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XST-CXS Strategy/Goals

Strategy

The XSD Computational X-ray Science (CXS) Group develops methodologies 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. Software engineers in the XSD Scientific Software Engineering & Data Management (SDM) Group then create professional software packages utilizing these results;
- 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 communicates APS computational needs to establish collaborations with other light sources and with mathematicians, computer scientists and other professionals in other divisions of Argonne. Through external coordination, large-scale APS computation is deployed on 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 offers its expertise 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.
- Demonstration of ground-breaking applications for Machine Learning and related methodologies for advancement of synchrotron-based data collection and data analysis.

Goals and Action Plan for FY2020 & FY2021

- Advanced 3D reconstruction capabilities for ptycho-laminography and ptycho-tomography; continued improvements in TomoPy.
- Development of synchrotron implementations for masked-aperture and timing-sequence reconstruction.
- Numerical methods development for multimodal nanometer-scale fluorescence tomography.
- Generalized frameworks and workflows for streaming data analysis and analysis-driven automated experimental control.

- Improved capabilities for crystallographic/PDF data reduction and modeling using GSAS-II.
- Deployment of streaming HEDM processing at LCRC via on-demand scheduling; provision of off-line computation for user-driven reprocessing; extend methods for highly deformed materials.
- Methodology for identification and masking of spurious signals in Bragg coherent diffraction imaging.
- 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 CELS divisions will help increase interactions with non-APS experts. • Opportunities for computational support from ALCF, LCRC and NERSC can allow beamlines to access leadership-scale resources. • 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.