January 1, 2023

XSD-XST Strategy Document

Mission

The X-ray Science Technologies (XST) section of the X-ray Science Division (XSD) aims to deliver innovative instrumentation and concepts to further the XSD mission. XST contributes to the success of XSD, APS, and APS-U by providing integrated technology solutions that make possible forefront scientific research with synchrotron X-rays.

Organization

The XST section comprises the Beamline Instrumentation (BI), Beamline Controls (BC), Computational X-ray Science (CXS), Detectors (DET), Optics (OPT), and Scientific Software and Data Management (SDM) groups. It also includes the Nanopositioning Support Laboratory (NPL). These groups are in a single structural organization as part of a strategic effort to accelerate the development of integrated forefront beamline instrumentation.

Vision

XST will transform beamline planning, design, and implementation from assembling individual components, e.g., insertion device, monochromator, optical components, detectors, data acquisition, data reduction, etc., to an approach that optimizes all beamline building blocks in context. For example, can downstream optical components actively compensate for monochromator vibrations? Can novel data acquisition and reduction paradigms reduce the effect of mechanical stability and reproducibility in scanning sample stages?

XST is more than the sum of its constituent groups. Project teams from across XST groups collaborate with XSD stakeholders to develop and equip x-ray beamlines to perform cutting-edge science. XST delivers integrated, optimized and unique instruments from concept through to operation. The XST management structure within XSD enables the XST technical groups to pursue this vision.

Strategy – Objectives

To achieve our mission, we are investing in R&D and technical activities to take full advantage of APS and APS-U. We are pursuing projects that are key to exploiting the APS-U source characteristics, in particular the development of high stability and/or high precision instrumentation, as well as concepts and infrastructure to handle the continuous increase in experiment complexity and data stream rates appropriately.

Pursuant to our vision, we are developing new approaches that take a holistic view of the experiment, starting at the experimental model through experiment setup, control, data acquisition, analysis, and visualization. These include:

- Modeling of instrumentation to carry out *in silico* prototype versions of experiments in advance of actual experiments.
- Development of fast, flexible, and precise data acquisition so that
  - Data acquisition time is maximized in relevant areas of interest
  - Experiments can achieve the highest spatial resolution and sensitivity (e.g., <5 nm positional control @1kHz).
- Real-time tools for computationally intensive data analysis to evaluate and interpret acquired

data in a time scale relevant to the experiment.

- New 'intelligent' analysis algorithms to
  - Drive and control instrumentation
  - Correct for instrumentation limitations
  - Significantly expand experimental capabilities (e.g., BCDI, ptychography, tomography, etc.)

We are developing and exploring new instrumentation platforms capable of data acquisition at the required speed, stability, precision, efficiency, frame rate, etc. Specific examples include:

- High-speed scanning (<5 nm, >1 kHz) on a high-stability platform
- Novel optics, e.g., wavefront preserving mirrors, nano-focusing optics, thin film optics
- Sensors implementing on-chip compression or edge computing for techniques like microscopy, ptychography and XPCS
- Energy resolving detectors, e.g., TESs for higher x-ray energies and Ge strip detectors
- Data management (acquisition, streaming, transfer, quality control, reduction) at multiple GB/s sustained rate

These developments will enable novel, innovative x-ray techniques and scientific approaches orders of magnitude faster and more sensitive than today.

<u>Strategy – Tools</u>

1. Communicate effectively

An essential aspect of our strategy is effective communication within XST, with our stakeholders (e.g., beamline personnel; XSD, APS, and APS-U management), and with our collaborators (e.g., APS users; other APS and Argonne divisions; other national laboratories).

2. Focus on XSD priorities

XST will accomplish its vision to deliver integrated technical solutions by focusing on the design, development, and construction of instruments for current and future APS beamlines in support of these XSD priorities:

- Brightness- and coherence-driven beamlines and techniques
- High-energy beamlines and techniques (> 20 keV x-rays)
- Timing and high-speed imaging capabilities
- Beamline operations and development

These priorities derive from the strengths of the APS Upgrade (APS-U) and the goal of sustained successful operation of APS beamlines.

3. Think strategically at the group level

Each XST group has a strategy to support the overarching XSD mission. Group strategy documents are updated to reflect changes in XSD and APS priorities, evaluate the impact of advances in our fields of expertise (e.g., emerging technologies), and document our activities and available resources. The strategy documents for each XST group and the Nanopositioning Support Laboratory are here: https://www.aps.anl.gov/X-ray-Science-Division/XSD-Strategic-Plans

4. Assemble crosscutting teams for XSD/APS high-priority strategic projects

Based on XST group strategies, we identify projects where an integrated design and implementation approach will result in a superior product. Teams formed across XST and APS plan and execute these projects.

5. Pursue sustained R&D efforts

Excellent beamline performance and best-in-class instruments require up-to-date skills and technology and the insight afforded by R&D projects. The strategy document of each XST group identifies areas where we will concentrate our R&D efforts.

6. Develop well-engineered and widely applicable solutions.

As we focus on a team approach to instrument development, we will balance novel "one-off" applications with the pursuit of solutions for use across the facility. This strategy can satisfy individual beamline needs and drive efficiency across the facility.

Strategy – Implementation

The APS Upgrade provides a focal point for organizing XST efforts and identifying strategic paths for each group. Crosscutting teams will collaborate with beamline scientists and other resources to design, construct, and deploy integrated beamlines, instruments, and facilities. In contrast with prior approaches to beamline or instrument development, the team will be involved in the design, planning, and execution for the full scope and duration of the project, with particular emphasis on identifying and leveraging synergies and interactions among beamline and experiment components. We will identify team members based on project requirements, staff expertise, and availability, but be mindful of XST-staff career and performance stretch goals.

Effective communication is crucial for the success of this project team approach. In particular, for APS-U projects, we define and coordinate clear boundaries for work implemented by either APS-U or APS operations.

Five-year Goals

Links to the strategy document for each XST group are provided at the URL listed above. The strategy documents include goals for each group. The goals listed here and in the next section are a subset of those goals, namely the ones that will require the participation of several, if not all, XST groups.

- Develop stable, rapid scanning, nano-positioning capable end stations to exploit the upgraded source—support nm metrology for data acquisition and diagnostics.
- Develop wavefront-preserving crystal and mirror optics, including related modeling, simulation tools, and metrology.
- Develop and deploy a robust set of high-performance computing (HPC) enabled software for data-intensive techniques that can leverage DOE leadership computing facilities (LCFs) seamlessly integrated with data processing pipelines.
- Develop AI-enabled digital twin beamlines providing control algorithms integrated with wavefront diagnostic tools to support beamline auto-alignment, adaptive optics control, and wavefront and beam focus optimization.

Goals and Action Plan for FY2023

- Continue to execute and support APS-U beamline projects; FY2023 (and FY2024) is an especially critical year with the one-year APS-U dark period scheduled to begin April 17, 2023
- Continue to execute and support priority DOE and XSD Operations projects such as the cavity-based x-ray free electron oscillator (CBXFEL), DOE Early Career Awards, LDRDs, and other operational priorities established by XSD management.
- Continue to advance the beamline data pipeline (BDP) project both in elucidating requirements for multimodal data acquisition and in building solutions for feature and enhanced beamlines that leverage the toolbox of supported infrastructure and that satisfy APS-U beamline requirements.
- Demonstrate the utility of a data processing unit (DPU) or SmartNIC to perform high bandwidth data processing impactful for APS beamlines.
- Continue to advance mirror zoom optics, including *in situ* metrology and feedback control.

XST SWOT Analysis

This SWOT analysis relates to XST as a whole, not to its constituent technical groups.

Strengths	Weaknesses
• XST personnel have strong technical skills and are highly motivated. • APS-U beamline requirements provide a focal point for XST activities. • Interaction between XST personnel across technical groups enables cross-pollination of ideas. • Shared management with XSD beamline personnel decreases barriers to execution. • Can leverage knowledge and expertise of XSD beamline scientists and APS users.	• Some technical areas are not represented or do not have sufficient depth, i.e., skills are concentrated in a few key personnel. • Need to leverage resources outside of XST more effectively. • Existing 20+-year-old infrastructure may constrain innovation.
Opportunities	**Threats**
• Bring successful implementation of mechatronics (combined electronics and mechanical engineering) to APS-U beamlines, e.g., active monochromator vibration control. • Develop beamline instruments that are "integrated by design," i.e., address all aspects of implementation and performance from concept to deployed instrument. • Become a world leader in experiment feedback, mechatronics, and adaptive coherence-preserving optics. • Build on synergies with other ANL Directorates to further impact. • Develop cross-platform sample environments optimized for APS-U feature and enhanced beamlines.	• Competition for scarce resources. • Failure to realize the XST vision in a timely manner could cause our stakeholders and sponsor to stop trusting us. • Increasingly stringent standards due to the characteristics of the APS-U x-ray beam, e.g., vibration control, coherence preservation, and increased data rates. • Adapting to new techniques and experiment requirements, e.g., on-the-fly scanning, real-time analysis, and multimodal data sets.