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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

Established in July 2015, the XST section comprises the Beamline Instrumentation (BI), Beamline Controls and Data Acquisition (BC), Computational X-ray Science (CXS), Detectors (DET), Optics (OPT), and Scientific Software & Data Management (SDM) groups, and the Nanopositioning Support Laboratory. All of these groups existed in some fashion prior to the creation of XST, but are now in a single structural organization as 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 technical groups work in collaboration with XSD stakeholders to develop x-ray beamlines for 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 hardware 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, etc.)

We are developing 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, nanofocusing optics, thin film optics;
- Sparsified readout detectors for XPCS, e.g., VIPIC;
- Energy resolving detectors, e.g., TES for energies 10-20 keV, Ge strip detectors; and
- Data handling (acquisition, streaming, transfer, reduction) @ 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.

<u>Strategy – Tools</u>

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; and
- 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 the ones that require additional resources. The strategy documents for each XST group and the Nanopositioning Support Laboratory are in
https://www1.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 have **identified projects where an integrated design and implementation approach will result in a superior product.** We will form teams across XST and APS to plan and execute these projects.

5. Pursue sustained R&D effort.

Excellent beamline performance and best-in-class instruments require not only up-to-date skills and technology, but also most importantly the vision, forward thinking, and prototyping afforded by R&D projects. The strategy document of each XST group identifies areas where we will concentrate our R&D effort.

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 driving efficacy and efficiency across the facility.

<u>**Strategy – Implementation**</u>

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 the typical prior approach to beamline/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 develop a **process to identify project team members** based on project requirements. 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 must **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 will deploy this team approach in the development of the **APS-U R&D beamline**, slated for 28-ID. 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.

We will pursue **projects for APS operations** prior to the upgrade, such as the **MONA project**, "Monitoring, Optimizing, Navigation, Adaptation," currently in its planning phase. MONA will be an acquisition system having autonomous decision capability in performing experiments. D. Gursoy (CXS) leads a team with representation from BC, CXS, and SDM, and that may expand to include other XST and APS Engineering Support division groups.

Five-year Goals

Links to the strategy document for each XST group are in the Appendix. 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.

- Validate and refine the XST team model, including processes and management tools, for integrated beamline & instrument development.
- Implement MONA for several techniques, e.g., full-field transmission microscopy, fluorescence tomography, and 3D ptychography, as an example of adaptive control strategies for experiment steering without human intervention.
- Develop stable, rapid scanning, nanopositioning 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 1-megapixel VIPIC detector and hard x-ray TES spectrometer.
- Integrate data acquisition scripting with data reduction/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. Implement routine integration of streaming data analysis and visualization using DOE leadership-scale computing facilities as 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 FY2019

- MONA – Further research on coupling data collection, analysis, and instrument feedback. Extend project to XRF microscopy technique.
- Continue to execute and support APS upgrade and operations projects, e.g., 28-ID IDEA, RAVEN, 25-ID ASL, 4-ID XTIP, 6-ID HT-HEDM.
- Demonstrate 1-D mirror zoom optics, including *in situ* metrology and feedback control (Q4 FY2019).
- Complete the stacked zone plates project for APS-U, with an optimized design for the precision alignment apparatus (Q3 FY2019).
- Modular Deposition System: Optimize velocity profiling capability for laterally-graded multilayers. Test components and instrumentation for *in situ* metrology (Q4 FY2019)
- Deploy 128-pixel TES array to 1-BM (Q3 FY2019).
- Develop advanced multimodal modeling and optimization that combine nanometer-scale fluorescence-tomography and ptychography-tomography modalities, and realize robust near real-time software.
- Continue to support HPC-enabled tools aligned with strategic techniques, e.g., XPCS, XRF, and Ptychography (Q4 FY2019).
- Deploy streaming tomography reconstruction.
- Redeploy HEDM analysis with MPI; extend the scientific scope and improve detector corrections.

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.	• Need to sharpen strategic focus in the management of XST groups' portfolios. • Some technical areas are not represented or do not have sufficient depth, i.e. skills are concentrated in a few key personnel. • Can 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 world leader in experiment feedback, mechatronics, and adaptive coherence preserving optics.	• Competition for scarce resources. • Disconnect with APS-U efforts. • Failure to realize the XST vision in a timely manner could cause our stakeholders and sponsor to stop trusting XST. • 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 multi-technique data sets.