MS08-2-2 OM and Cheetah: a common framework for online and offline analysis in serial crystallography #MS08-2-2

A. Tolstikova [1], V. Mariani [2], T.D. Grant [3], A. Barty [1]
[1]DESY - Hamburg (Germany), [2]SLAC - Menlo Park (United States), [3]Jacobs School of Medicine and Biomedical Sciences - Buffalo (United States)

Abstract
OM, formerly known as OnDA [1], is a software framework for real-time monitoring of X-ray imaging experiment data and experimental conditions. OM provides users with a set of stable and efficient real-time monitors for the most common types of experiments, which can be used immediately without modifications or can be easily adapted to meet the users' requirements. Since its first release OM has proven to be an invaluable tool for monitoring of diffraction data and quick decision making during serial crystallography experiments at both free-electron laser and synchrotron sources. OM focuses on scalability and portability, to facilitate its adoption for a wide array of current and future instruments, and strives for stability and performance, relying on free and open-source libraries and protocols.
Although OM has been originally designed for real-time data processing, the flexibility of its core parallelization and data recovery strategies as well as its highly modular architecture have allowed it to be used as a new processing core for Cheetah, a software package for high-throughput reduction and analysis of serial diffraction data [2]. Merging online and offline analysis for serial crystallography into a single software framework offers numerous advantages. Support for new facilities, detectors and data sources can be shared between the OM and Cheetah packages, facilitating the development work and reducing the time needed to adapt both packages to new experiments and processing workflows. Using the same algorithms and features in both OM and Cheetah, additionally, allows the processing parameters optimized for one of the packages to be used for the other, avoiding duplication of effort. OM has, for example, recently gained the ability to stream data via a network socket to the CrystFEL software package [3], to get real-time feedback on the indexing rate and unit cell parameters during data collection. Cheetah can use the same technology to send detector frame to CrystFEL for further processing, without writing intermediate file to disk. As new, high-throughput facilities and detectors come online, and generate data at an unprecedented rate, avoiding writing files to disk can result in a strong reduction of storage needs, with its associate costs.
This contribution will give an overview of the new features in both the OM and Cheetah software packages, introducing recent development and discussing possible directions of future development.

References
1. Mariani, V., Morgan, A., Yoon, C.H., Lane, T.J., White, T.A., O'Grady, C., Kuhn, M., Aplin, S., Koglin, J., Barty, A. and Chapman, H.N., 2016. OnDA: online data analysis and feedback for serial X-ray imaging. Journal of applied crystallography, 49(3), pp.1073-1080.
2. Barty, A., Kirian, R.A., Maia, F.R., Hantke, M., Yoon, C.H., White, T.A. and Chapman, H., 2014. Cheetah: software for high-throughput reduction and analysis of serial femtosecond X-ray diffraction data. Journal of applied crystallography, 47(3), pp.1118-1131.
3. White, T.A., Kirian, R.A., Martin, A.V., Aquila, A., Nass, K., Barty, A. and Chapman, H.N., 2012. CrystFEL: a software suite for snapshot serial crystallography. Journal of applied crystallography, 45(2), pp.335-341.