MS3-P10 Data acquisition and analysis software at the Swiss Light Source macromolecular crystallography beamlines

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Data acquisition software is an essential component of modern macromolecular crystallography (MX) beamlines, allowing for efficient use of beamtime at synchrotron facilities. Coupled with automatic data processing routines it allows assessment of data quality on the fly. Developed at the Paul Scherrer Institut, the DA+ data acquisition software is implemented at all three MX beamlines. DA+ consists of services and components written in Python and Java, which are connected *via* messaging and streaming technologies. The major components of DA+ are the user interface, acquisition engine, hardware/detector and online processing. The DA+ provides a simple and easy to use GUI, which supports standard, as well as advanced data acquisition protocols, such as multi-orientation SAD, energy interleaved MAD, raster scan and serial crystallography. Automatic data processing routines utilize freely available crystallographic data analysis programs and deliver near real time results for data collected with PILATUS (CBF format) and EIGER (HDF5 format) detectors. Resulting metadata are stored and analyzed in the dedicated MongoDB database. The software architecture enables exploration of the full potential of the latest instrumentations at beamlines. For example, real time evaluation of continuous raster scan data collected with a EIGER 16M detector at high frame-rate and delivered via streaming interface has been implemented at X06SA beamline recently.

Keywords: data acquisition, user gui, automatic data processing, Eiger, database

MS3-P11 High-speed detectors enable synchrotron serial crystallography

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With the recently introduced EIGER, hybrid photon counting enters a new dimension of spatial and temporal resolution and expands the field of x-ray experimentation. The absence of detector noise in combination with an image bit depth of 32 bit and high spatial resolution ensure uncompromised data quality. Continuous read-out with frame rates in the hundreds of hertz and a pixel size of 75 μm open EIGER detectors to various time-resolved and high-throughput experiments.

A short outline of the differences between EIGER and PILATUS3 will highlight key aspects of the new detector technology. The main focus of the presentation will be on synchrotron serial crystallography. This novel approach to data collection brings strategies developed at X-ray free-electron lasers (XFEL) to synchrotron beamlines. Appropriate sample supports (e.g. mesh loops or mesophase sandwiches) can be automatically screened for the presence of crystals by their diffraction [1]. Identified crystals are targeted for the acquisition of partial datasets that are then merged until sufficient data has been acquired for structure solution. Alternatively, crystals can be injected into the beam in glass capillaries, grease matrices, lipidic cubic phase jets [2] or on standing ultrasonic waves [3]. Individual diffraction images from non-oriented crystals can be merged to yield complete datasets.

Synchrotron serial crystallography allows the study of crystals of sizes formerly thought to require highly restrictive XFELs for their structural study. The crystals can be prepared in aqueous solutions as well as in lipidic mesophases [4] and at room temperature as well as at cryogenic temperatures [5], and can be presented to the beam in a variety of ways. To be successful, the new methods critically depend on noise-free detectors operating at high speed, like EIGER.

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Keywords: HPC detectors, synchrotron serial crystallography