

MXCuBE / ISPyB meeting – spring 2024



MicroMAX – MXCuBE dev.

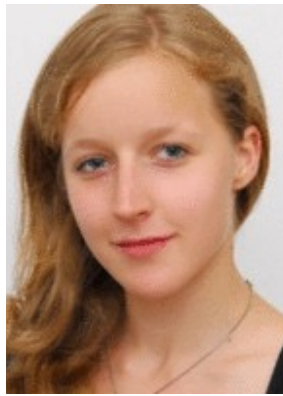
Outline

- **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?**

novonordiskfonden

Overview of main contributors to MicroMAX MXCuBE

Driving the implementation of MXCuBE at MicroMAX



Dominika



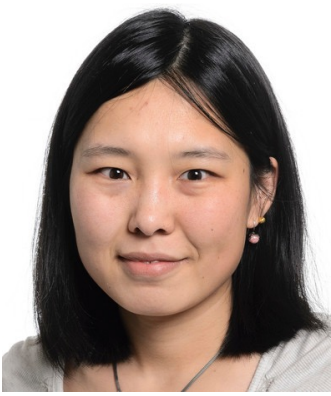
Elmir



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:



Hide motors

Z:

0.679 0.3 mm

Samp-X:

-0.220 0.1 mm

Samp-Y:

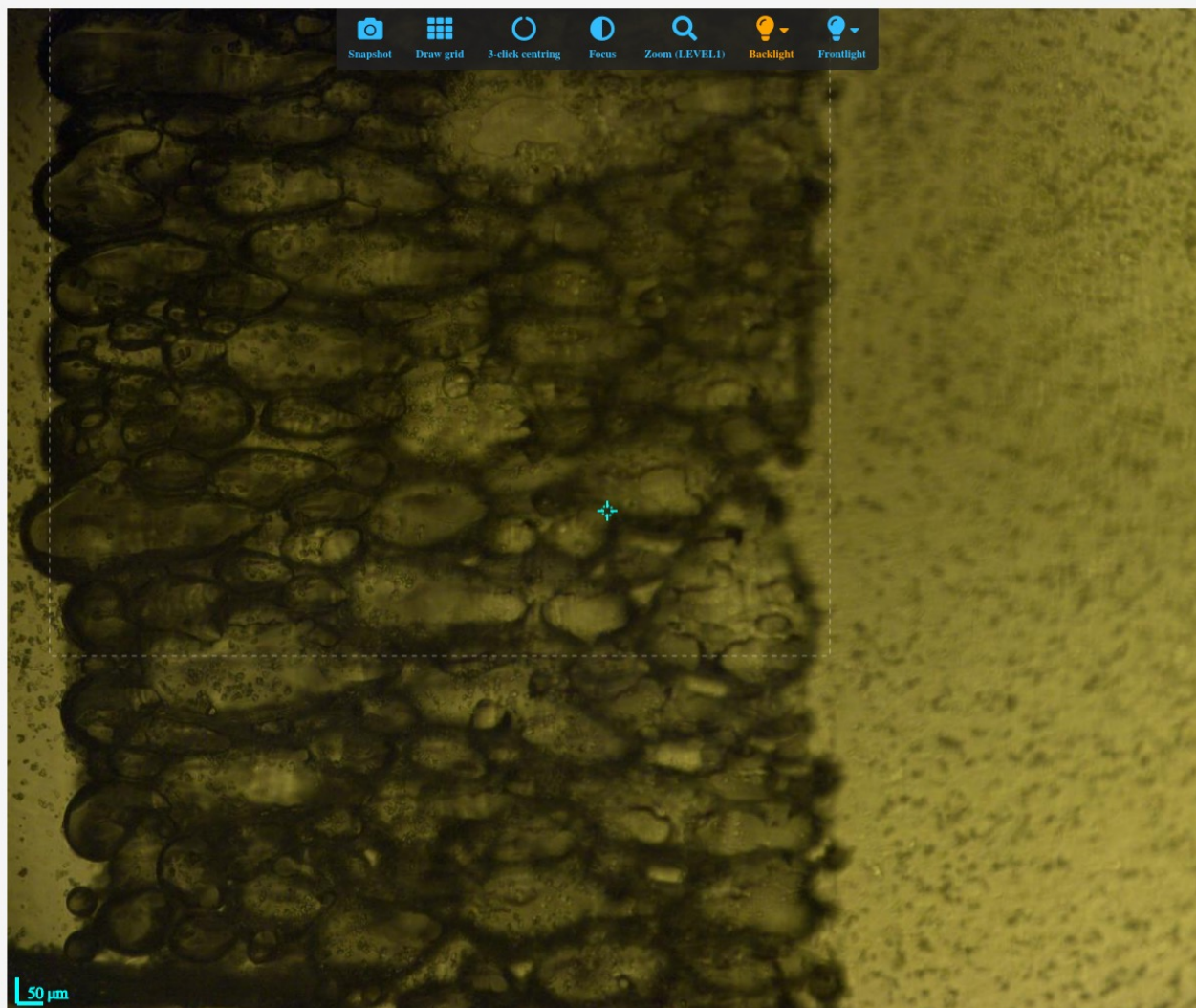
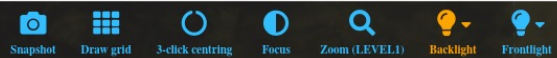
0.075 0.1 mm

Sample Horizontal:

0.679 0.1 mm

Sample Vertical:

-1.769 0.1 mm



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]?

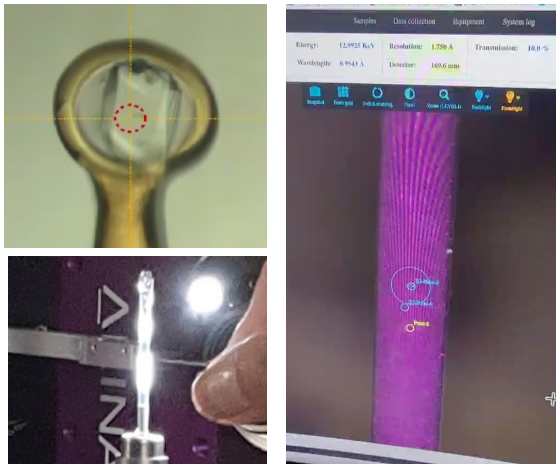
- Selection from [MAX IV] MX-group review report, end of 2023

#	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

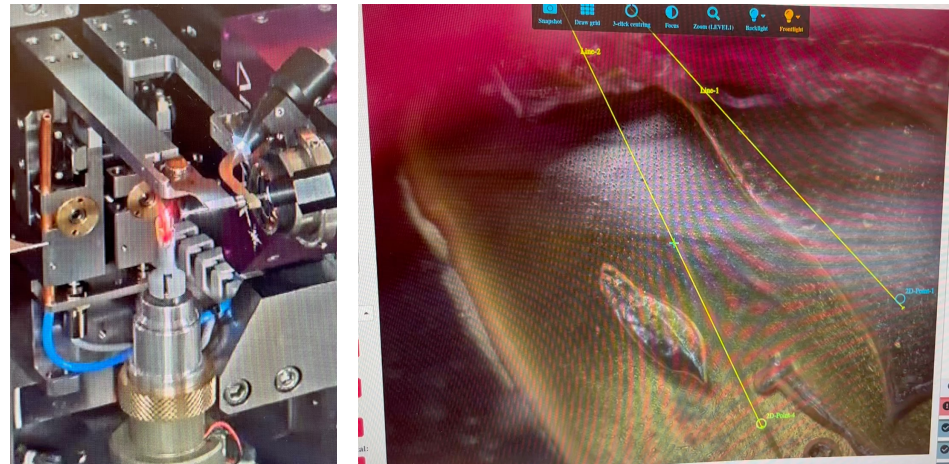
Spinning, running & flowing first experiments

- **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

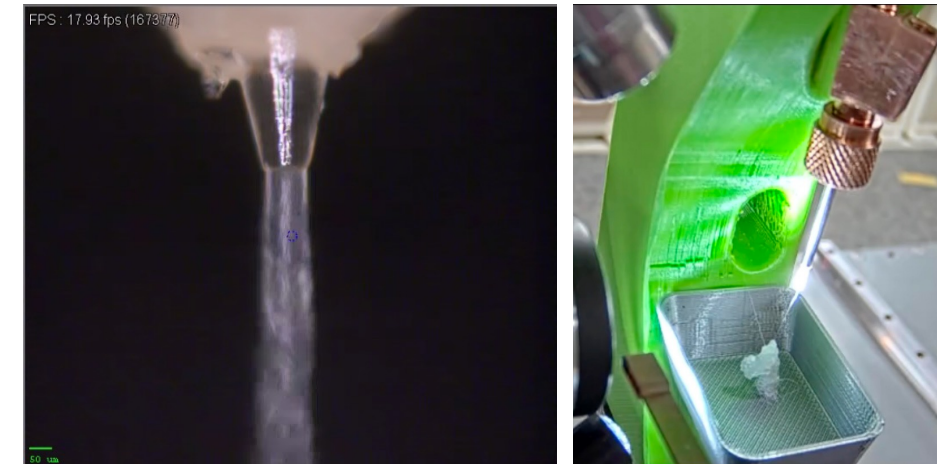
Spinning



Running

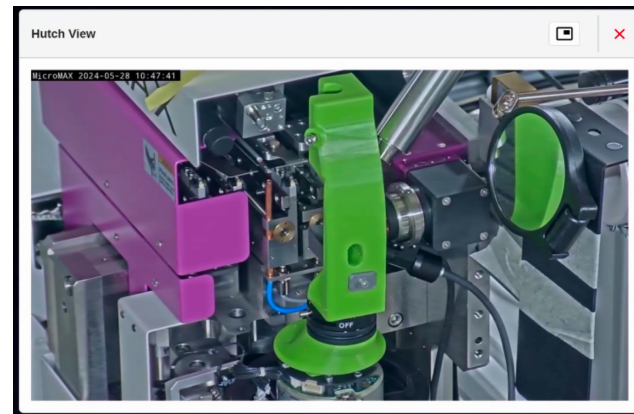
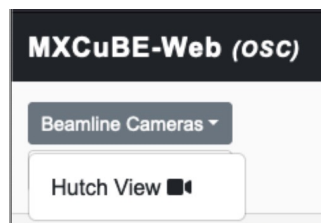


Flowing

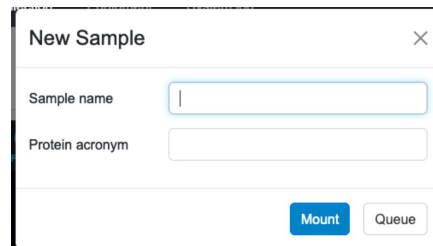
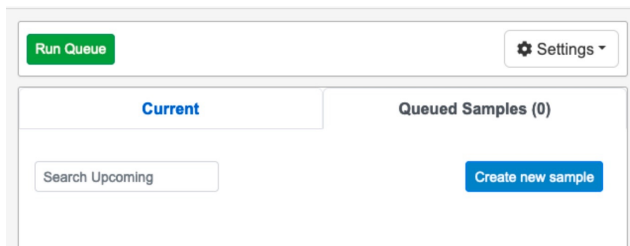


Revisiting old "new features"

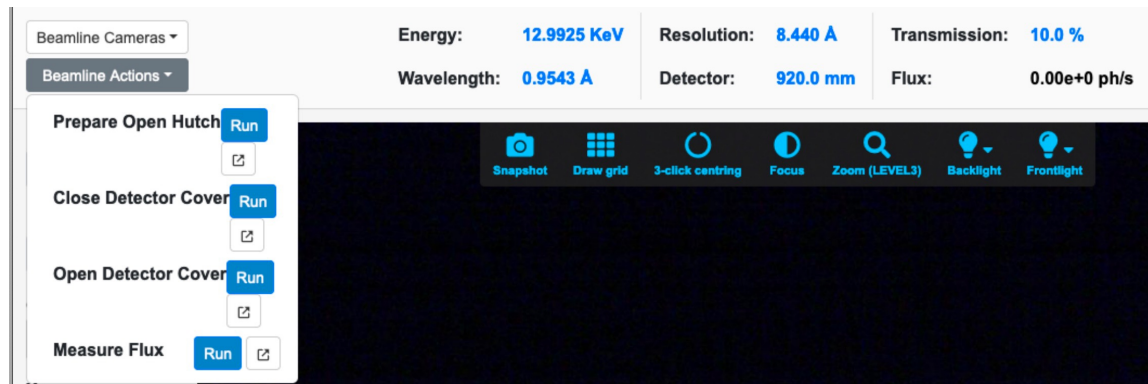
- Hutch cameras



- Sample creation



- Beamline actions

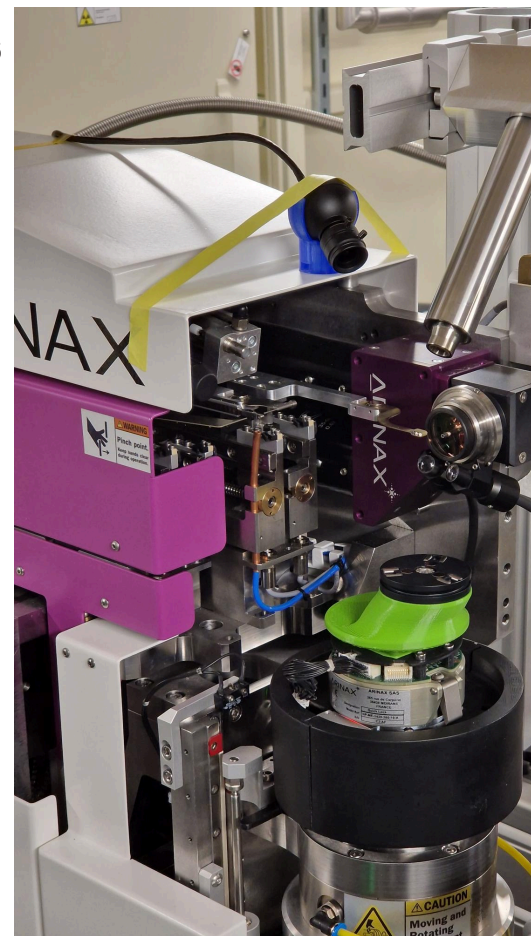


Minor (temporary?) features updates

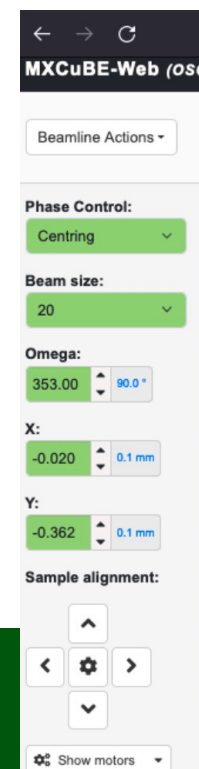
- **Universal goniometer head for fitting various sample environments**
 - Can use MD3 motion system for positioning
- **Awaiting MD3 software upgrade project with Arinax**
 - To allow custom interlocks and extended functionality
 - Currently identifies itself as a "plate manipulator"
- **Currently limited 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

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

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

Sample name: NoCryo/NoCryo-NoCrystal/

Prefix: NoCryo-NoCrystal

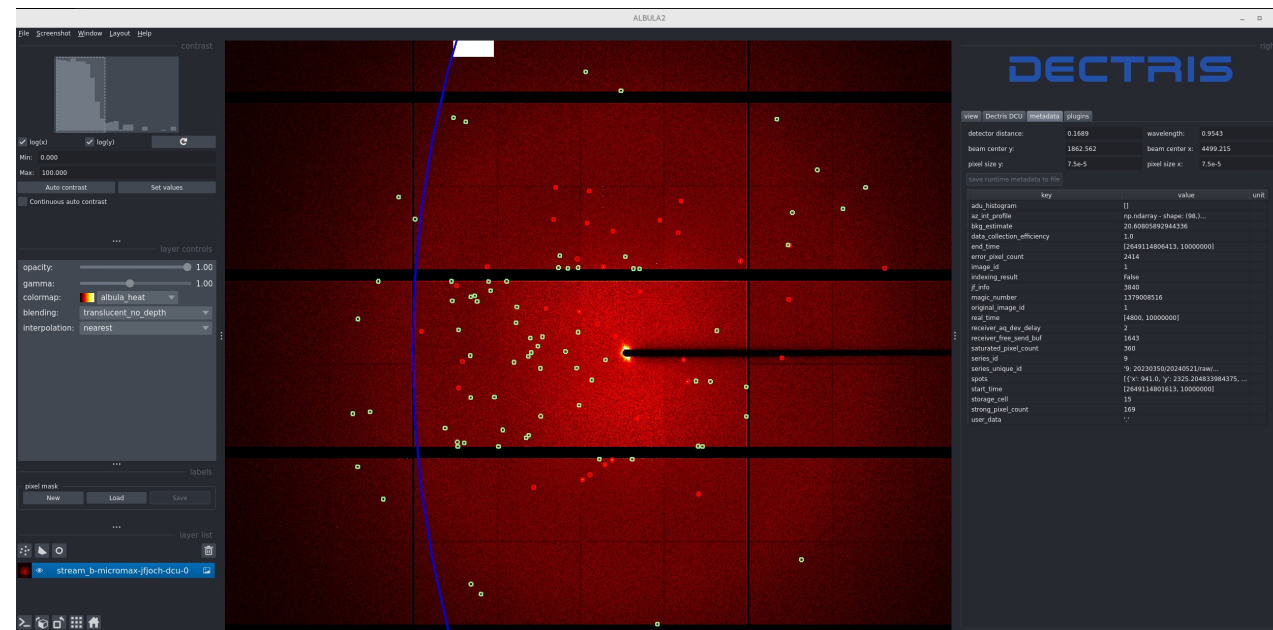
Acquisition

Number of images: 12000 Exposure time (s): 0.0001

Resolution*: 2.05 Energy*: 13.279

Cell A	64	Cell α	90
Cell B	64	Cell β	90
Cell C	135	Cell γ	90

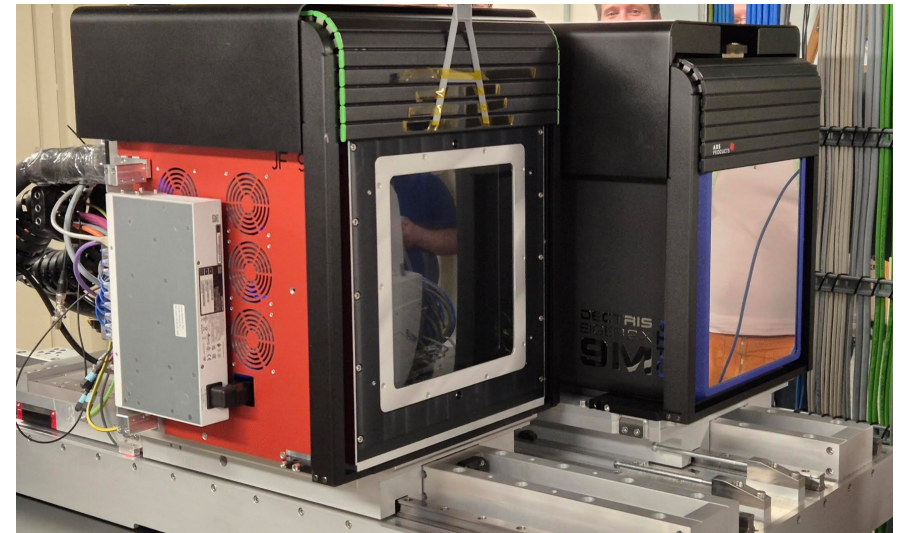
Default Parameters Run Now Add to Queue



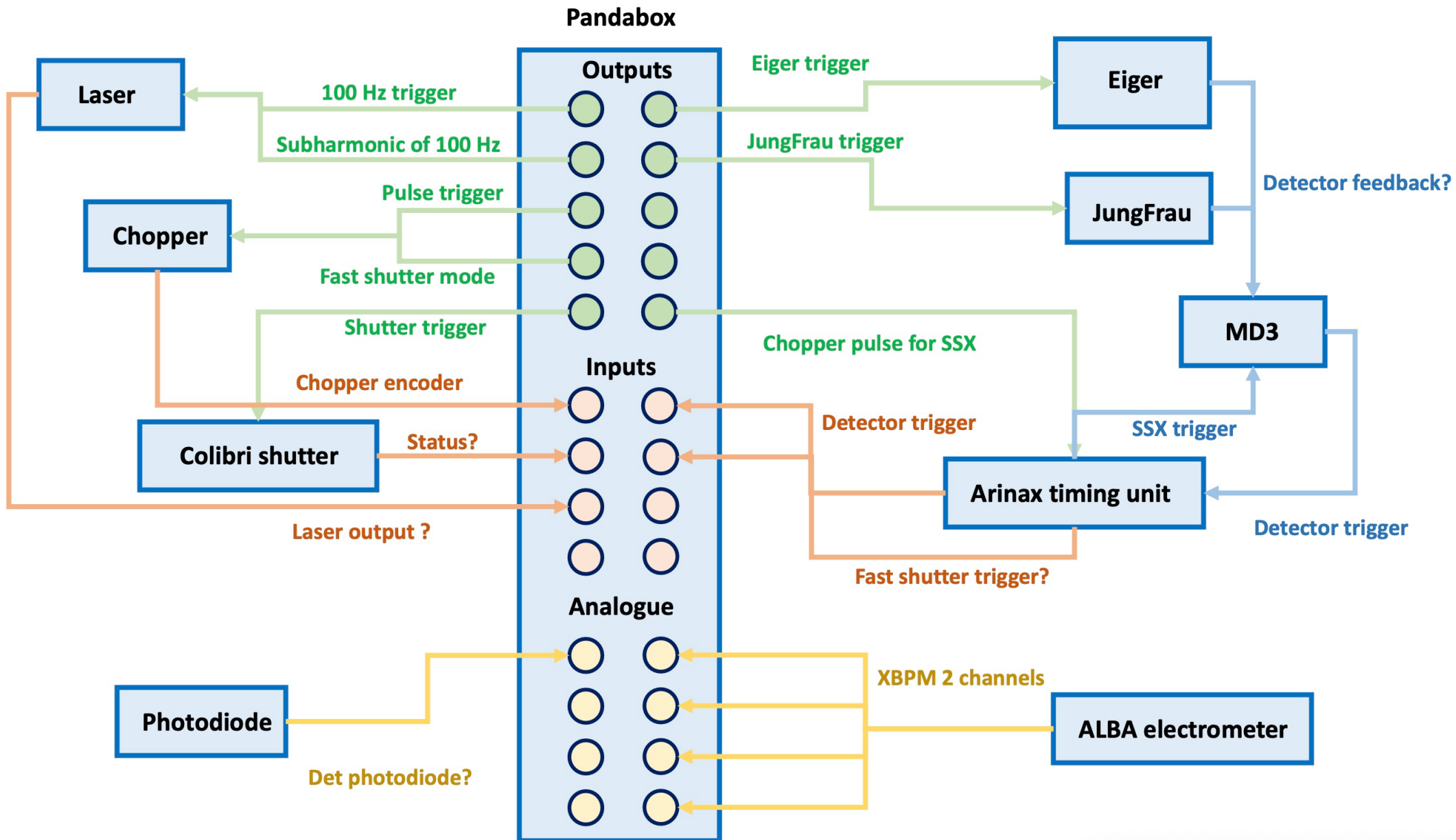
New complementary features to BioMAX functionality

- **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*

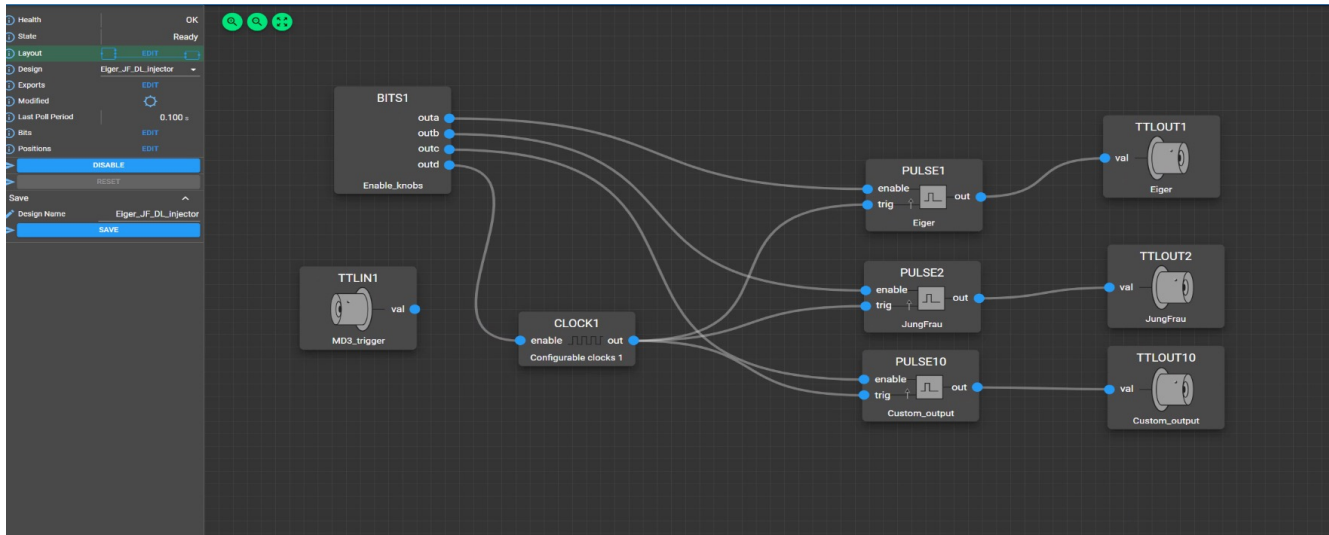
- **Handling more than 1x diffraction (area) detector**
 - Currently done by two branches of MXCuBE
 - Plan to merge so switch can be done within the same session
 - No technical details for implementation plan yet



Timing system



PandA configuration & Tango interfacing



Device Panel [B312A-A101232-CAB01/CTL/PANDA-01] on loca...

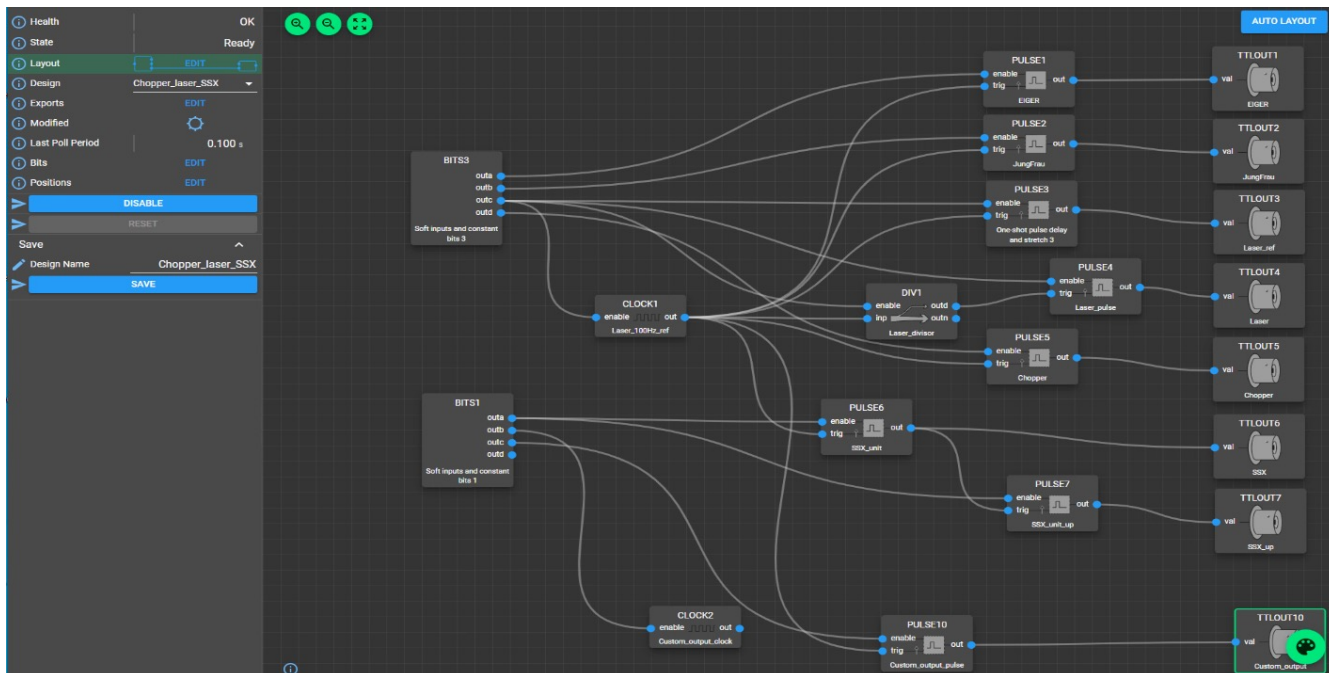
Commands | **Attributes** | Pipe | Admin

Argin value Ex: 2.3 (64bits float)

ClockFrequency	Name	ClockFrequency
ClockRunning	Label	ClockFrequency
CustomOutputDelay	Desc	No description
CustomOutputPulseWid	Writable	READ_WRITE
EigerDelay	Data format	Scalar
EigerPulseWidth	Data type	DevDouble
EnableCounterGate	Max Dim X	1
EnableCustomOutput	Max Dim Y	0
EnableEiger	Unit	
EnableJungfrauCount	Std Unit	No standard unit
EnableMeasurement	Disp Unit	No display unit
EnableShutterCount	Format	%6.2f
JungfrauCounts	Min value	Not specified
JungfrauDelay		

Read Write Plot

Clear history Dismiss



MXCuBE-side of timing

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

Exposure time (s): 0.0001

Energy*: 13.02

Laser pulse width (s): 0.00018

Cell A: 65

Cell B: 65

Cell C: 65

Number of images: 1500000

Resolution*: 2.05

Laser pulse delay (s): 0.00009

Cell α : 90

Cell β : 90

Cell γ : 90

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



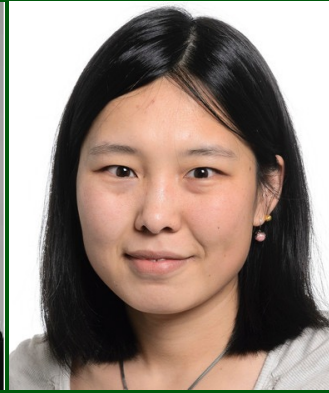
Elmir



Fabien



Ishkhan



Jie



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:



Hide motors ▾

Z:

0.949 ▾ 0.1 mm

Samp-X:

0.272 ▾ 0.1 mm

Samp-Y:

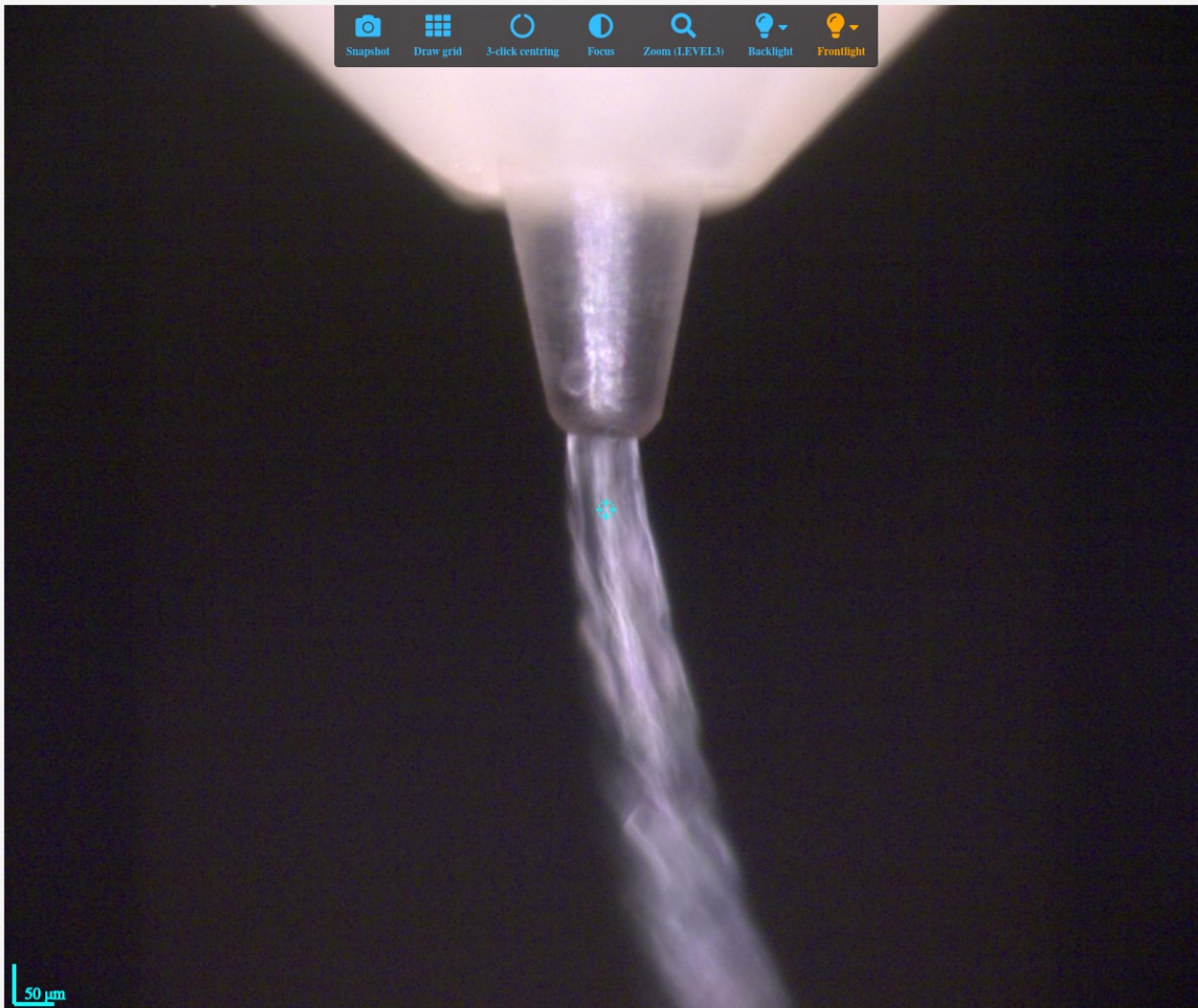
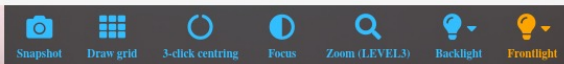
0.027 ▾ 0.1 mm

Sample Horizontal:

0.949 ▾ 0.1 mm

Sample Vertical:

-4.379 ▾ 0.1 mm



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)