Scientific Software Engineering & Data Management
X-ray Science Division (XSD), Advanced Photon Source
Effort Plan for FY21 and FY22

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 FY21 & FY22

High-level goals for FY21 & FY22 are:

- Continue to support HPC-enabled tools aligned with APS strategy for techniques such as XPCS, XRF, Ptychography by completing highest-priority goals in each area below.
- Meet FY21 goals for the BES Data Solutions Task Force Data Pilot Project.
- Meet FY21 and FY22 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 roll-out and support of the APS Data Management System at APS beamlines.

Project	Summary	FY21 SDM FTE	FY22 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.	0.25	0.25
BES Data Solution Task Force Pilot Project	Collaborate with the ALS, CAMERA, LCLS, NSLS-II, and SSRL to share common XPCS, tomography, and ptychography software tools.	2.50	0.00
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.	0.50	0.50
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	Provide ongoing support for ptychography reconstruction software and tools, and integration with complementary techniques.	0.75	0.75
X-ray Fluorescence Mapping (XFM) Software	Develop HPC-enabled fitting library and tools for fast elemental mapping.	0.75	0.75
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.	0.10	0.10
X-ray Emission Spectroscopy	Develop and support X-ray Emission Spectroscopy (XES) calibration, processing, and analysis tools.	0.10	0.10
Support for HT-HEDM Beamline Project	Develop and integration of auto-alignment/calibration tools and mail-in automation software with existing systems for the new HT-HEDM beamline.	0.20	0.20
In-operando AC scattering software	Continue development of software for in-operando AC scattering experiments.	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*
Visualization Tools	Application and/or development of advanced visualization tools for APS beamline data analysis and experiment feedback.	0.00**	0.00**
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 FY21 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 a number of 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.

FY21 SDM Effort: 0.25 FTE
FY22 SDM Effort: 0.25 FTE
Out Years: TBD

Goals for FY21 and FY22 include:
1. Continue to provide support and development.
2. Utilize ANL-593 status and badge status to appropriately authorize access.
3. Integrate with beamline scheduling system to automatically add/remove remote users to specific beamline computers.

BES Data Solution Task Force Pilot Project

Summary: Collaborate with the ALS, CAMERA, LCLS, NSLS-II, and SSRL to share common XPCS, tomography, and ptychography software tools.

Team: Faisal Khan (SDM), Miaoqi Chu (SDM), Qingteng Zhang (DYS), Pete Jemian (BC), Suresh Narayanan (DYS), Francesco De Carlo (IMG), Junjing Deng (MIC), Nicholas Schwarz (SDM), et al.

FY21 SDM Effort: 2.50 FTE
FY22 SDM Effort: 0.00 FTE

Collaborate with the Advanced Light Source (ALS) and CAMERA at Lawrence Berkeley National Laboratory, the National Synchrotron Light Source II (NSLS-II) at Brookhaven National Laboratory, and the Linac Coherent Light Source (LCLS) and Stanford Synchrotron Radiation Lightsource (SSRL) at the SLAC National Accelerator Laboratory, to share common software tools, algorithms and data formats. This project focuses on integrating and deploying common X-ray Photon Correlation Spectroscopy (XPCS) data collection and processing software, including Bluesky from Brookhaven, XPCS-Eigen from Argonne, PyDM from SLAC, and Xi-CAM from Lawrence Berkeley, at XPCS instruments at each of the five BES light sources.

Goals for FY21 include:
1. Integrate bluesky for operations at 8-ID-I.
2. Create a Python wrapper for XPCS-Eigen.
3. Collaborate on a GUI for XPCS data processing.

A Collaborative Machine Learning Platform for Scientific Discovery

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

Team: Nicholas Schwarz (SDM), New Hire Postdoc, et al.

FY21 SDM Effort: 1.00 postdoc

FY22 SDM Effort: 1.00 postdoc

Goals for FY21 and FY22 include:

1. TBD

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), Nicholas Schwarz (SDM), Junjing Deng (MIC), Roy Guerra (BC), Pete Jemian (BC), Peter Kenesei (MPE), Arthur Glowacki (SDM), Miaoqi Chu (SDM), Faisal Khan (SDM), Suresh Narayanan (DYS), Jun-Sang Park (MPE), Max Wyman (BC), et al.

FY21 SDM Effort: 0.50 FTE
FY22 SDM Effort: 0.50 FTE

Goals for FY21 and FY22 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: Arthur Glowacki (SDM), John Hammonds (SDM), Sinisa Veseli (SDM), New Hire (SDM), New Hire (SDM), APS-IT, et al.
FY21 SDM Effort: 2.50 FTE
FY22 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 FY21 and FY22 include:

1. Continue support and roll-out to more beamlines.
2. On-board 2 new staff members.
3. Interface with Argonne Leadership Computing Facility (ALCF) tape-based storage.
4. Develop web portal and a graphical user interface for workflow and data processing job management.
5. Enhance services and tools for beamlines with high data rates and large data volumes.
6. Enhance workflow engine and processing job management capabilities.
7. Provide support for automating beamline processing workflows.
8. Provide software packaging for individual software components.

9. Enhance installation with support for external site deployments.

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.

FY21 SDM Effort: 0.10 FTE
FY22 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.
FY21 SDM Effort: 0.50 FTE
FY22 SDM Effort: 0.50 FTE
Out Years: TBD

Processing time of a 100 MB sample using serial MATLAB code takes 60 minutes using limited parameters. Current data acquisition time for a 100 MB data set is 20 minutes, and will decrease after the completion of the AP-U. 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, the vast majority of 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 reccdi tool is a very performant 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. There is constantly maintained user documentation. Other distribution options are investigated as well.

The tools run on GPU or CPU. The GPU size is a limit to what data size can be reconstructed with the tools. 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. Another goal is to add the multi-phasing feature, the novel research in the CDI field.

Goals for FY21 and FY22 include:
1. Provide easy installation of the reconstruction tools.
2. Provide documentation.
3. Optimize for size and speed, considering APS-U era needs.
4. 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.

Proposed Team: Miaoqi Chu (SDM), Ashish Tripathi (DYS), Zhang Jiang (DYS), Jin Wang (TRR), et al.
FY21 SDM Effort: 0.50 FTE
FY22 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 FY21 and FY22 include:
1. Explore the physical nature that distinguishes between the CSSI's surface scattering and transmission type scattering.
2. Identify possible approaches to incorporate scattering physics.
3. Implement prototype algorithms 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: Faisal Khan (SDM), Miaoqi Chu (SDM), Qingteng Zhang (DYS), Suresh Narayanan (DYS), et al.
FY20 SDM Effort: 1.00 FTE
FY21 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 in order 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.

Last year we moved fully to next generation XPCS toolkit for both SA-XPCS and WA-XPCS at 8-ID. The plan it to continue improving this software. Additionally, the focus for FY21 will be to make the software more widely available as a python module. In this regard, greater effort is being undertaken as part of the BES Data Solution Task Force Pilot Project.

Goals for FY21 and FY22 include:
1. Continue supporting the current tool and adding new features.
2. A python interface that is more suitable for deployments at collaborating facilities.
3. Incorporate analysis from other light sources based on ongoing discussions.
4. Develop a new XPCS GUI.
5. Begin planning and implementing a new version that can address APS-U era data rates.

General-Purpose Reciprocal-Space Mapping (RSM) Tools

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

Team: John Hammonds (SDM), Jonathan Tischler (SSM), Zhan Zhang (SSM), et al.
FY21 SDM Effort: 0.10 FTE
FY22 SDM Effort: 0.10 FTE
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 FY21 and FY22 include:
1. Continue supporting the current tool and adding new features as requested.

Ptychography Software

Summary: Provide ongoing support for ptychography reconstruction software and tools, and integration with complementary techniques.

Team: Ke Yue (SDM), Junjing Deng (MIC), Stefan Vogt (XSD-ADMIN), et al.
FY21 SDM Effort: 0.75
FY22 SDM Effort: 0.75
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 existing GPU-based ptychography code base.

Goals for FY21 and FY22 include:
1. Develop CUDA and C++ implementation of ML ptychography reconstruction algorithms.
2. Support current ptychography reconstruction library, ptycholib, ptychopy.
3. Support GUI interface for reconstruction.
4. Support workflow tools.
5. Support HPC library on ALCF with ptychopy.

6. Develop framework for ML, DM, ePIE.
7. In developments, plan for needs of APS-U era instruments.

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.
FY20 SDM Effort: 0.75 FTE
FY21 SDM Effort: 0.75 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 so as 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. In order 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 FY21 and FY22 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. Create general dataset import feature as a Python extension to allow user custom loading of datasets.
4. Collaborate with Northwestern University (Andrew Crawford) to implement background correction from his software M-BLANK.
5. Begin designing and implementing software for APS-U era.

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.
FY21 SDM Effort: 0.10 FTE
FY22 SDM Effort: 0.10 FTE
Out Years: TBD

Algorithmic work is underway in the XSD-CXS group.

Goals for FY21 and FY22 include:
1. Develop an application from MATLAB-based algorithmic code.
2. Optimize MATLAB code to run on LCRC 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), et al.
FY20 SDM Effort: 0.20 FTE
FY21 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 FY21 and FY22 include:
1. Implement the given algorithm for performance and ready for data streaming.
2. Assist with other code for this project, as needed.

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.
FY21 SDM Effort: 0.10 FTE
FY22 SDM Effort: 0.10 FTE
Out Years: TBD

A project is underway to upgrade the miniXES spectrometer presently on Sector 20 moving to Sector 25. 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.

Support for HT-HEDM Beamline Project

Summary: Develop and integrate auto-alignment/calibration tools and mail-in automation software with existing systems for the new HT-HEDM beamline.

Team: Sinisa Veseli (SDM), Faisal Khan (SDM), Bob Suter (CMU), Jon Almer (MPE), et al.
FY21 SDM Effort: 0.10 FTE
FY22 SDM Effort: 0.10 FTE
Out Years: TBD

Work in this area will be applicable to many other APS beamlines, including 1-ID and 12-ID. Project deliverables are currently being scoped.

Goals for FY21 and FY22 include:

1. Provide support for HT-HEDM data acquisition and processing workflows.
2. Implement additional alignment algorithms.
3. Integrate alignment with data acquisition workflow.
4. Test the technique developed for alignment and calibration at 1-ID and 6-ID.
5. Integration of data from the HT-HEDM beamline with third-party data analysis and mining tools.

In-operando AC scattering software

Summary: Continue development of software for in-operando AC scattering experiments.
Proposed Team: John Hammonds (SDM), Henry Smith (SDM Co-op student), Philip Ryan (MM), et al.
FY21 SDM Effort: 0.10 FTE
FY22 SDM Effort: 0.10 FTE
Out Years: TBD

Continue development of the xPlotUtil in-operando AC scattering software.

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), Ned Arnold (CTL), John Carwardine (APS-U), et al.
FY21 SDM Effort: 0.75 FTE*
FY22 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.

Goals for FY21 and FY22 include:

1. Develop and deploy production version of the DAQ data correlation/alignment service.
2. Develop and deploy production version of the DAQ orbit service.
3. Develop and deploy production version of the high-level integrated control of capture & processing.
4. Enhance and refine DAQ IOC drivers for consistency and support of all acquisition modes.
5. Enhance processing services.
6. Provide DAQ support for AOP use cases and applications.
7. Provide support for development of new DAQ IOCs.
8. Provide support for production packaging and deployment of DAQ IOCs, tools and services.

Visualization Tools

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

Proposed Team: TBD SDM Member, et al.
FY21 SDM Effort: 0.00 FTE
FY22 SDM Effort: 0.00 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 in the near future. 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, such as ParaView, on advanced computational resources are needed in order to cope with these large and complex data streams.

Multi-modal Diffraction Tomography

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

Proposed Team: TBD SDM Member, et al.
FY21 SDM Effort: 0.00 FTE**
FY22 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.
FY21 SDM Effort: 0.00 FTE**
FY22 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.