MS41 Automation in data collection and processing

MS41-02
Real-time pre-processing of serial crystallography

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Abstract
This contribution presents recent advances on real-time analysis of diffraction images acquired at high frame-rate (1 kHz) and their application to macro-molecular serial crystallography. A new signal separation algorithm is presented, able to distinguish amorphous (or powder diffraction) component from the signal originating from larger (single) crystals. The main improvement comes from the calculation of azimuthal uncertainties and relies on the ability to work efficiently in azimuthal space. This work is built on top of pyFAI, the fast azimuthal integration library and take benefits of running on graphical processors.
Two applications, built upon this separation algorithm are presented:
1. A lossy compression algorithm whose performances are evaluated on rotational and serial crystallography data. Performances are compared with uncompressed data using the XDS tool for the rotational part and CrystFEL for serial data.
2. A peak-picking algorithm which is able to assess the diffraction quality of crystals in real-time, with fast user feedback using the NanoPeakCell application. The quality of picked peaks is evaluated through the indexing rate in CrystFEL.
This algorithm will be the core of data processing of the new serial crystallography beam-line at ESRF-ID29.

References
Debionne, S., Homs, A., Claustre, L., Kieffer, J., De Sanctis, D., Santoni, G., Goetz, A. & Meyer, J. (2022). In Proceedings of the 14 th international conference on Synchrotron Radiation Instrumentation (SRI2021). https://indico.desy.de/event/27430/abstracts/

Background analysis of MX diffraction frame