

MXCuBE / ISPyB meeting – spring 2024



MicroMAX – MXCuBE dev.

Outline

- **Overview of team**
- The road to MXCuBE at MicroMAX
- **Spinning, running and flowing first experiments**
- The different MXCuBE integration topics compared to BioMAX
- **What comes next?**

novo nordisk fonden

MAX IV

Overview of main contributors to MicroMAX MXCuBE

Driving the implementation of MXCuBE at MicroMAX



Dominika



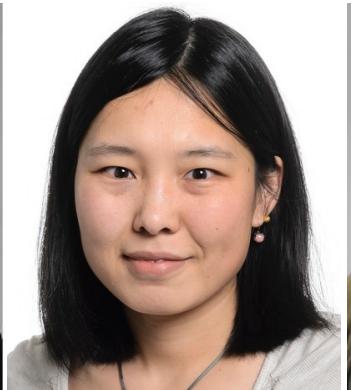
Elmir



Fabien



Ishkhan



Jie



Meghdad



Mikel

MX-group



The road to MXCuBE at MicroMAX

- **Legacy and divergence**
 - BioMAX MXCuBE3 was forked and not up to speed with main branch
- **Wish to be more involved in contributing and benefitting from the collaboration**
 - Keep up with main branch
- **Invest in new feature sets to cover experiment types that have not been routine at BioMAX**
 - Make SSX and time-resolved experiments more routine

MXCuBE-Web

MXCuBE-Web (osc)

Samples Data collection Equipment System log Help Remote Select proposal (MX20230350) Sign out (dworkowski)

Beamline Cameras Beamline Actions

Energy: 12.9923 KeV Resolution: 1.750 Å Transmission: 10.0 %
Wavelength: 0.9543 Å Detector: 168.9 mm

Sample Changer: DISABLED Safety shutter: OPEN Detector: READY Diffractometer: READY Ring Current: 398.3 mA

Phase Control: Centring

Beam size: 20

Omega: 289.00 90.0 °

X: -0.050 0.1 mm

Y: -1.769 0.1 mm

Sample alignment:

Z: 0.679 0.3 mm

Samp-X: -0.220 0.1 mm

Samp-Y: 0.075 0.1 mm

Sample Horizontal: 0.679 0.1 mm

Sample Vertical: -1.769 0.1 mm

50 μm

Snapshot Draw grid 3-click centring Focus Zoom (LEVEL1) Backlight Frontlight

Run Queue Unmount Settings

Sample: FixedTarget_MLMDual - lysozyme1 Queued Samples (0)

Grid-1: MESH (FixedTarget_MLMDual-lysozyme1_1_%004d.h5)

Log messages:

- [10:35:24]: Moving point x: 94.86, y: 667.08 to beam
- [10:35:20]: Moving point x: 1089.3600000000001, y: 698.7 to beam
- [10:33:37]: Diffractometer phase changed to Centring
- [10:33:37]: Diffractometer phase changed to Centring

What will MicroMAX actually do [next]?

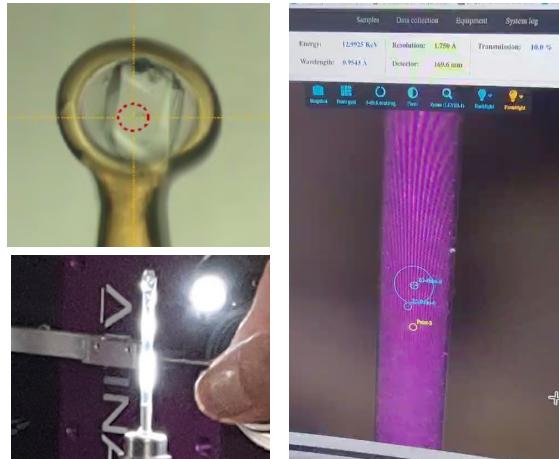
- Selection from [MAX IV] MX-group review report, end of 2023

#	Milestone	Timing	Goal
M1	Friendly user rotation data collection	2023 Q4	First external user experiment: SPINE rotation data collection using MD3 diffractometer
M2	Routine remote rotation data collection	2024 Q1	Remote users operating MicroMAX at fixed-energy and fixed-focus for cryogenic data collection, assisted by the ISARA2, MD3, Cryostream, EIGER2 and data auto-processing
M3	Fixed-target SSX with SPINE-like sample supports	2024 Q1	Collect SSX data from SPINE-like fixed-target mounts, with live image analysis Sample changer assisted and variable temperature [cryogenic and non-cryogenic]
M4	First injector experiment	2024 Q2	Simple injector experiment on MD3 with basic MXCuBE integration User-provided setup if performing pump-probe
M5	Extended SSX early user program	2024 Q4	Open up for sample feasibility checks for users [fixed-target and flow-cell] – proposal-less screening beamtime Collect MLM data for such an experiment and easily switch between the 3 available photon energy bandwidths and variable attenuation
M6 (F)	High data-rate injector pump-probe experiment	2025 Q1	HVE and JUNGFRAU used for chopper pump-probe experiment with nanosecond laser, using pink beam

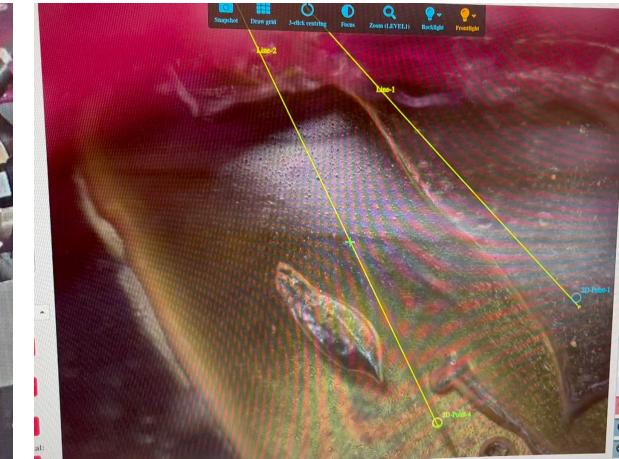
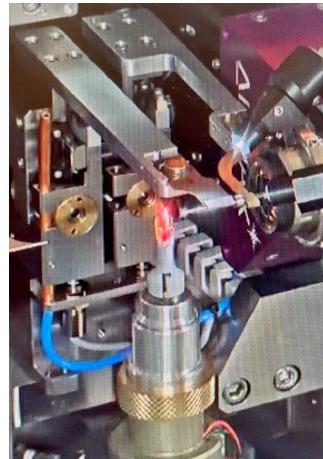
Spinning, running & flowing first experiments

- Not started using different MXCuBE Web configurations outside of “OSC”
 - Temporarily been running injector and fixed-target experiments also in “OSC” configuration
 - Will migrate SSX functionality to custom configuration - “Injector”, “Fixed-target”
- Used for first data collection of
 - Rotation data
 - Fixed-target SSX
 - Injector

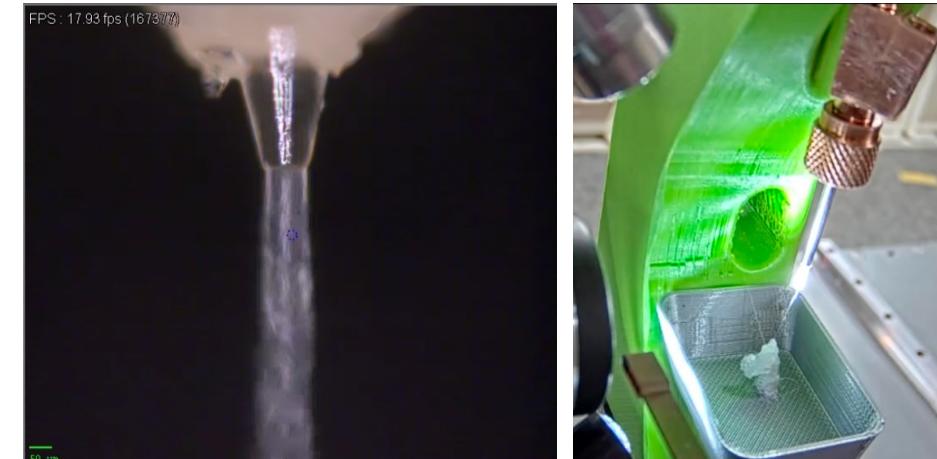
Spinning



Running

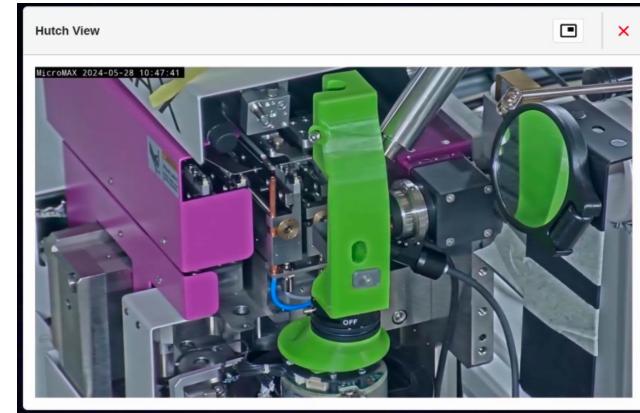
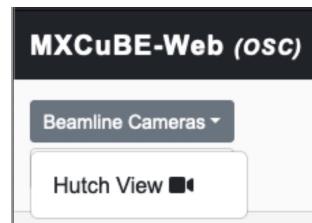


Flowing

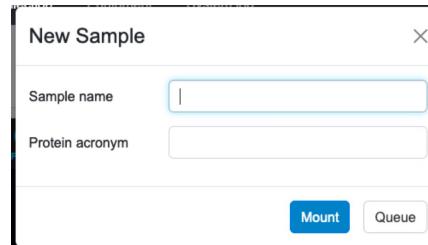
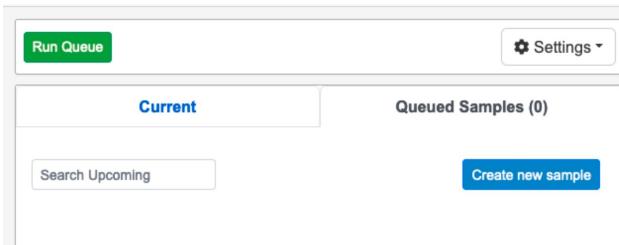


Revisiting old "new features"

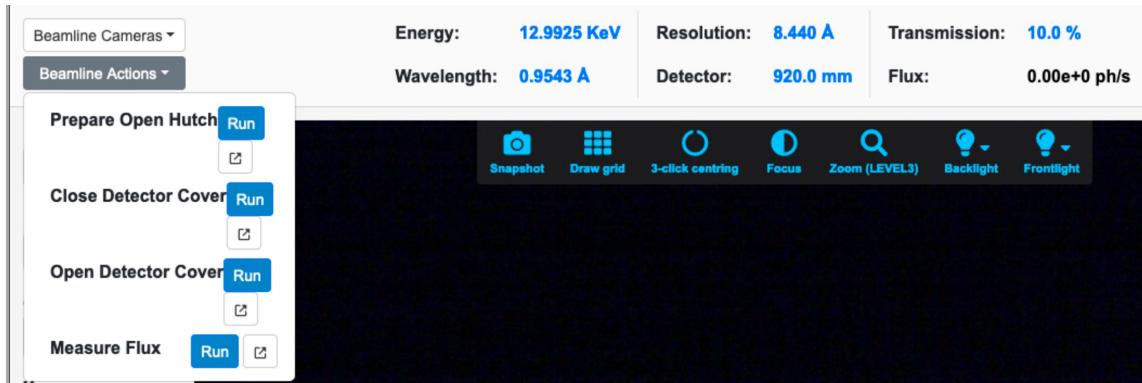
- Hutch cameras



- Sample creation



- Beamsline actions

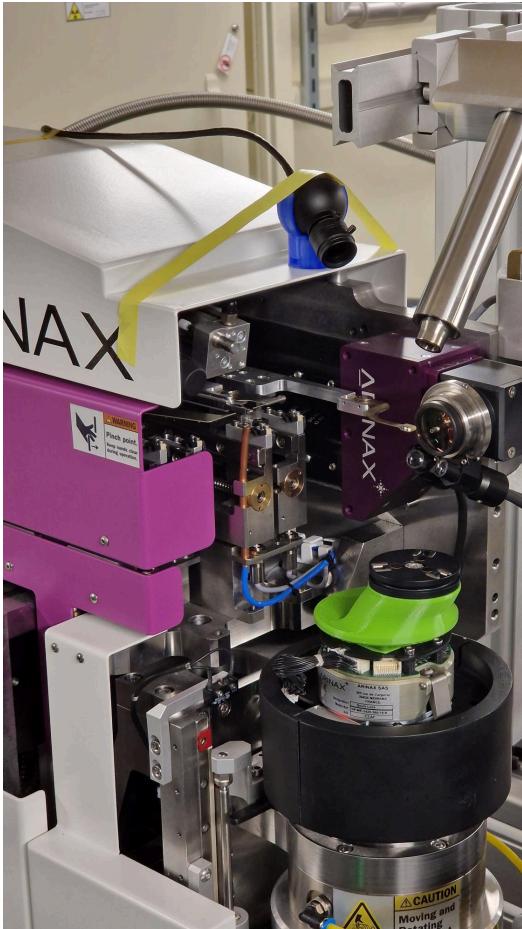


Minor (temporary?) features updates

- Universal goniometer head for fitting various sample environments
 - Can use MD3 motion system for positioning
- Awaiting MD3 software upgrade project with Arinax
 - To allow custom interlocks and extended functionality
 - Currently identifies itself as a "plate manipulator"
- Currently limited by interlock mismatches prior to software update
 - MXCuBE equivalence to MD3 phases
 - MXCuBE individually moves motors and performs checks, instead of standard MD3 phase control



"Empty" goniometer head

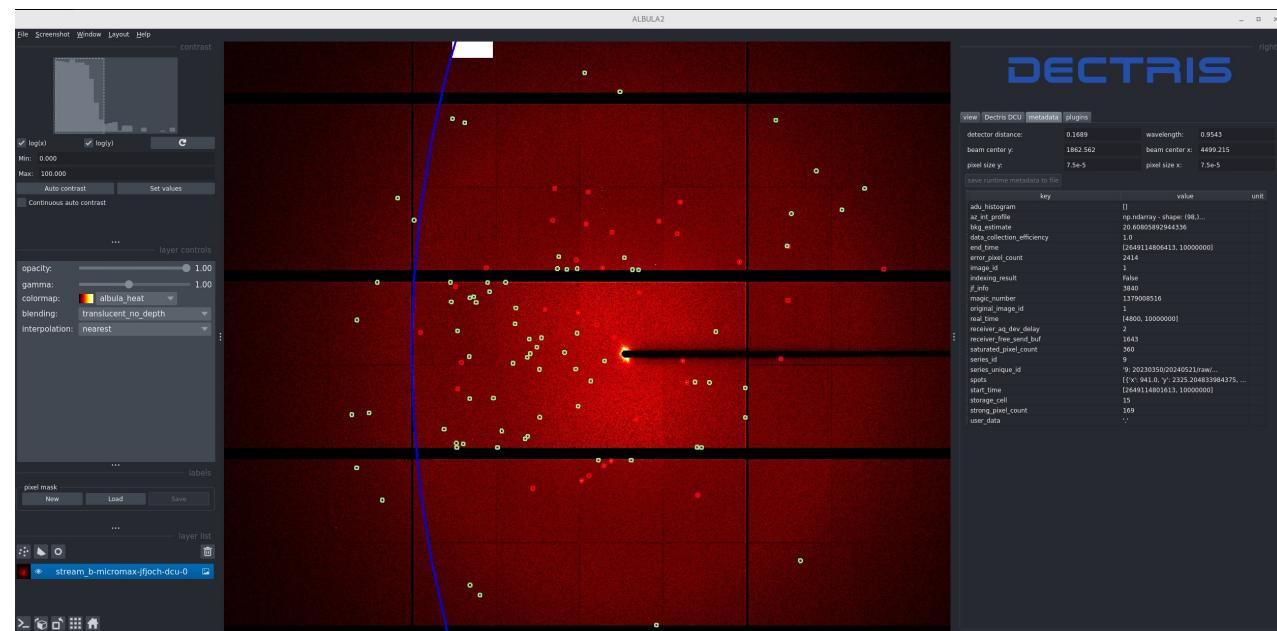
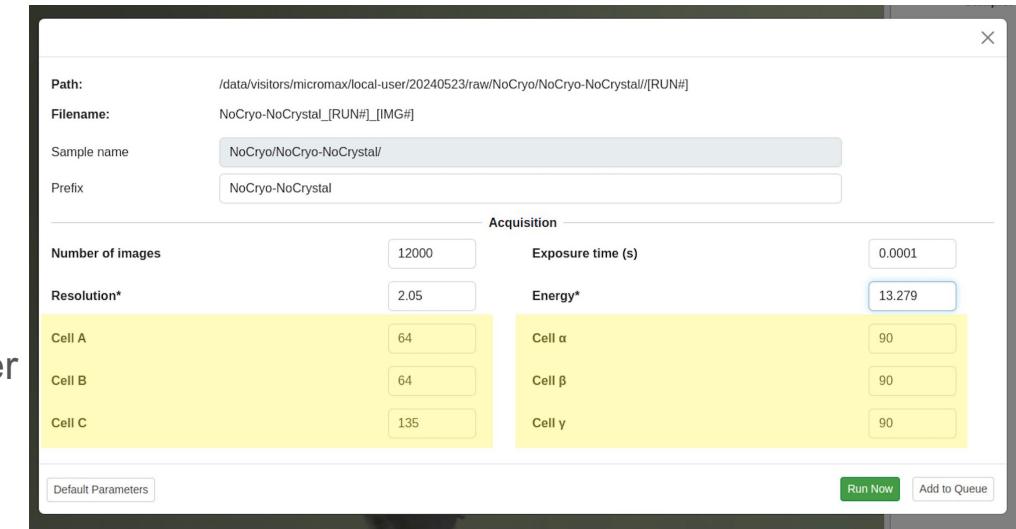
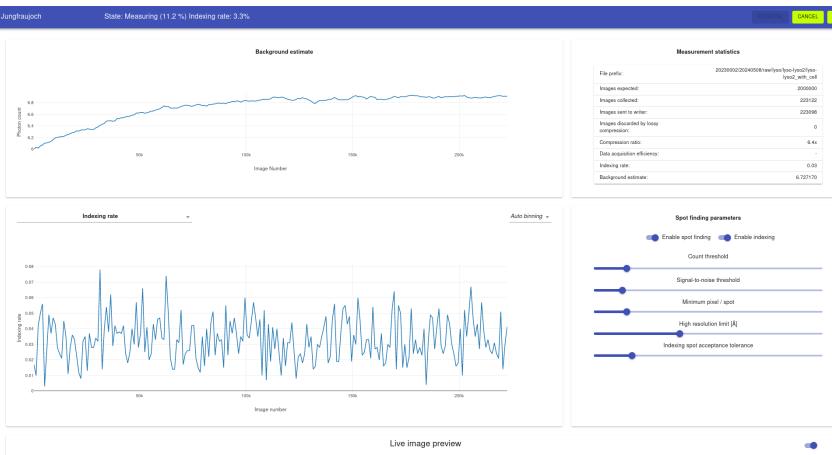


3D-printed HVE-injector holder on kinematic mount



SSX live data analysis

- Currently no visualisation or feedback to MXCuBE
- Different analysis workflows between EIGER2 and JUNGFRAU
 - In-house pipeline by Cecilia Casadei, and previously Aleksander Cehovin, for EIGER2 spot-finding [as presented by Jie]
 - Jungfraujoch also includes indexing and cell parameters are parsed from MXCuBE currently
- CrystFEL input files auto-generated

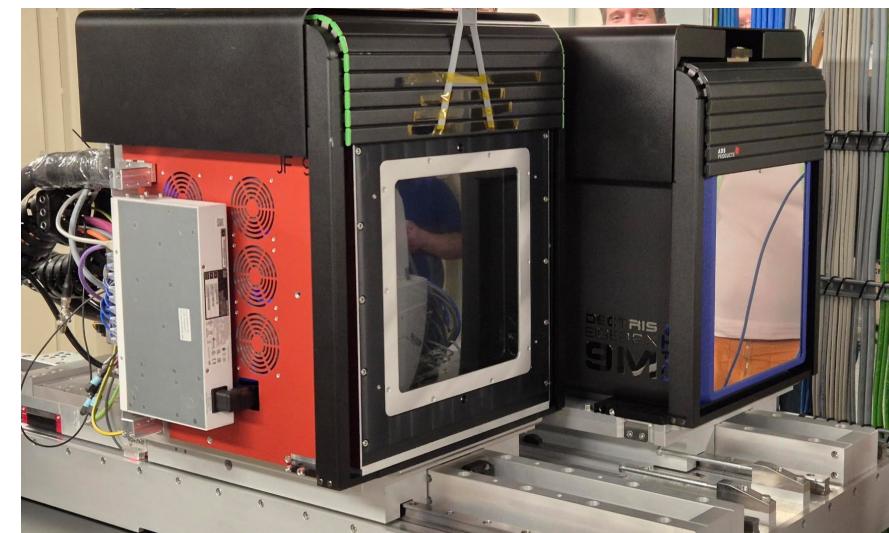


Green – peak

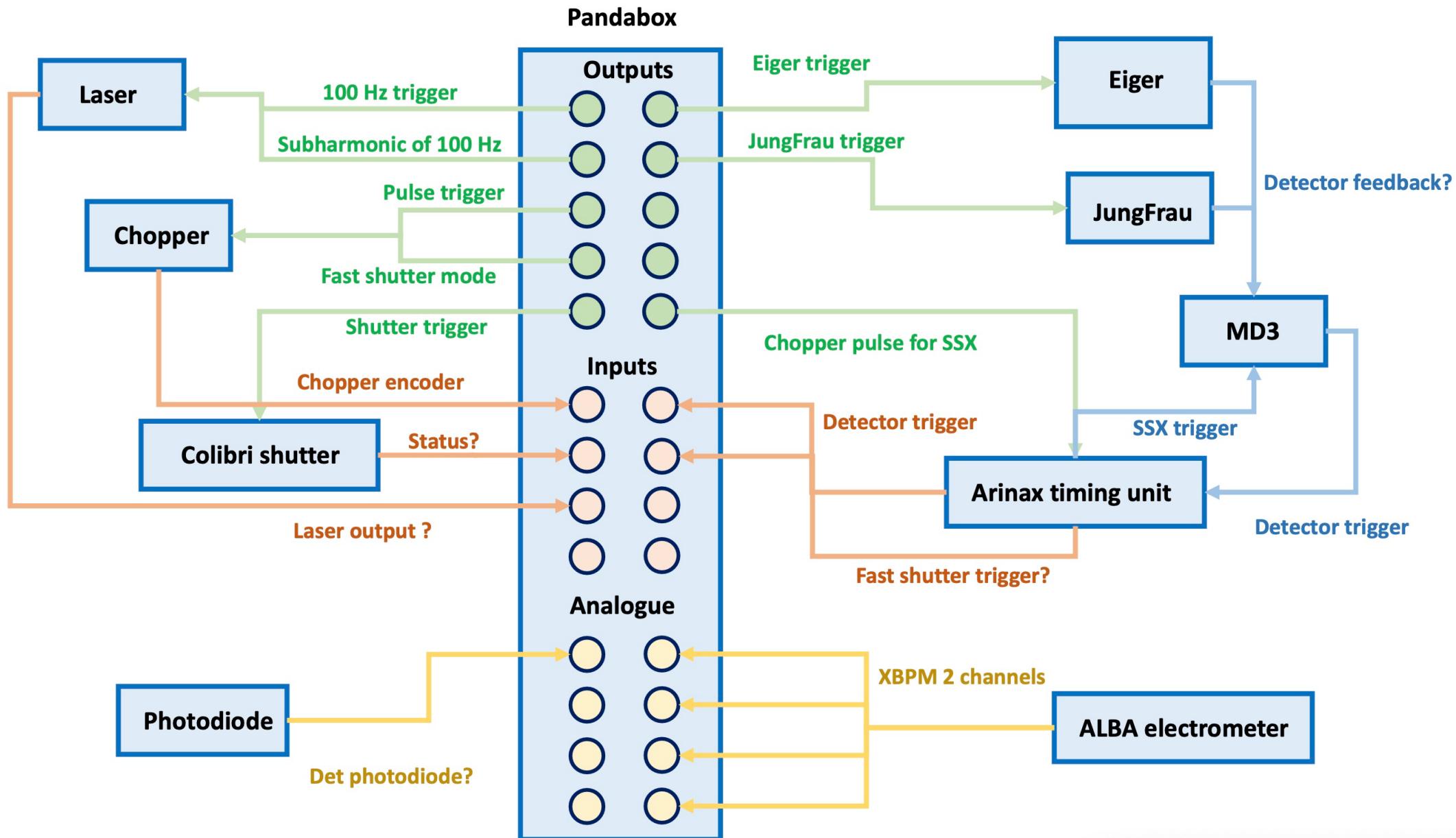
Red – indexed solution

New complementary features to BioMAX functionality

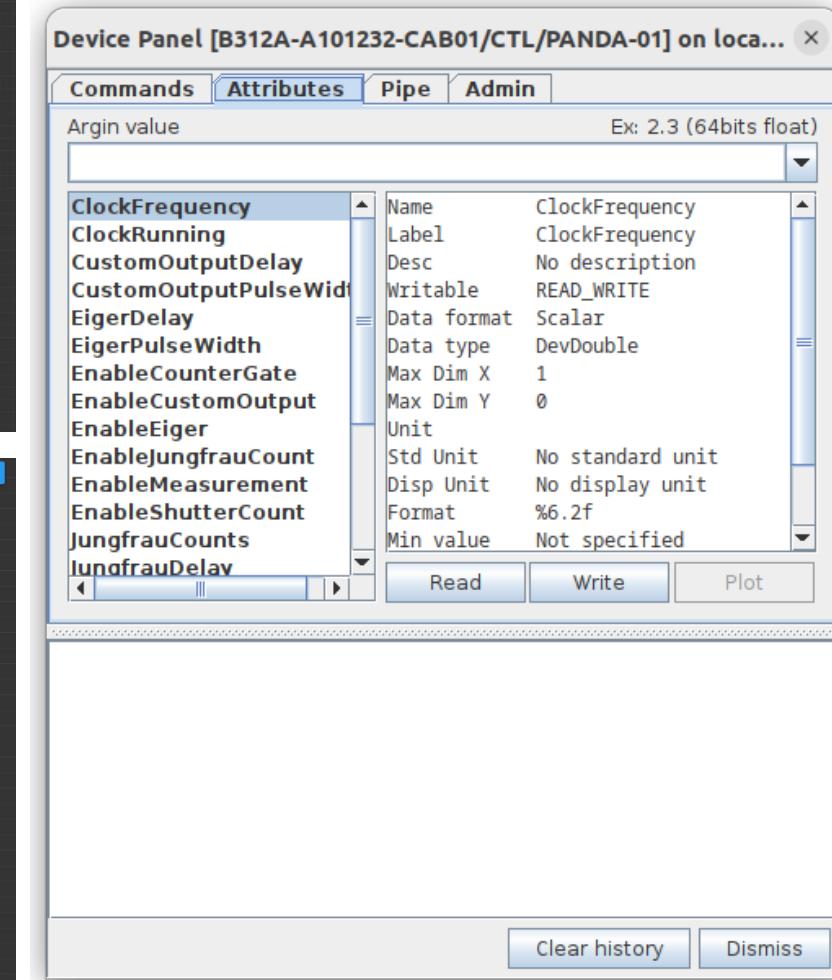
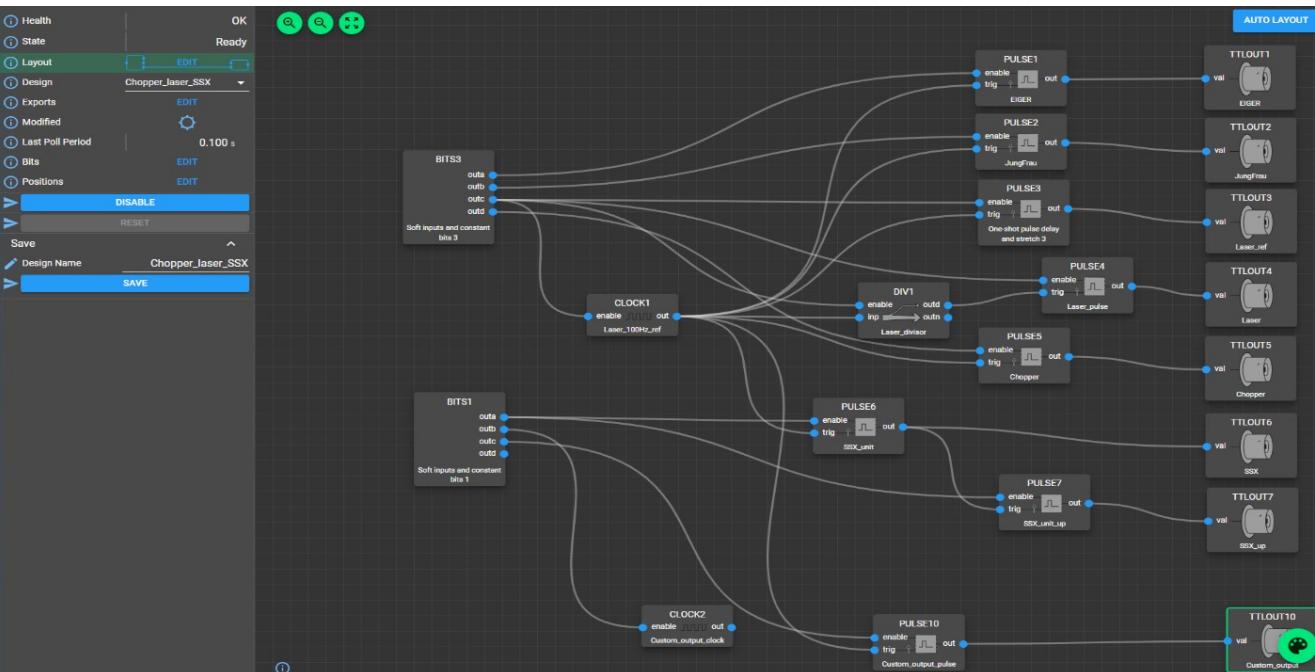
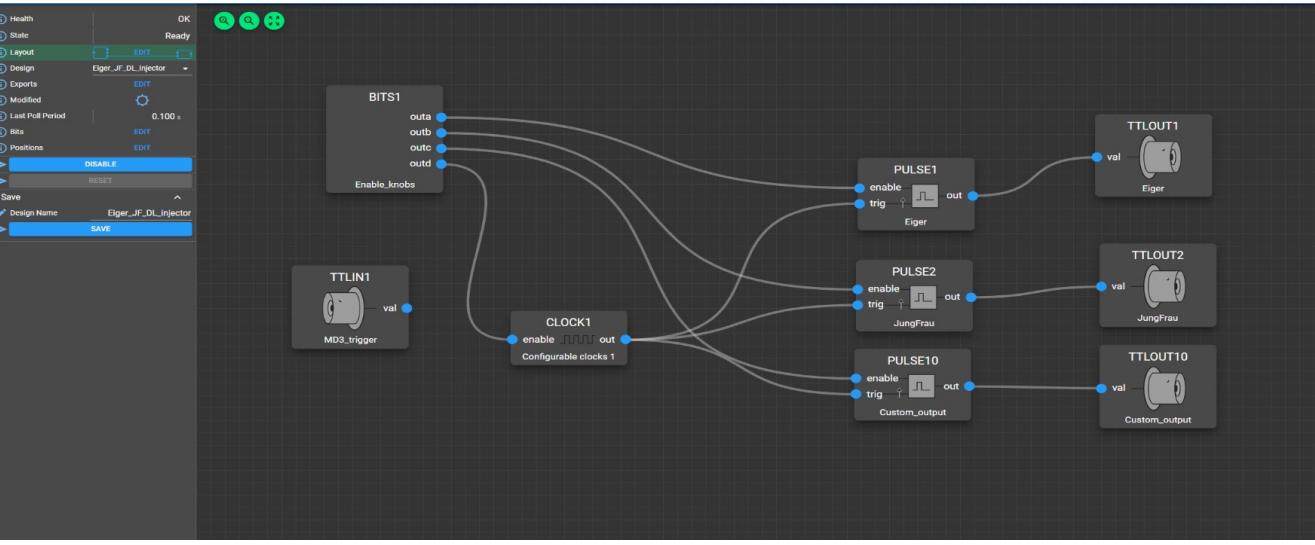
- Multi-configuration experiment timing control
 - PandA-box as a central point for timing control
 - Introduce timing offsets
 - Interfacing both with beamline and user equipment
 - *Covered further in later slides*
- Handling more than 1x diffraction (area) detector
 - Currently done by two branches of MXCuBE
 - Plan to merge so switch can be done within the same session
 - No technical details for implementation plan yet



Timing system



PandA configuration & Tango interfacing



MXCuBE-side of timing

X

Go To Beam

Measure Distance

Draw Grid

Data Collection (Limited OSC)

Characterisation (1 Image)

Create 2D point

SSX Injector Collection

SSX Injector Time Resolved

Path: /data/visitors/micromax/20230002/20240523/raw/NoCryo/NoCryo-NoCrystal//[RUN#]

Filename: NoCryo-NoCrystal_[RUN#]_[IMG#]

Sample name NoCryo/NoCryo-NoCrystal/

Prefix NoCryo-NoCrystal

Acquisition

Number of triggers 100000

Number of images 1500000

Exposure time (s) 0.0001

Resolution* 2.05

Energy* 13.02

Laser pulse delay (s) 0.00009

Laser pulse width (s) 0.00018

Cell α 90

Cell A 65

Cell β 90

Cell B 65

Cell γ 90

Cell C 65

Default Parameters

Run Now

Add to Queue

Wrapping up

Outlook and main conclusions

- Increase activities towards new features and to participate in the collaboration
 - Will depend on an investment from the beamline/MX-group -side to produce detailed user stories
- Move different “packaged” feature sets into separate MXCuBE configurations
 - “Injector”, “fixed-target”, ... modes
- Develop timing control and try to learn from experiences on UI work in Qt-MXCuBE at T-REXX
 - For user friendliness, but also to cover more complex experiment control within MXCuBE
- Make detector changes trivial within MXCuBE and with minimal (software-related) downtime
 - Handle reconfigurations of detector parameters, triggering, data analysis, flux estimations, and motor positions
- Increase presence and interaction with user group to tweak/adjust target functionality
 - Aided by now being in user operation and performing experiments beyond pure commissioning work

Timely acknowledgement



Dominika



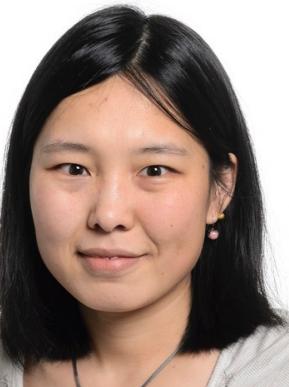
Elmir



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Meghdad



Mikel

MX-group



Questions?

HVE run

Beamline Cameras ▾ Beamline Actions ▾

Energy: **12.9925 KeV** Resolution: **2.200 Å** Transmission: **10.0 %**

Wavelength: **0.9543 Å** Detector: **223.6 mm**

Sample Changer: **DISABLED** Safety shutter: **OPEN** Detector: **BUSY** Diffractometer: **READY** Ring Current: **397.8 mA**

Phase Control: DataCollection ▾

Beam size: 20

Omega: 264.26 ▾ 90.0 °

X: -3.230 ▾ 0.1 mm

Y: -4.379 ▾ 0.1 mm

Sample alignment:

Z: 0.949 ▾ 0.1 mm

Samp-X: 0.272 ▾ 0.1 mm

Samp-Y: 0.027 ▾ 0.1 mm

Sample Horizontal: 0.949 ▾ 0.1 mm

Sample Vertical: -4.379 ▾ 0.1 mm

50 μm

Snapshot Draw grid 3-click centring Focus Zoom (LEVEL3) Backlight Frontlight

Stop Pause Settings ▾

Sample: Lyz_HEC1 - MK_lyzozyme Queued Samples (0)

SSX Injector Collection

SSX Injector Collection

Path: .../raw/Lyz_HEC1/Lyz_HEC1-MK_lyzozyme/Lyz_HEC1-MK_lyzozyme_0_%004d.h5

Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (keV)
264.26	0.10	0.000500	500000	10.00	2.200	12.9925

Log messages:

- [14:14:52]: Diffractometer phase changed to DataCollection
- [14:14:51]: Creating (MAXIV-MicroMAX) processing input file directories
- [14:14:49]: Not mounting next sample automatically (Auto mount next)
- [14:14:01]: Not mounting next sample automatically (Auto mount next)