

September 1, 2021

## **XSD-XST Strategy Document**

### **Introduction: XSD-XST Mission**

The mission of the X-ray Science Technologies (XST) section of the X-ray Science Division (XSD) is 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 technical solutions that make possible forefront scientific research with synchrotron X-rays.

### **XSD-XST 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). All of these groups existed in some fashion prior to the creation of XST, but are now in a single structural organization as part of a strategic effort to accelerate development of integrated forefront beamline instrumentation.

### **Vision – XST 2025**

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 assembled from across XST groups work in collaboration 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 operations. A common 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 appropriately the continuous increase in experiment complexity and data stream rates.

Pursuant to our vision, we are developing new approaches that take a holistic view of the experiment, starting at the experimental model, all the way 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 on relevant areas of interest; and
  - experiments can achieve 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; and
  - 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., wave front 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

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

## **Strategy – Tools**

### **1. Communicate effectively**

An important 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 from the goal of sustained successful operation of APS beamlines.

### **3. Think strategically at group level**

Each XST group has developed its own strategy to support the overarching XSD mission. We will keep group strategy documents updated to reflect changes in XSD and APS priorities, to evaluate the impact of advances in our fields of expertise (e.g., emerging technologies), and to document our activities and available resources. Up-to-date XST group strategies will make clear the projects we can pursue and ones that require additional resources. The strategy documents for each XST group and the Nanopositioning Support Laboratory are in <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 not only up-to-date skills and technology, but also, most importantly, the vision and experience 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 pursuit of solutions to common beamline requirements for use across the facility, as well as look for ways to repurpose one-off solutions globally. This strategy has the advantage of satisfying individual beamline needs but also driving efficiency across the facility.

#### **Strategy – Implementation**

The feature beamlines, beamline enhancements, and instrumentation of the APS Upgrade provide the focal point for organizing the XST effort and for identifying strategic paths for each XST group. XST crosscutting teams will collaborate with beamline scientists and other APS, APS-U, and/or Argonne resources in the design, construction, and deployment of integrated beamlines, instruments, and facilities, both for APS operations up to the upgrade and for APS-U beamlines. In contrast with typical prior approaches to beamline or instrument development, the team will be involved in design, planning, and execution for the full scope and duration of the project, with particular emphasis in identifying and leveraging synergies and interactions among beamline/experiment components.

We will identify project team members based on project requirements and staff expertise and availability but being mindful of XST-staff career and performance stretch goals. A balance is necessary between groups that are too wide, where some may not play a role, and too narrow, where the benefits of experience, diversity, and flexibility are lost. We will engage APS-U staff in developing the team selection process.

Effective communication between all parties involved will be 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. We will develop clear procedures to define and facilitate interactions.

In collaboration with APS-U staff and beamline scientists, we are deploying this team approach for the development of the APS-U IDEA beamline at 28-ID (this beamline will become CHEX after the APS dark period for APS-U). This beamline will serve as a test bed for APS-U optical components and will house the demonstration phase of the fast ptychography RAVEN project.

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## **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 participation of several, if not all, XST groups.

- Implement and refine the XST team model, including processes and management tools, for integrated beamline and instrument development.
- 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.
- Deploy a multipixel hard x-ray TES detector and sensors with edge computing capabilities.
- Integrate data acquisition scripting with data reduction and analysis pipelines.
- Expand fly-scanning capabilities.
- Develop and deploy a robust set of high-performance computing (HPC) enabled software for coherence, imaging, high energy, and multi-modal data. Provide streaming data analysis and visualization using DOE leadership computing facilities (LCFs) where appropriate.
- Deploy automated data management tools and storage, including archival storage, for high data volume and data rate XSD beamlines, in collaboration with the AES-IT and AES-IS groups.

## **Goals and Action Plan for FY2022**

- Continue the deployment of Bluesky (<https://www.aps.anl.gov/BCDA/Bluesky>) to beamlines.
- Integrate EPICS v7 data structures into device support as appropriate.
- Continue to execute and support APS-U, DOE, and Operations projects such as 28-ID IDEA, RAVEN, 25-ID ASL, the cavity-based x-ray free electron oscillator (CB-XFEL) as well as a recent DOE Early Career Award
- Continue to execute and support APS-U in the completion of FDRs, procurement readiness reviews and procurements for APS-U feature beamlines and enhancements.
- Continue to support HPC-enabled tools aligned with APS strategy for techniques such as XPCS, XRF, and ptychography especially oriented towards seamless integration with on-demand high performance computing
- In collaboration with the Globus team, deliver science data portals and workflow automation tools at select APS beamlines.
- Continue deployment and support of the APS Data Management System at APS beamlines including increased data confidentiality.
- Continue development and support of remote access tools for APS beamlines.
- Advance 3D reconstruction capabilities for nano-imaging
- Development of numerical methods for multimodal nanometer-scale fluorescence tomography.
- Continued development of AI-enabled high-resolution coherent imaging methods and continued exploration of unsupervised deep learning (DL) techniques for phase retrieval.
- Improved capabilities for crystallographic/pair distribution function data reduction and modeling using GSAS-II.
- Extend HEDM techniques to highly deformed materials by developing point-focus FF-HEDM and full-field NF-HEDM modes; implement AI driven peak detection systems to speed up reconstruction times.
- Increase the number of active pixels in the TES array at 1-BM-C.
- Build the first complete MM-PAD v2.1 detector and an improved high-energy germanium strip detector.
- Continue to advance the 1-D mirror zoom optics, including *in situ* metrology and feedback control.
- Supply high-quality multilayers to beamlines by request.

## XST SWOT Analysis

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

<b>Strengths</b>	<b>Weaknesses</b>
<ul style="list-style-type: none"><li>• XST personnel have strong technical skills and are highly motivated.</li><li>• APS-U beamline requirements provide a focal point for XST activities.</li><li>• Interaction between XST personnel across technical groups enables cross-pollination of ideas.</li><li>• Shared management with XSD beamline personnel decreases barriers to execution.</li><li>• Can leverage knowledge and expertise of XSD beamline scientists and APS users.</li></ul>	<ul style="list-style-type: none"><li>• Some technical areas are not represented or do not have sufficient depth, i.e., skills are concentrated in a few key personnel.</li><li>• Need to leverage resources outside of XST more effectively.</li><li>• Existing 20+-year-old infrastructure may constrain innovation.</li></ul>
<b>Opportunities</b>	<b>Threats</b>
<ul style="list-style-type: none"><li>• Bring successful implementation of mechatronics (combined electronics and mechanical engineering) to APS-U beamlines, e.g., active monochromator vibration control.</li><li>• Develop beamline instruments that are “integrated by design,” i.e., address all aspects of implementation and performance from concept to deployed instrument.</li><li>• Become world leader in experiment feedback, mechatronics, and adaptive coherence preserving optics.</li><li>• Build on synergies with other ANL Directorates to further impact.</li><li>• Develop cross-platform sample environments optimized for APS-U feature and enhanced beamlines.</li></ul>	<ul style="list-style-type: none"><li>• Competition for scarce resources.</li><li>• Failure to realize the XST vision in a timely manner could cause our stakeholders and sponsor to stop trusting XST.</li><li>• Increasingly stringent standards due to the characteristics of the APS-U x-ray beam, e.g., vibration control, coherence preservation, and increased data rates.</li><li>• Adapting to new techniques and experiment requirements, e.g., on-the-fly scanning, real-time analysis, and multi-technique data sets.</li></ul>