MS08-1-2 User support for time-resolved SFX data processing at XFELs
#MS08-1-2

T. Zhou [1], P. Aller [1], R. Bosman [1], J.J.A.G. Kamps [1], A. Shilova [1], A. Brewster [2], F. Dall'Antonia [3], A.M. Orville [1]
[1]XFEL Hub, Diamond Light Source - Harwell Science and Innovation Campus, Didcot OX11 0DE (United Kingdom), [2]Molecular Biophysics and Integrated Bio imaging Division, Lawrence Berkeley National Laboratory - 1 Cyclotron Road, Berkeley, CA 94720, (United States), [3]European XFEL - Holzkoppel 4, 22869, Schenefeld (Germany)

Abstract

A frontier challenge of structural biology is to determine high-resolution structures of catalytic systems in the fourth dimension (time) to reveal the intermediate state of catalysis. Serial crystallography methods at synchrotrons (SSX) and XFELs (SFX) are particularly well suited for time-resolved studies using micro-crystal slurries. Specifically, the intense beam generated at XFEL enables the study of smaller crystals and, thereby, reduces the ligand diffusion time allowing for more reaction time control.

Two important questions that need to be answered during the SFX experiments are: **a)** "Have we obtained sufficient data?" During SSX and SFX experiments, "still" diffraction patterns are collected at random orientations, which need to be processed individually and merged for a complete dataset. Merging statistics and assessment of the quality of electrons density maps ultimately determines whether sufficient data has been collected. **b)** "Does the equilibration/reaction time need to be adjusted?" Again, the electron density maps for a given time point must be checked during time-resolved studies to evaluate interpretability of atomic models with respect to the proposed reaction mechanisms and/or anticipated catalytic reaction intermediates. Therefore, answering both questions during SSX/SFX experiments requires collected data to be processed in as near to real-time as possible. Further, the fast data collection rate at XFELs, which currently can go up to 3520 images per second with an AGPID 1M at the European XFEL, makes real-time data processing challenging and an optimized data processing strategy is required for maximum data processing efficiency. The XFEL Hub at Diamond Light Source has been helping users/collaborators during SSX and SFX experiments, from set up software packages to process collected data. I will present our works relating to user support at several XFELs (LCLS, PAL-XFEL and EuXFEL), focusing on real-time data processing using dials and cctbx packages (script based data processing and cctbx.xfel GUI)[1, 2].

References

[1] Winter, G., *et al.*, (2018). "DIALS: implementation and evaluation of a new integration package." *Acta Crystallogr D Struct Bio*l 74(Pt 2): 85-97.

[2] Brewster AS, *et al.*, (2019): Processing serial crystallographic data from XFELs or synchrotrons using the cctbx.xfel GUI. *Computational Crystallography Newsletter* 10, 22 - 39