MS08-1-11 Automated data processing and analysis of serial crystallography experiments #MS08-1-11

G.M. Assmann [1], F. Leonarski [1], F. Dworkowski [1], T. Tomizaki [1], C.Y. Huang [1], M. Wang [1], J.A. Wojdyla [1]
[1]Swiss Light Source, Paul Scherrer Institute - Villigen (Switzerland)

Abstract
To collect a complete data set with little radiation damage, serial crystallography (SX) data collection strategies have recently experienced a renaissance. In serial synchrotron crystallography (SSX) experiments either partial data sets from a few degrees of rotation or zero-rotation stills are collected. Serial femtosecond crystallography (SFX) collects stills using X-ray pulses generated by a FEL before destruction of the crystal occurs (Chapman *et al*., 2011; Boutet *et al*., 2012). SX experiments produce large datasets, which require automated data-processing pipelines and sufficient merging strategies. An automated pipeline should analyze and archive raw data and support users in decision-making on merging strategies.
At the beamline X06SA at the Swiss Light Source, VESPA, a dedicated, versatile and universal endstation for SSX experiments supporting sample delivery methods including HVE (high viscosity ejectors), ALD (acoustic levitation diffractometry) and FT (fixed targets), was recently installed. The SSX stills, collected during commissioning beamtime at the VESPA endstation with a Jungfrau 4M detector (Leonarski *et al*., 2018), were used to compare different data processing steps (spot finding, indexing, integration and merging) offered by existing SFX data processing packages (such as CrystFEL (White, 2019), nXDS (Kabsch, 2014)). The VESPA setup, the first results of comparative analysis and the implementation of a combined automated data-processing pipeline, to be deployed at the SLS and the SwissFEL facilities, will be presented.

References
Boutet, S. *et al.* (2012). Science, 337, 362–364 ; Chapman, H., *et al.* (2011). Nature, 470, 73–77

Kabsch, W., (2014) Acta Cryst., D70, 2204-2216

Leonarski F., *et al.* (2018) Nature Methods, 15(10): 799-804

White, T.A., (2019) Acta Cryst., D75.