XSD-CXS Strategy and Goals

Strategy:

The XSD-Computational X-ray Science (CXS) group develops the methods and computational tools used by beamline scientists and APS users to process and interpret experimental data. Our efforts are directed both towards the development of techniques and software to quickly and efficiently analyze data from existing x-ray characterization tools at the APS, and towards the development of new computational and AI-enabled methods that expand the suite of x-ray characterization tools at the APS. Our efforts are driven by a diverse group of computational scientists with expertise in beamline science, algorithms, applied math, theory, physical sciences, optimization and machine learning (ML). Members include joint appointees with the Data Science and Learning (DSL) division, the Math and Computer Science (MCS) division and the physics department at Northern Illinois University (NIU). We also work closely with the Software and Data Management (SDM) group to translate methods developed in the CXS group into user-friendly software packages, and with the Beamline Controls and Data Acquisition (BCDA) group on the development of methods for experimental automation.

Five-year goals:

The CXS group's 5-year goals are aimed at the development of capabilities that will enable the maximum utilization of the dramatically improved brightness, coherence and high energy x-rays provided by APSU. We identify four high priority research and development areas:

- **Real-time analysis and visualization**: Streaming data analysis, data abstraction, enhancement and visualization across various high-data-rate APSU feature beamlines, employing high-performance computing facilities on-demand. Real-time error detection and mitigation.
- **Experimental automation**: AI-guided steering of experiments removing too-slow human decision making from the loop and allowing autonomous tracking and targeted acquisition of data in a rapidly evolving material.
- **Multimodal data analysis**: Methods to derive maximum insight from multimodal data streams.
- **Novel characterization methods**: Couple advances in AI and computation with the enormous coherent flux provided by APSU to create new characterization methods that go beyond current hardware limitations.

Goals and Action Plan for FY2021 & FY2022

- Strengthen collaboration with beamlines, BCDA and SDM to translate methods, software and algorithms developed in the group to user-friendly software packages.
- Advanced 3D reconstruction capabilities for nanoimaging including ptycho-laminography, ptycho-tomography, micro-CT, XRF-tomography, Bragg coherent diffraction imaging (BCDI), Bragg ptychography and Laue micro-diffraction. Explore use of convolutional neural networks (CNNs) for improving the reconstruction quality and performance on GPUs. Continue exploration of self-supervised ML techniques for phase retrieval that will accelerate and improve quality of reconstructions.
- Continue development of efficient distributed optimization techniques for tomography and ptychography to address the experimental challenges such as drifts, noise, errors, etc.

- Explore feasibility of tensor-field reconstruction methods for dichroic 3D ptychography; expand current 3D ptychography software for simulating magnetization and for imaging tensor-fields.
- Numerical methods development for multimodal nanometer-scale fluorescence tomography.
- Continued development of AI-enabled high-resolution coherent imaging methods including sparse-sampled ptychography, Bragg ptychography with dynamical effects and *operando* Lorentz TEM.
- Development of structured illumination techniques such as masked-aperture and timing-sequence reconstruction.
- Generalized frameworks and workflows for streaming data analysis and automated experimental control.
- Improved capabilities for crystallographic/pair distribution function data reduction and modeling using GSAS-II.
- Extend HEDM techniques to highly deformed materials by developing peak-focus FF-HEDM and full-field NF-HEDM modes; implement AI driven peak detection systems to speed up reconstruction times.
- 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 of the CXS group:

Strengths	Weaknesses
• World-leading expertise in algorithms, theory, modeling and machine learning applied to x-ray science. • Diversity in x-ray characterization techniques supported by the group.	• Current funding and staffing levels limit the number of beamlines and techniques supported by the group. • Successfully translating methods, algorithms and software developed by the group into user-friendly packages.
Opportunities	**Threats**
• Unique computational resources at ANL including the world's first exascale machine (Aurora) and the world's largest AI chip (Cerebras). • Development of ML frameworks and hardware for edge computing.	• Data rates post APSU will exacerbate inadequacies in current data analysis methods. • Effect of the COVID19 pandemic on scientific collaborations and personnel efficiency.