September 28, 2018

XST-CXS Strategy/Goals

Strategy

The XSD Computational X-ray Science (CXS) Group develops mechanisms for understanding complex phenomena from APS measurement data. To do this:

- CXS computational scientists develop theory, mathematical models, algorithms and prototype software in collaboration with XSD beamline scientists and software engineers in the XSD Scientific Software Engineering & Data Management (SDM) Group. CXS focus is on methodology development, rather than creating professional-quality software packages;
- CXS also seeks to improve the effectiveness of next-generation beamline experiments through data analysis, visualization, modeling and adaptive control strategies, which are implemented in collaboration with engineers in the SDM and Beamline Controls (BC) Groups;
- CXS establishes collaborations in data analysis methods with scientists in other user facilities and with mathematicians, computer scientists and other professionals in other divisions of Argonne.
- CXS works to increase use of large-scale computational facilities within the DOE complex;
- CXS performs outreach to improve software development skills amongst APS beamline scientists and teaches techniques in data analysis using locally-developed software to APS users.
- CXS provides expertise as consultants in areas such as tomography, crystallography, spectroscopy theory, applied mathematics, leadership-scale parallelization and experimental design to aid in XSD projects.

Five-year goals

The CXS group develops advanced algorithms and strategies for data analysis in support of XSD beamlines. In cooperation with the BCDA and SDM groups, results are deployed as open source software packages for users and beamline scientists. Specific targets are:

- Routine integration of streaming data analysis and high-level visualization across XSD high-data rate beamlines, employing DOE leadership-scale computing facilities, where appropriate;
- Prototyping adaptive control strategies that allow for steering of experimental conditions from streamed data analysis to perform experiments on timescales too fast for human-instrument interaction;
- Development of multimodal data analysis methodology to derive results that fully utilize the measurements possible with the APS-U.

Goals and Action Plan for FY2019 and beyond

- Port Midas from Swift-k (now deprecated) to MPI; develop corrections for pixel-array detection. Extend the scope of HEDM to smaller grained and heavily deformed materials. Initiate educational outreach on HEDM analysis using Midas
- Further research on coupling experimental data collection and analysis via MONA
- Deploy streaming tomography analysis
- Novel algorithm development for joint reconstruction of ptychography-tomography data
- Research on novel 1D masked aperture diffraction reconstruction algorithms
- Advanced modeling and optimization combining multimodal tomography modalities including fluorescence and ptychography imaging
- HPC-implemented scheme for correcting positioning errors in tomographic reconstruction
- Completion of few remaining analysis applications so that GSAS-II can be a fully comprehensive

materials crystallography analysis package; document the computations in a monograph.
- Theoretical study of pump-probe X-ray spectroscopies on systems excited away from equilibrium using ultra-high performance computing. Development of new theoretical methodologies in X-ray spectroscopy.
- Theory support of experimental groups in X-ray spectroscopy and elastic/inelastic X-ray scattering.

SWOT Analysis for Scientific Data Analysis Methodologies

Strengths	Weaknesses
• World-leading computational experience in a number of scientific areas. • World-class beamline staff and user groups that spur new analysis approaches. • Ability to form teams pairing computation scientists with software and beamline engineers. • XSD scientists have extensive interest and experience with scientific software; ~25 tools, some best-in-field, have been developed. • ANL has world-class expertise in applied math, computer science, HPC as well as data and computation facilities.	• Foreseeable funding levels will require triaging of projects. • CXS expertise does not cover the breadth of XSD techniques; domain-specific skillsets are time consuming to develop • Few examples exist for successful scientific development as a cooperative effort between small teams of computational scientists and software/beamline engineers.
Opportunities	**Threats**
• Having shared staffing with MCS will help increase interactions with non-APS experts. • Interest in experimental support from ALCF, LCRC and NERSC is allowing beamlines to expand computational resources to leadership-scale. • The APS Upgrade will allow the opportunity to rethink the entire data acquisition / reduction / analysis / data delivery chain, which to date has been engineered piecemeal. • Other light sources wish to collaborate on data analysis activities	• The APS is world-leading in the majority of techniques; a small number of staff must support a broad range of efforts or the APS will lose ground; users will seek beamlines where they can be most productive • Collaborative projects with external organizations may not produce code meeting APS needs. • Users/staff will be overwhelmed and unable to analyze data from APS-U beamlines due to lack of HPC-ready software.

FY19 Milestones:

1st Quarter:

- Discussions with ALCF and/or LCRC on streaming tomography analysis deployment
- GSAS-II: Complete commensurate magnetism treatment & image calibration/integration API
- Initial demonstration of optimal aperture design for diffraction depth reconstruction

2nd Quarter:

- Validation of a MPI-implemented Midas starts

3rd Quarter:

- Deploy streaming tomography analysis for one APS beamline
- Demonstration of HPC-based tomography error correction.
- Implement spatial corrections for Pilatus & Dexela detectors

4th Quarter:

- GSAS-II: Complete incommensurate magnetism treatment and stacking fault refinement