Scientific Software Engineering & Data Management
X-ray Science Division (XSD), Advanced Photon Source
Effort Plan for FY20 and FY21

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 XSD-CXS group to implement new algorithms and mathematical methods, and with the XSD-BC group to integrate data analysis with beamline data acquisition systems. This document will be reviewed and updated at least once a year.

Five-year Goals

The SDM group's goals over the next five years 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 FY20 & FY21

High-level goals for FY20 & FY21 are:

- Integrate the APS Data Management System with Argonne Leadership Computing Facility (ALCF) tape-based storage. (Q1 FY20)
- 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 FY20 & FY21 goals for the BES Data Solutions Task Force Data Pilot Project.

Project	Summary	FY20 SDM FTE	FY21 SDM FTE
BES Data Solution Task Force Pilot Project	Collaborate with the ALS, CAMERA, LCLS, NSLS-II, and SSRL to share common XPCS software tools.	1.00	1.00
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
MONA	Project aimed at integrating bluesky with APS HPC data analysis packages and other tools to enable automated experiment feedback.	0.50	0.50
APS / NSLS-II Data Collaboration	Synergize collaborations and best leverage scarce resources to provide optimal value and interoperability among facilities in the area of data acquisition, management, analysis, and visualization.	0.25	0.25
Bragg Coherent Diffraction Imaging (CDI) Software	Implement and parallelize genetic algorithms and phase retrieval methods for the Bragg CDI technique.	0.50	0.50
Correlation Toolkit	Develop a real-time HPC-enabled set of tools for time-based correlation data analysis.	0.75	0.75
General-Purpose Reciprocal-Space Mapping (RSM) Tools	Continue development and deployment of high-performance RSM tools.	0.20	0.20
Support for 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.	0.20	0.20
Laue Diffraction	Develop 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	0.25	0.25
Data Quality, Feedback & Control Tools	Toolkit and framework to verify quality of collected data and provide feedback during and after acquisition.	0.20	0.20
Workflow & Data Management Tools	Continue application of analysis workflow, web portals, and data management and distribution tools at APS beamlines.	0.50	0.50

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
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*
Component Database (CDB) for APS-U	An electronic system for tracking and documenting accelerator and beamline components.	0.75*	0.75*
Coherent Surface Scattering Imaging (CSSI) Software	Implementation of high-performance CSSI and GISAXS software applications.	0.00	0.00
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 FY20 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

BES Data Solution Task Force Pilot Project

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

Team: Faisal Khan (SDM), Qingteng Zhang (DYS), Pete Jemian (BC), Suresh Narayanan (DYS), Nicholas Schwarz (SDM), et al.

FY20 SDM Effort: 1.00 FTE
FY21 SDM Effort: 1.00 FTE
Out Years: TBD

Summary: 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. 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.

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.

FY20 SDM Effort: 0.10 FTE
FY21 SDM Effort: 0.10 FTE
Out Years: TBD

MONA

Summary: Project aimed at integrating bluesky with APS HPC data analysis packages and other tools to enable automated experiment feedback. The current focus is on XRF streaming and Laue reconstructions.

Team: Barbara Frosik (SDM), Arthur Glowacki (SDM), Faisal Khan (SDM), Ke Yue (SDM), Doga Gursoy (CXS), Tekin Bicer (CXS/MCS), et al.

FY20 SDM Effort: 0.50 FTE
FY21 SDM Effort: 0.50 FTE
Out Years: TBD

APS / NSLS-II Data Collaboration

Summary: Synergize collaborations and best leverage scarce resources to provide optimal value and interoperability among the APS and NSLS-II in the area of data acquisition, management, analysis, and visualization.

Team: Arthur Glowacki (SDM), Doga Gursoy (CXS), John Hammonds (SDM), Faisal Khan (SDM), Pete Jemian (BC), Nicholas Schwarz (SDM), Brian Toby (CXS), Andrey Yakovenko (SRS), NSLS-II Staff, et al.
FY19 SDM Effort: 0.25 FTE
FY20 SDM Effort: 0.25 FTE

Synergize collaborations and best leverage scarce resources to provide optimal value and interoperability among the APS and NSLS-II in the area of data acquisition, management, analysis, and visualization. The APS will target the adoption of bluesky for new beamlines, including the APS-U suite of beamlines. The NSLS-II and the APS will aim to share APS developed HPC code bases and modify them for use by both facilities. Both facilities will integrate existing data management tools with the bluesky suite of acquisition tools, and with streaming HPC-enabled data analysis tools. Together both facilities will investigate tools and technologies for advanced visualization capabilities.

Effort in this area may overlap significantly with other projects described in this document. See the *APS / NSLS-II Data Acquisition, Management, Analysis, and Visualization Working Group Collaboration Report* and the *APS / NSLS-II Data Acquisition, Management, Analysis, and Visualization Working Group FY18 – FY19 Plan* for more detailed information and timelines.

Goals for FY20 and FY21 include:
1. Utilizing bluesky.
2. Sharing APS developed XPCS and XRF software with the NSLS-II.
3. Common metadata formats between the APS and NSLS-II for a few targeted techniques.

Bragg Coherence Diffraction Imaging (CDI) Software

Summary: Implement and parallelize genetic algorithms and phase retrieval methods for Bragg CDI techniques.

Team: Barbara Frosik (SDM), Ross Harder (MIC), et al.
FY20 SDM Effort: 0.50 FTE
FY21 SDM Effort: 0.50 FTE
Out Years: TBD

A genetic algorithm approach to CDI phase retrieval will improve coherent imaging in two aspects. The first is to enable the recovery of highly reproducible images from a given data set. The second is to render previously impossible to image samples amenable to CDI, opening the door to a greater scientific impact for the method. The basic idea is to do the same phasing process with tens to thousands of random starting points. The diversity of results is then exploited to arrive at a highly reproducible image of the sample. Another aspect of genetic algorithm approaches is in the "fitness" criterion used to evaluate the population of results. This can be tuned to enable phase retrieval of datasets that have previously been impossible to produce images from. It is desired to implement and parallelize software for fast processing by non-expert beamline users.

Current 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.

Goals for FY20 and FY21 include:
1. Add alternative algorithms.
2. Make system use resources in a more economic manner when running in parallel.
3. Improve performance in Python code for preparation and display phases.

Correlation Toolkit

Summary: Real-time HPC-enabled set of tools for time-based correlation data analysis.

Team: Faisal Khan (SDM), Qingteng Zhang (DYS), Suresh Narayanan (DYS), et al.
FY20 SDM Effort: 0.75 FTE
FY21 SDM Effort: 0.75 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.

The current-generation HPC-enabled correlation system has been in use since February 2013, primarily by the Small-Angle X-ray Photon Correlation Spectroscopy (SA-XPCS) beamline at 8-ID-I, where it has been used by every user group at that beamline for multi-tau, and, more recently, two-time correlation analysis. These and other correlation algorithms will be critical to the techniques used by many APS-U first experiments. In order to serve a larger community of dynamics driven experiments, such as image correlations for materials exploration and high-speed imaging techniques, a real-time, general-purpose correlation toolkit implementing more advanced correlation methods using parallel computational and algorithmic techniques, and deployed on high-performance computing (HPC) resources is required. This work will leverage effort related to workflow and management tools, and data streaming and analysis tools for real-time correlation analysis.

Goals for FY20 and FY21 include:
1. Implementing additional analysis algorithms.
2. Implement a robust and fully featured Python wrapper.
3. Supporting data from multiple detector types.
4. Deploying for Wide Angle XPCS.
5. Evaluating Python-based Jupyter notebooks for interactive analysis.

General-Purpose Reciprocal-Space Mapping (RSM) Tools

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

Team: John Hammonds (SDM), Jonathan Tischler (SSM), et al.
FY20 SDM Effort: 0.20 FTE
FY21 SDM Effort: 0.20 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.

Support for 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), Youssef Nashed (MCS), et al.
FY20 SDM Effort: 0.75
FY21 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 FY20 and FY21 include:
1. Develop CUDA and C++ ML ptychography reconstruction algorithms.
2. Support current ptychography reconstruction library, GUI interface, and HPC library on ALCF.

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 (CXS), Stefan Vogt (MIC), 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 FY20 and FY21 include:
1. Continue developing a graphical user interface for XRF-Maps.
2. Use interferometer data for precision coordinates.
3. Investigate feasibility of tomography alignment algorithms for XRF tomography alignment in XRF-Maps.

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 (CXS), et al.
FY20 SDM Effort: 0.20 FTE
FY21 SDM Effort: 0.20 FTE
Out Years: TBD

Algorithmic work is underway in the XSD-CXS group.

Goals for FY20 and FY21 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. The new algorithm uses physical mask that is being relocated for several “masked” scans. The initial data, (i.e. without mask) together with the altered data, and the mask, is used to find the orientation of grains in the subject.

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

Goals for FY20 and FY21 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.

FY20 SDM Effort: 0.25 FTE
FY21 SDM Effort: 0.25 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.

Data Quality, Feedback & Control Tools

Summary: Toolkit and framework to verify quality of collected data and provide feedback during and after acquisition.

Team: Barbara Frosik (SDM), Francesco De Carlo (IMG), Doga Gursoy (CXS), Jonathan Almer (MPE), Byeongdu Lee (CMS), et al.
FY20 SDM Effort: 0.20 FTE
FY21 SDM Effort: 0.20 FTE
Out Years: TBD

Confirming the quality of data that has been and is being collected is critical to the efficient and effective use of experiment beam time at the APS. Without such quality checks experimenters are collecting "in the dark" and may discover issues only after beam time is over. As data volumes and rates increase due to the further deployment of higher frame-rate detectors and the increase in flux and coherence afforded by the APS-U project, and due to the complexity of novel experiments enabled by the APS-U project, the ability to check data quality in real-time in order to alert experimenters to potential data collection issues, and to be able to provide feedback and automatically adjust experiment parameters is necessary.

These tools and framework provide a mechanism for monitoring data and applying appropriate and user definable quality checks to experiment data. It can verify that EPICS PV values are within expected ranges, monitor files and compare them against predefined schemas, and apply mean, standard deviation, and delta mean statistical methods to data. Further work is required in order to catalog results for use as a log, and as input to machine learning algorithms for real-time, automated feedback. This work will synergize with other effort related to workflow and management tools, and real-time data streaming and analysis tools.

Controller will use the feedback from verifier in form of process variables and will determine how the experiment instruments need to adjust. The tool will provide a framework so it can be adopted to other beamlines in the future.

Goals for FY20 and FY21 include:

1. The initial project will be implemented for the 12-ID-C beamline.

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), Dariusz Jarosz (SDM), Sinisa Veseli (SDM), et al.
FY20 SDM Effort: 0.50 FTE
FY21 SDM Effort: 0.50 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 FY20 and FY21 include:

1. Interface with Argonne Leadership Computing Facility (ALCF) tape-based storage.
2. Develop web portal and a graphical user interface for workflow and data processing job management.
3. Enhance services and tools for beamlines with high data rates and large data volumes.
4. Enhance workflow engine and processing job management capabilities.
5. Provide support for automating beamline processing workflows.

Support for HT-HEDM Beamline Project

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

Proposed Team: Sinisa Veseli (SDM), Faisal Khan (SDM), Bob Suter (CMU), Jon Almer (MPE), et al.
FY20 SDM Effort: 0.20 FTE
FY21 SDM Effort: 0.20 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 FY20 and FY21 include:

1. Integration of the APS Data Management System with the HT-HEDM control system.
2. Integration of data from the HT-HEDM beamline with third-party data analysis and mining tools.

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 (SDM), Ned Arnold (CTL), John Carwardine (APS-U), et al.
FY20 SDM Effort: 0.75 FTE*
FY21 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 FY20 and FY21 include:
1. Design and prototype DAQ data correlation/alignment service.
2. Design and prototype DAQ orbit service.
3. Design and prototype 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. Design and prototype framework for production packaging and deployment of DAQ IOCs, tools and services.

Component Database (CDB) for APS-U

Summary: An electronic system for tracking and documenting accelerator and beamline components.

Proposed Team: Dariusz Jarosz (SDM), Sinisa Veseli (SDM), Ned Arnold (CTL), John Carwardine (APS-U), et al.
FY20 SDM Effort: 0.75 FTE*
FY21 SDM Effort: 0.75 FTE*
Out Years: TBD

The APS-U project aims to replace the existing APS storage ring under an aggressive one-year schedule for removal, installation and testing. Management of the thousands of components to be installed in such a short time represents a significant challenge. The Component Database (CDB) is a tool for organizing and tracking components and designs used for the APS storage ring upgrade. It helps capture component documentation, provides a repository for inspection and measurement data (e.g. electronic travellers), and supports logging of component history through the component's life cycle. CDB is built around relational database, web portal, and REST web service technologies, and provides users with a number of options for accessing the system. In particular, it serves as a user portal for finding all known information about a specific component or a design. To that end, CDB provides links and interfaces to external systems commonly used at APS, such as various drawing and document management systems, procurement applications, etc. Future efforts will focus on extending the system capabilities to capture cable connections, enabling access via mobile applications, and providing custom views for different user groups.

Goals for FY20and FY21 include:
1. Machine Design UI Enhancements.
2. CDB Relationships.
3. Continue working with the traveler working group to ensure application support requirements for receiving components and APS-U.
4. Integration of CDB with a cable tracking application.

5. Provide support for APS-U data management use cases.
6. Enhance capabilities of the CDB mobile application.

Coherent Surface Scattering Imaging (CSSI) Software

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

Proposed Team: Ke Yue (SDM), Zhang Jiang (DYS), Jin Wang (DYS), et al.
FY20 SDM Effort: 0.00 FTE
FY21 SDM Effort: 0.00 FTE
Out Years: TBD

CSSI and the non-coherence dependent complementary technique, GISAXS, will be critical techniques used at a number of APS-U beamlines. Algorithm and model development are currently underway. Proposed LDRDs will further required development in this area, however, software coding effort will be needed in order to fully realize the benefit of these developments once sufficient algorithmic advances are made.

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.
FY20 SDM Effort: 0.00 FTE
FY21 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.
FY20 SDM Effort: 0.00 FTE**
FY21 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.
FY20 SDM Effort: 0.00 FTE**
FY21 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.