SAT B: Dynamic X-ray Crystallography

Time: 2 Full-days
Date: Thursday, April 23 – Friday, April 24
Course location: Sectors 84, 19, and 23
Organizers: Darren Sherrell (SBC/APS) and David Kissick (GMCA/APS)

The APS-U will provide a highly brilliant beam ideally suited for serial crystallography methods. In preparation for the new source, GM/CA and SBC at the APS propose a collaborative workshop for user training 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 bright APS-U beam. Participants will receive hands-on 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. SMX 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 and BioCARS, and SBC recently began offering fixed-target SMX to 'friendly' users. GM/CA has worked to advance this method by improving signal-to-noise with tapered beam stops 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. Experimenters now have access to well-rehearsed methods and free, data processing software packages, such as CrystFEL and DIALS.

SMX 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. However, the wider user community is not yet aware of SMX capabilities and developments. This workshop will advertise the method and familiarize the attendees with the new experimental setup, processes, and potential outcomes. In this way, users will be able to maximize their data collection experience and tailor their experiments to biological problems and challenges. Importantly this will also provide us with feedback for future needs, improvements, and developments.

Participants will need to be registered APS users with all training up to date at the time of the training. At GM/CA, participants will receive training with a viscous jet injector, and at SBC, they will use the high-speed fixed-target method. On the first day, the users will be trained in methods of sample delivery and data collection using either their samples or standard samples provided by the organizers. On the second day, participants unfamiliar with the SMX technique will explore approaches to data processing and analysis.