1. Continue supporting the tike ptychography software.
2. Refactor and integrate features from the ptychopy software into the tike ptychography software.
3. Assist with the development of distributed-memory, multi-GPU implementations.
4. Assist with the deployment of ptychography tools on Polaris.
5. Develop plans for APS-U Era ptychography needs.

X-ray Fluorescence (XRF) Microscopy Software

Summary: High-performance computing (HPC) enabled fitting library and tools for fast elemental mapping of x-ray fluorescence microscopy software.

Team: Arthur Glowacki (SDM), Wendy Di (MCS/CXS), Olga Antipova (MIC), Si Chen (MIC), Lu Xi Li (MIC), Barry Lai (MIC), Stefan Vogt (XSD/ADM), at al.
FY22 SDM Effort: 0.70 FTE
FY23 SDM Effort: 0.70 FTE
Out Years: TBD

XRF imaging typically involves the creation and analysis of 3D data sets, where at each scan position the full spectrum is recorded. This allows one to later process the data in a variety of different approaches, e.g., by spectral region-of-interest (ROI) summation with or without background subtraction, principal component analysis, or fitting. Additionally, it is possible to sum up the per pixel spectra over selected spatial ROIs to improve the photon statistics in such a spectrum.

The XRF microscopy technique is a staple technique that will be used by many APS-U beamlines in combination with other x-ray acquisition modalities, such as fluorescence tomography and fluorescence ptychography. The increase in intensity and smaller spot size due to benefits of the APS-U will drastically increase data size and data rates for this technique. To facilitate real-time data analysis and fast feedback for experiment steering, HPC-enabled implementations of common elemental mapping algorithms and data I/O schemes that facilitate streaming data, and appropriate user interfaces are required. This work will leverage effort related to workflow and management tools, and data streaming and analysis tools for real-time analysis, and can serve in conjunction with existing tomography software to provide analysis code for fluorescence tomographic reconstructions.

Goals for FY22 and FY23 include:
1. Continue developing a graphical user interface for XRF-Maps.
2. The new algorithm uses a physical mask that is being relocated for several "masked" scans. The initial data, (i.e. without a mask) together with the altered data, and the mask, is used to find the orientation of grains in the subject. Use interferometer data for precision coordinates.
3. Collaborate with Northwestern University (Andrew Crawford) to implement background correction from his software M-BLANK.
4. Continue implementing software for APS-U era needs.

Multi-modal XRF/Ptychography Tomography Alignment

Summary: Develop robust near real-time software for XRF/Ptychography tomographic alignment.

Proposed Team: Arthur Glowacki (SDM), Wendy Di (MCS/CXS), et al.
FY22 SDM Effort: 0.10 FTE
FY23 SDM Effort: 0.10 FTE
Out Years: TBD

Algorithmic work is underway in the XSD-CXS group.

Goals for FY22 and FY23 include:
1. Develop an application from MATLAB-based algorithmic code.
2. Optimize MATLAB code to run on LCRC, ALCF, and other HPC computers, and benchmark it to see how feasible it would be for large ptychographic tomography scans.

Laue Diffraction

Summary: Develop high-performance computing tool kit for the new Laue depth reconstruction algorithm.
Proposed Team: Barbara Frosik (SDM), Doga Gursoy (CXS), Jon Tischler (SSM), Dina Sheyfer (SSM), et al.
FY22 SDM Effort: 0.20 FTE
FY23 SDM Effort: 0.20 FTE
Out Years: TBD

The new algorithm uses a physical mask that is being relocated for several "masked" scans. The initial data, (i.e. without a mask) together with the altered data, and the mask, is used to find the orientation of grains in the subject.

Goals for FY22 and FY23 include:
1. Implement the given algorithm for performance and ready for data streaming (CXS).
2. Assist with other code for this project, as needed (SDM).

X-ray Emission Spectroscopy

Summary: Develop and support X-ray Emission Spectroscopy (XES) calibration, processing, and analysis tools.

Team: John Hammonds (SDM), Chengjun Sun (SPC), et al.
FY22 SDM Effort: 0.10 FTE
FY23 SDM Effort: 0.10 FTE
Out Years: TBD

A project is underway to upgrade the miniXES spectrometer. This purpose of this upgrade is to allow simultaneous non-resonent XES measurements at multiple edges and potentially measure sequential resonant XES at multiple edges at the same experimental condition. These changes are made possible by replacing the current analyzer array with a larger 2D crystal array with multiple crystal types and a larger detector to collect the resulting larger data set.

Software updates are needed to allow processing of data coming from each data set, which now contain data from multiple edges in one set. In addition to processing more data in each image, the software will need to be adapted to process a 2D map of XES data over the sample surface collected by performing a fly scan of the surface of the sample.

In-operando AC scattering software

Summary: Continue development of software for in-operando AC scattering experiments.
Proposed Team: John Hammonds (SDM), Henry Smith (SDM), Philip Ryan (MM), et al.

FY22 SDM Effort: 0.10 FTE (staff), 1 Research Aide Technical
FY23 SDM Effort: 0.10 FTE (staff), 1 Research Aide Technical
Out Years: TBD

Goals for FY22 and FY23 include:
1. Continue development of the xPlotUtil in-operando AC scattering software.
2. Continue space-mapping GUI development.

Real-time Feedback & Data Acquisition System for APS-U Accelerator

Summary: Software framework and tools for the collection of data used for controls, statistics, and diagnostics of technical systems for the MBA accelerator.

Proposed Team: Sinisa Veseli (PSC/SDM), Guobao Shen (CTL), John Carwardine (APS-U), et al.
FY22 SDM Effort: 0.75 FTE*
FY23 SDM Effort: 0.75 FTE*
Out Years: TBD

The real-time feedback and data acquisition (RTFB/DAQ) system is a software framework and associated tools that enable fast data collection for controls, statistics, and diagnostics associated with the state-of-the-art embedded controllers utilized by the APS-U project MBA-based accelerator design. The DAQ software interfaces with several technical subsystems to provide time-correlated and synchronously sampled data that can be used for commissioning, troubleshooting, performance monitoring, and early fault detection. The key features of the system include capability to acquire data from multiple subsystems at various sample rates, support for continuous data acquisition, and the ability to route data to any number of applications. Future work will focus on extending system functionality to provide access to BPM turn-by-turn data, as well as power supply monitoring.

Visualization Tools

Summary: Application and/or development of advanced visualization tools for APS beamline data analysis and experiment feedback.

Team: Arthur Glowacki (SDM), Alexis Quental (CMS), et al.
FY22 SDM Effort: 0.10 FTE
FY23 SDM Effort: 0.10 FTE
Out Years: TBD

Visualization is often critical to experiment data analysis. Visualization of data from tomographic imaging, micro-diffraction, and high-energy diffraction beamlines is already a challenge that will become more pressing soon. With the increase in data volumes being generated by higher frame-rate detectors, and as novel multi-modal techniques are enabled due to the benefits of the APS-U project and planned as a part of the APS-U's first experiments, e.g. x-ray fluorescence microscopy data coupled with coherent diffraction imaging, advanced visualization techniques will be needed in order to gain understanding and insight from this data, both as a part of post-acquisition processing and to allow user intervention during data collection. The application, augmentation, and/or development of capable data visualization tools on advanced computational resources are needed to cope with these large and complex data streams.

Goals for FY22 and FY23 include:
1. Develop PV's heads up display for Sector 12.
2. Explore use-cases for visualizing data with the Microsoft HoloLens 2 hardware.

Multi-modal Diffraction Tomography

Summary: Develop robust near real-time software for diffraction tomography.

Proposed Team: TBD SDM Member, et al.
FY22 SDM Effort: 0.00 FTE**
FY23 SDM Effort: 0.00 FTE**
Out Years: TBD

Algorithmic work is currently underway in the XSD-CXS group. Performance and engineering work will commence once algorithmic proof-of-concept is complete.

Multi-modal XRF Ptychography

Summary: Develop robust near real-time software for XRF ptychography.

Proposed Team: TBD SDM Member, et al.
FY22 SDM Effort: 0.00 FTE**
FY23 SDM Effort: 0.00 FTE**
Out Years: TBD

Algorithmic work is currently underway in the XSD-CXS group. Performance and engineering work will commence once algorithmic proof-of-concept is complete.