Computing in Fragment Screening

Fully automated data collection and data management at the Swiss Light Source

K. Smith¹, E. Panepucci¹, S. Aumonier¹, D. Eris¹, C.Y. Huang¹, D. Eris¹, D. Buntschu¹, N. Meier¹, W. Glettig¹, K. McAuley¹, M. Sharpe¹, M. Wang¹, J. Wojdyla¹

¹Paul Scherrer Institute (PSI), 5232 Villigen, Switzerland
Kate.smith@psi.ch

Keywords: automation, crystallography, data acquisition, databases, fragment screening

With the advent of fragment screening and increased industrial demands for beamtime, synchrotrons have had to adapt their services to provide reliable high throughput systematic data collections. The Swiss Light Source (SLS) has recently upgraded their data acquisition hardware and software to meet automation needs at the macromolecular crystallography (MX) beamlines [1, 2, 3]. Unattended data collection at the SLS is best suited for single crystals from well characterized crystallization systems, such as crystals from high-throughput screening or fragment-based drug discovery pipelines. The recent development of the SLS MX Fast Fragment and Compound Screening (FFCS) platform [4, 5] has produced large quantities of fragment-soaked crystals for a number of academic and industrial targets, which were successfully measured with the smart digital user (SDU).

I will first present the development of SDU, automatic loop centring (ALC) and the expansion of our software microservice framework [6]. The SDU is a sophisticated communications and decision-making software which performs systematic, fully automated data collection at all three MX beamlines with a maximum throughput of 25 samples per hour. I will also present the migration of our mongo database (MXDB) to the cloud and how this is central to our current and future samples management, data acquisition, automation and data processing pipeline strategies. The current external webpage allows users to validate excel sample spreadsheets prior to their experiment, in the future this will be modernized to provide users with extensive sample management capabilities, including logistics, data acquisition, data processing and post-experiment analysis.