MS01 - Micro & nano crystals in MX

Chairs: Dr. Helen Ginn, Dr. Thomas White

MS01-P06

New Beamlines for Macromolecular Crystallography at MAX IV

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MAX IV is the first operational 4th generation storage ring offering synchrotron radiation for many scientific communities. Among the first beamlines in user operation, BioMAX, the first macromolecular crystallography (MX) beamline, can be used to create high resolution 3D data from crystalline macromolecules to better understand the structure functional relationship of this complex matter. BioMAX has been designed as a work horse beamline to support all kinds of established crystallography methodologies and runs at a high automation level. The experimental station is equipped with a MD3 micro-diffractometer, an Eiger 16M hybrid pixel detector and an ISARA sample changer, which allows for complete data collections in seconds.

Recently a second MX beamline has been funded by the Danish Novo Nordisk Foundation. MicroMAX will become a micro-focusing beamline, which will allow for investigating micrometer sized protein crystals at room temperature using serial crystallography. Here the complete diffraction dataset is composed of several thousand single frames, partial datasets of a large number of crystals. Using a wide bandpass option, MicroMAX can be exploited also for time resolved crystallography down to the microsecond time resolution range. After a four-year construction period, the beamline will be ready for first experiments.

Keywords: Beamlines, Macromolecular crystallography, Serial crystallography

MS02 - From data collection to structure finalization: getting the most from your crystal

Chairs: Dr. William Shepard, Dr. Katherine McAuley

MS02-P14

Scaling data in the DIALS framework

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The process of scaling crystallographic data aims to put all reflections on a common scale, by correcting for experimental effects such as sample illumination, absorption and radiation damage. Here we present the implementation and evaluation of a new scaling framework in the DIALS diffraction integration package[1], for scaling of macromolecular and chemical crystallographic data. We discuss the details of the scaling models used to correct the data and of the algorithm choices available. Our framework allows a new incremental workflow for multi-crystal scaling, allowing finer control of the scaling models for individual datasets, as well as further analysis tools for scaling model validation. We demonstrate the use of and the results of our scaling programs on a number of example datasets, including thin-wedge rotation data and weak-intensity data.

References:

[1] Winter G., Waterman D.G., Parkhurst, J.M., Brewster A.S., Gildea R.J., Gerstel M., Fuentes-Montero L., Vollmar M., Michels-Clark T., Young I.D.,Sauter N.K., Evans G. 2018 Acta Cryst. D74 85-97

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