APS Training #6: Dynamic X-ray Crystallography

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The APS-U will provide a highly brilliant beam ideally suited for serial crystallography methods. In preparation for the new source, GM/CA@APS, SBC, and BioCARS at the APS are hosting this collaborative workshop for user demonstrations in sample preparation, data collection, and data processing for serial millisecond crystallography (SMX). This method has the potential to visualize dynamic processes in macromolecules and to address the substantially faster x-ray damage that will occur with the brighter APS-U beam. Participants will receive demonstrations and training with crystal handling, sample delivery to the x-ray beam, data collection approaches, beamline controls as well as auto- and post-processing and structure determination.

Serial crystallography methods have many advantages: low dose per crystal, room-temperature collection, and reduced radiation damage per crystal, allowing the use of small or x-ray sensitive samples and the ability to perform time-resolved measurements. Initially developed at XFELs, serial experiments have been implemented and expanded at synchrotron sources. Advances in SMX experiments are paramount for the APS-U, as this method is expected to flourish with the significant increase in x-ray flux density and a concomitant rise in multi-crystal datasets. Proof-of-principle and groundbreaking experiments using the injection method were conducted by GM/CA@APS and BioCARS, and SBC recently began offering fixed-target collaborative users. GM/CA@APS has worked to advance this method by improving signal-to-noise with tapered beamstops and focusing via compound refractive lenses. SBC has worked on sample preparation, delivery, ease-of-use, and developed collaborations within Argonne, including the supercomputing group, for automatic data analysis and feedback. BioCARS uses Laue crystallography technique for time-resolved studies and has expanded its use to fixed-target serial crystallography compatible with use of short laser pulses for reaction initiation. Experimenters now have access to well-rehearsed methods and free data processing software packages such as CrystFEL and DIALS. Serial crystallography is now feasible at the APS and is becoming routine at these beamlines. Interest in the scientific community is growing for those who have seen that the method can be straightforward.

At GM/CA@APS, participants will receive demonstrations and training with a viscous jet injector, and at SBC, they will gain exposure to the high-speed fixed-target equipment. Users will see demonstrations in methods of sample handling, delivery, and data collection using standard samples provided by the organizers. Participants unfamiliar with the serial techniques will explore approaches to data processing and analysis.