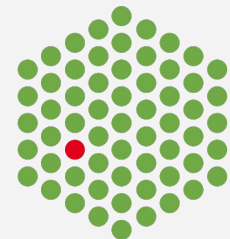


MXCuBE status report

Ivars Karpičs (EMBL Hamburg)

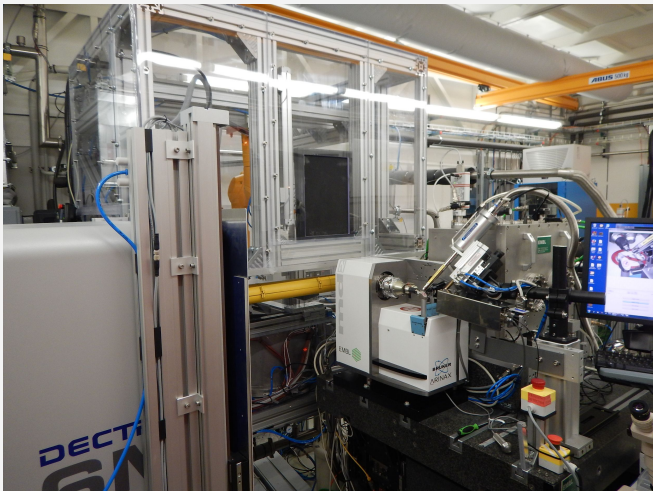
EMBL



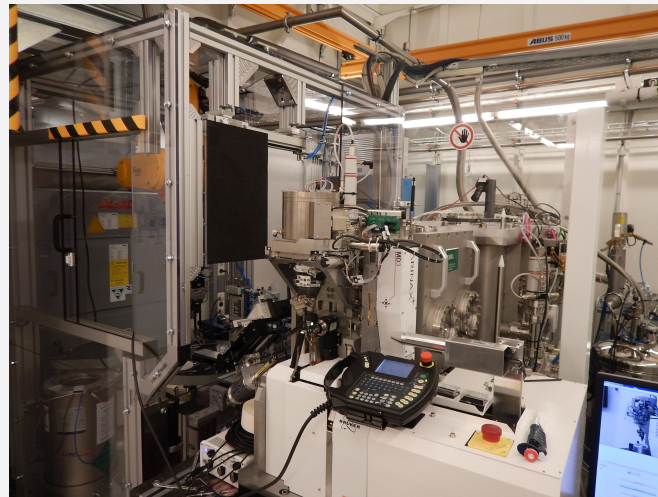
MX @ EMBL Hamburg



MX beamlines P13, P14

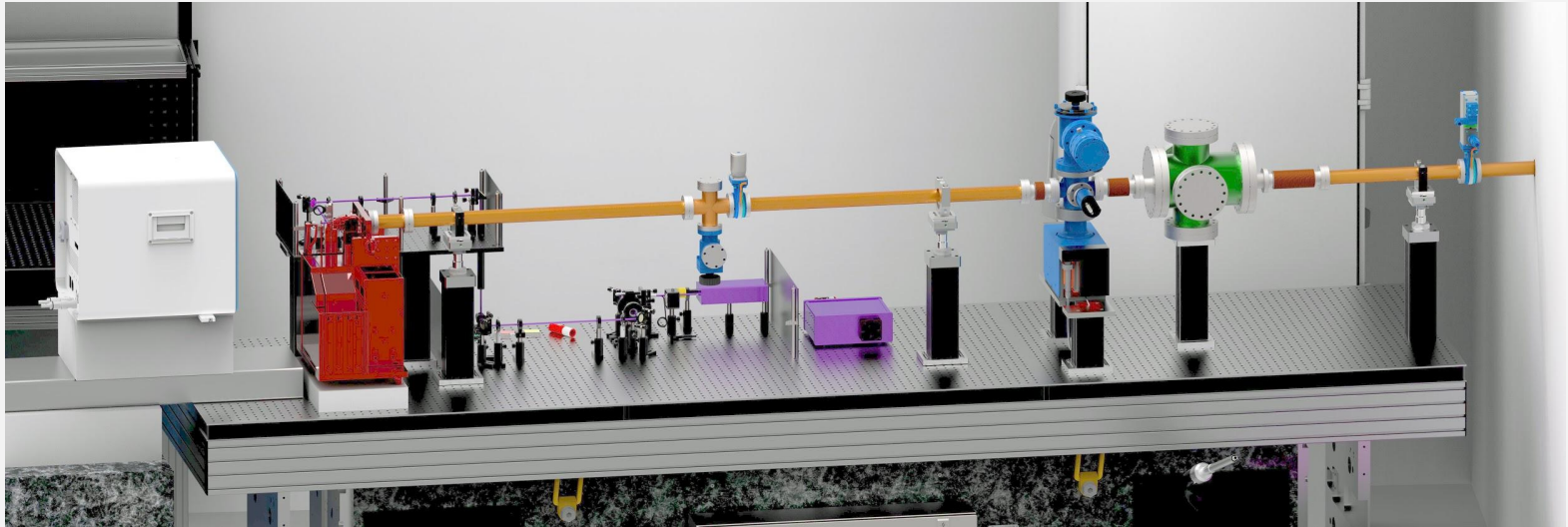


- Variable beam size and high flux
- Tunable energy between 4.5 and 17.5 KeV
- MD2 diffractometer and Pilatus6MF
- EMBL Marvin sample changer with 16 pucks



- Micro-beam conditions with 5 x 5 micron beam
- On the fly changeable focusing of the beam
- Tunable energy and CRLs (ESRF/CINEL)
- MD3 diffractometer and Eiger16M
- EMBL Marvin sample changer with 16 pucks
- Plate scanning possibilities

P14eh2 aka Pe2



- Time-resolved crystallography.
- In collaboration with Prof. Arwen Pearson (University of Hamburg).
- MD3 without a goniostat, CRLs, Eiger4M.
- Simplified MXCuBE will be used.

MXCuBE deployment

- Deployed from the master branch.
- Prosilica camera running without sudo via pymba library (Qt4_VimbaVideo).
- Dozor real time plots on the main window.
- HD screen at P14.

The screenshot displays the MXCuBE software interface, which is used for controlling and monitoring X-ray diffraction experiments. The main window is divided into several sections:

- Top Left:** A live camera feed showing a sample mounted on a goniometer. The feed is labeled "Sample B11.1".
- Top Right:** A panel for "Standard Collection" parameters, including acquisition settings like "Number of images: 100", "Exposure time (s): 0.01", and "Energy (keV): 12.0237".
- Right Side:** A detailed "Sample loaded" section showing the sample name "msh0021_1_#####.cif.gz", the file path, and various experimental parameters such as "Energy: 12.0237 keV" and "Wavelength: 0.1016 Å".
- Bottom Left:** A "Beam size" section with fields for "Horizontal" and "Vertical" dimensions, and a "Phase Centring" button.
- Bottom Center:** A "Log" window displaying a list of system events and messages, such as "Data collection finished" and "Sample change".
- Bottom Right:** A "Status" panel with buttons for "Full shutter", "Imaging", "Ready", and "Temperature: 27.0°C".

Latest GUI developments

On-the-fly processing results:

- Dozor score
- Number of spots
- Resolution

Statusbar:

- Queue
- Diffractometer
- Sample changer
- Last collection

The screenshot displays the MXCuBE/ISPyB control interface. At the top, there are control buttons for 'Collect', 'Exp', 'Reset', and 'Sample centring'. The main window shows a diffraction image with a grid overlay. To the right, there are panels for 'Standard Collection' (with parameters like Oscillation start, Exposure time, Energy, Resolution), 'ISPyB proposal' (with parameters like Mode, Sample tray, Cooling), and 'Machine current' (with parameters like Machine state, Front end, Hatch temperature, Flux, Cryoprotect in place, Sample changer, Storage disk space, Energy, Wavelength, Status, Transmission, Current, Resolution, Beamstop distance, Current, Door interlock, Safety shutter, Fast shutter, Image tracking, Detector status, Frame rate, Temperature, Humidity). At the bottom, a log window shows a list of events with timestamps, such as '2018-09-04 14:23:04 Collection: started' and '2018-09-04 14:23:27 Collection: finished'. Red arrows point from the text labels on the left to these specific GUI elements.

Queue item tooltip

- Collection parameters
- Info about processing

Processing info in the log bar

Status indicators:

- File system
- EDNA
- ISPyB

Latest GUI developments

The screenshot displays the MXCuBE GUI with several key features highlighted by red boxes:

- Acquisition Parameters Panel (Top Left):** A panel containing fields for Oscillation middle (180.277), Osc. range per frame (0.076), Number of images (5324), Total osc. range per line (18.5378), First image (1), Exposure time (s) (0.001343), Detector mode (4M), Kappa (0), Phi (0), Energy (keV) (12.6957), and MAD (unchecked).
- Grid Parameters Panel (Middle Right):** A panel showing Grid settings: Horizontal spacing (10.00), Vertical spacing (1.00), and Adjust size (1.00). It also includes Move horizontal and Move vertical options.
- Acquisition Parameters Panel (Bottom Right):** A duplicate of the top-left panel, also containing the 'Full osc. range' checkbox, which is checked.
- Compress data Button (Bottom Right):** A button labeled 'Compress data' with a question mark icon.
- Collect Now Button (Bottom Center):** A button labeled 'Collect Now' with a play icon.

The main window shows a diffraction image with a grid overlay. The grid is centered on the image, and the 'Collect Now' button is highlighted with a red box. The 'Compress data' button is also highlighted with a red box. The 'Full osc. range' checkbox is checked in the acquisition parameters panel.

Full oscillation range:

- Checkbox to use full the oscillation scan range.
- Range is based on the ac(de)celeration and is solved in the EMBLMiniDiff.
- For mesh scans parameters are optimized after drawing the grid.
- For standard collections range is defined by the number of images.

Other features:

- Collect Now button adds item to the queue and executes it without the confirmation dialog.
- Compress data checkbox to compress data on the fly.
- Centering points used in the data collection are painted red.

Auto processing at EMBL Hamburg

- P13: EDNAProc (XDS), Xia2/Dials, autoPROC with staraniso, dozor (via EDNA). Pilatus6M, cbf.
- P14: EDNAProc (XDS), dozor (as library for streaming data). Eiger16M, cbf, gz.
- All results stored in ISPYB.
- Short term plan is to upgrade the processing cluster.

03-09-2018 10:11:26
icsIP13/201810695_206pompidor/20180903/RAW_DATA/Prot_K

Workflow: Res. (corner) **1.15 Å (A)** P 41 21 2 Completeness **99.4%** Res. **43.5-1.2** Rmerge **6.7**

Protein: En. (Wave) **12.700 keV (0.9763 Å)** Overall **94.3%** 43.5-3.3 2.3

Sample: Phi range **0.10 °** Inner **99.6%** 1.22-1.20 58.0

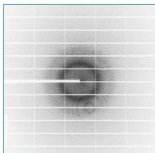
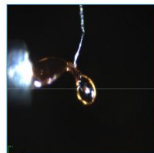
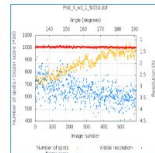
Prefix: Prot_K_w1 Phi start (total) **132.00 ° (69°)** Outer **99.6%** 1.22-1.20 58.0

Run # 1 Exposure Time **0.04 s**

Images (Total) **590 (590)** Flux start **5.26e+11 ph/sec**

Transmission **18.3 %** Flux end **5.26e+11 ph/sec**

	a	b	c
	68.02 Å	68.02 Å	102.19 Å
	α	β	γ
	90 °	90 °	90 °

OSC Prot_K_w1 1 Nb images: 590
Exp. time: 0.040 s
Phi range: 0.10 °
Flux: 5.26E11 ph/sec
Detector resolution: 1.15 Å
Transmission: 18.32
Wavelength: 0.976 Å
Total expo time: 23.60 s

EDNA_proc autoPROC XIA2_DIALS

Space Group: P 41 21 2
Completeness:




Pipeline	SpaceGroup	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Shell	Resolution (Å)	Multiplicity
BEST autoPROC	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.2	4.2
								Inner	43.5-3.3	4.1
								Outer	1.2-1.2	4.1
autoPROC_staraniso	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.1	4.3
								Inner	43.5-3.1	4.2
								Outer	1.1-1.1	3.2
XIA2_DIALS	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.1	3.9
								Inner	43.5-3.0	4.2
								Outer	1.1-1.1	2.5
EDNA_proc	P 4	68.0	68.0	102.2	90.0	90.0	90.0	Overall	48.1-1.1	2.2
								Inner	48.1-4.3	2.5
								Outer	1.1-1.1	1.7
BEST autoPROC	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.2	2.3
								Inner	43.5-3.3	2.5
								Outer	1.2-1.2	2.2
BEST autoPROC_staraniso	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.1	2.3
								Inner	43.5-3.0	2.4
								Outer	1.1-1.1	2.0
BEST XIA2_DIALS	P 41 21 2	68.0	68.0	102.2	90.0	90.0	90.0	Overall	43.5-1.1	2.1
								Inner	43.5-3.0	2.4
								Outer	1.1-1.1	1.8
BEST EDNA_proc	P 4	68.0	68.0	102.2	90.0	90.0	90.0	Overall	48.1-1.1	0.8
								Inner	48.1-4.3	1.5
								Outer	1.1-1.1	1.3

Experiment parameters | Beamline parameters | **AutoProcessing**

Autoprocessing Summary (click on an entry for more details)

Method	Point Group	Cell A	Cell B	Cell C	Cell Alpha	Cell Beta	Cell Gamma
Anomalous: OFF (Friedel pairs merged) (4 items)							
autoPROC_staraniso	P 41 21 2	68	68	102.1	90	90	90
XIA2_DIALS	P 41 21 2	68	68	102.2	90	90	90
autoPROC	P 41 21 2	68	68	102.1	90	90	90
EDNA_proc	P 4	68	68	102.1	90	90	90
Anomalous: ON (Friedel pairs unmerged) (4 items)							
autoPROC	P 41 21 2	68	68	102.1	90	90	90
autoPROC_staraniso	P 41 21 2	68	68	102.1	90	90	90
XIA2_DIALS	P 41 21 2	68	68	102.2	90	90	90
EDNA_proc	P 4	68	68	102.1	90	90	90

Reprocessing

To submit a new autoprocessing task upload edited XDS.INP file and press Start processing.

EDNAProc

Thank you for your attention!

Acknowledgments:

- T. Schneider group: G. Bourenkov, T. Schneider, and others.
- Instrumentation group: M. Nikolova, M. Bueno, U. Ristau, and others.
- EMBL Grenoble: J. Sinoir, and others.
- MXCuBE community.