

MXCuBE / ISPyB meeting



# MAX IV MXCuBE Status Report

Jie Nan on behalf of the MX-group

2024 May 29th



# MX beamlines at MAX IV

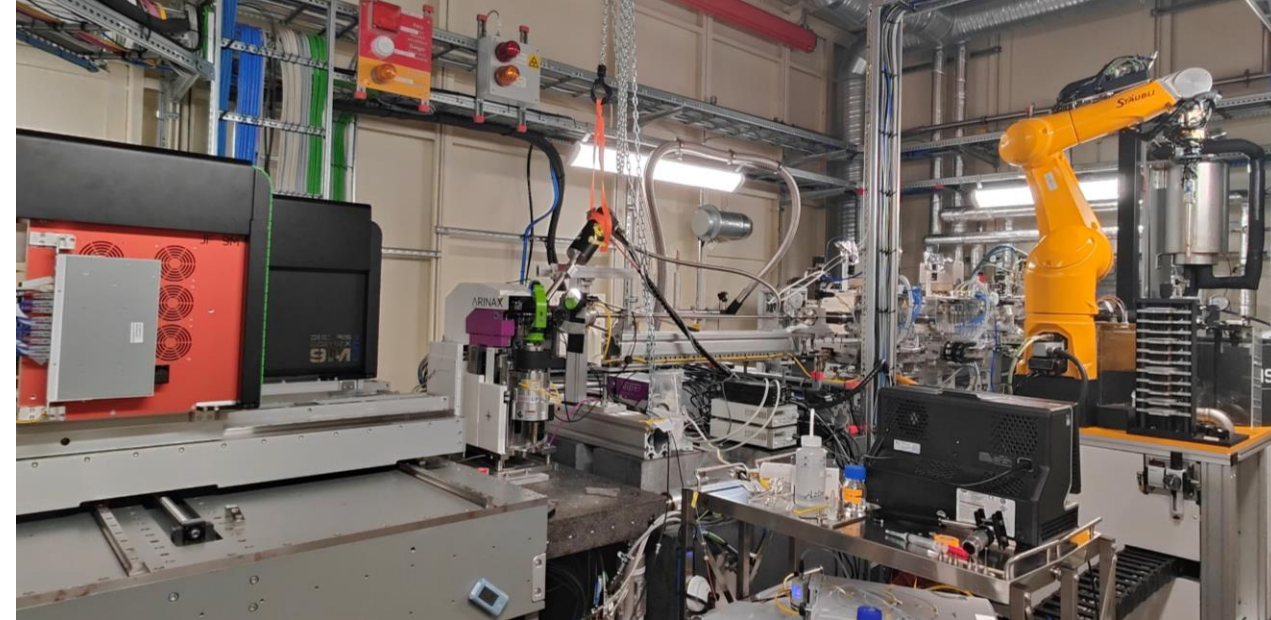
## BioMAX



- Tunable Energy (6-24keV)
- hDCM,  $10^{13}$  ph/s,  $20 \times 5 \mu\text{m}^2$
- **Eiger2 CdTe 16M XE**
- MD3-down
- ISARA
- Amptek fluorescence detector
- REX, Cryojet5, HC-lab

MXCuBE3 v3.0  
hwobj v2.2

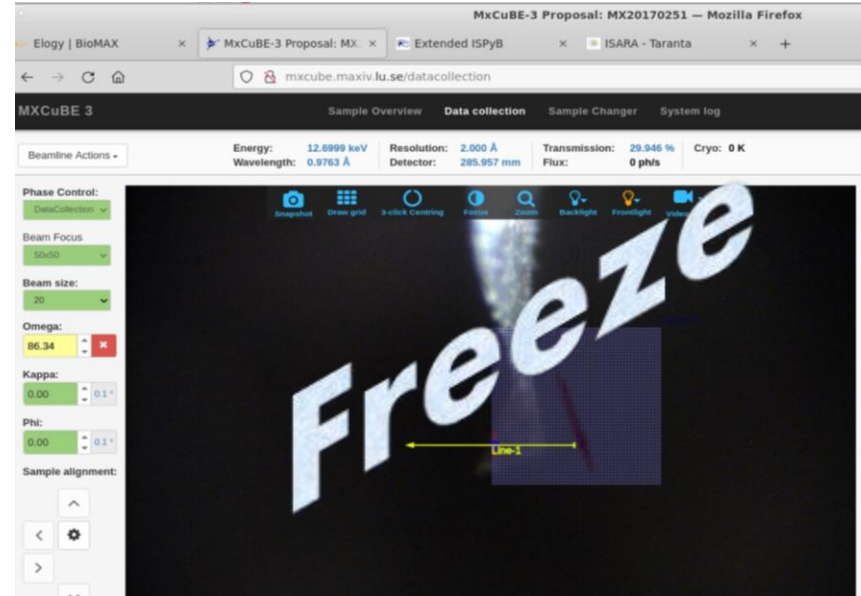
## MicroMAX



- Tunable Energy (5-25keV)
- hDCM,  $10^{13}$  ph/s, now  $14 \times 4 \mu\text{m}^2$  ( $1 \mu\text{m}$  with mirrors)
- MLM,  $>10^{14}$  ph/s
- Eiger2 CdTe 9M
- **Jungfrau 9M**
- MD3-up
- ISARA2
- Cryostream 1000

MXCuBE-web latest  
mxcubecore develop

## MXCuBE, web3.0, HWR 2.2

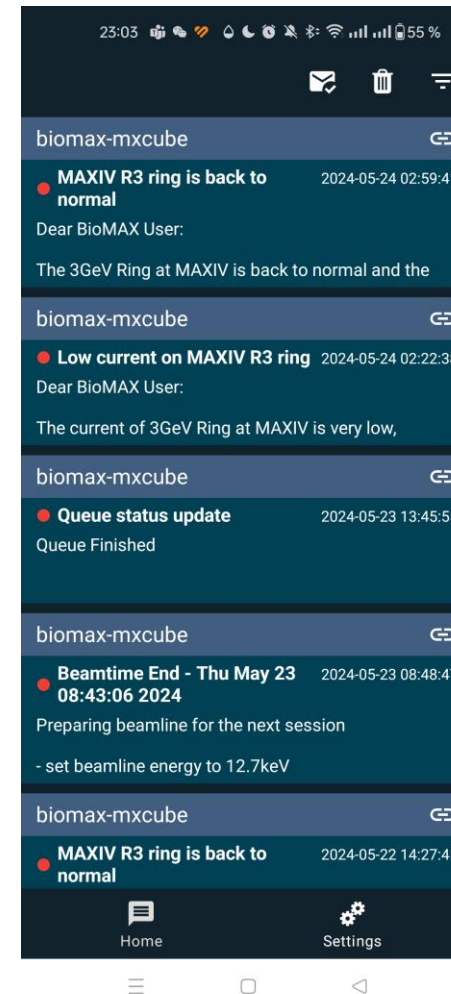


**Upgrade to mxcubecore /mxcube-web latest**

## Recent developments (MXCuBE3)

Improvements of automatic data collection (Ana's talk)

- Import data collection plan from ISPyB
- Inform users of queue change by email
- Notification emails to users are also sent to MAXIV notify app



# BioMAX – Eiger2 CdTe 16M XE

- In operation since 2024 April
- Transition from Eiger 16M
- some minor modification of tango server and MXCuBE
- we stay with Filewriter1 and Stream1, (Filewriter2 and Stream2 available)
- Planning to have 17keV as default energy for operation

# MicroMAX

## X-ray delivery system

- DCM and MLM are in operation, which give  $1e13$  and  $1.5e14$  ph / s respectively
- Beam focusing currently with X-ray lenses; X-ray chopper available in the autumn, KB-mirrors planned for 2025

## Experiment setup

- MD3-up, an empty goino base is used for injector-based experiment
- Jungfrau 9M (on loan from PSI)
- Laser diode installed
- PandABox for timing and trigger control

See Oskar's talk





# MicroMAX –mxcubecore / web4

## Recent development

- Hutch view
- Integration with Jungfrau detector operation
- injector-based (time-resolved) collection
- Phase control for MD3 injector head
- Flux measurement

The screenshot displays the MicroMAX web interface. At the top, a status bar shows Energy: 12.9925 KeV, Resolution: 2.200 Å, Transmission: 10.0 %, Wavelength: 0.9543 Å, and Detector: 223.6 mm. Below this, a central panel shows a live hutch view of the sample area with a 50 µm scale bar. To the left of the hutch view is a 'Phase Control' panel with a 'DataCollection' dropdown, 'Beam size' set to 20, 'Omega' at 264.26°, 'X' at -3.230 mm, 'Y' at -4.379 mm, 'Sample alignment' buttons, 'Z' at 0.949 mm, 'Samp-X' at 0.272 mm, 'Samp-Y' at 0.027 mm, 'Sample Horizontal' at 0.949 mm, and 'Sample Vertical' at -4.379 mm. To the right of the hutch view is a 'Sample' panel showing 'Sample: Lyz\_HEC1 - MK\_lysozyme' and 'Queued Samples (0)'. Below this is a table for 'SSX Injector Collection' with columns: Start °, Osc. °, t (s), # Img, T (%), Res. (Å), and E (keV). The table contains one row of data. At the bottom right is a 'Log messages' panel showing several status messages.

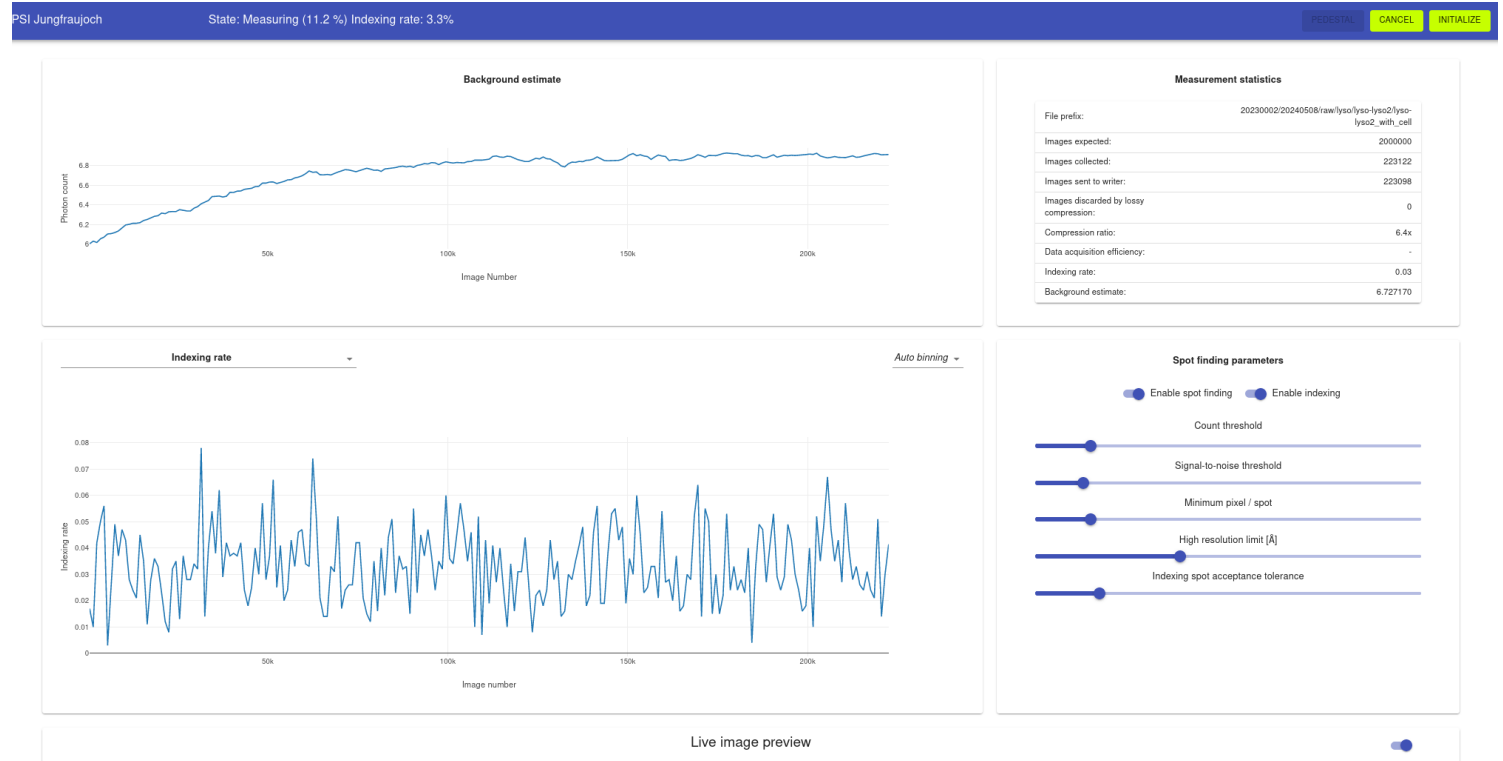
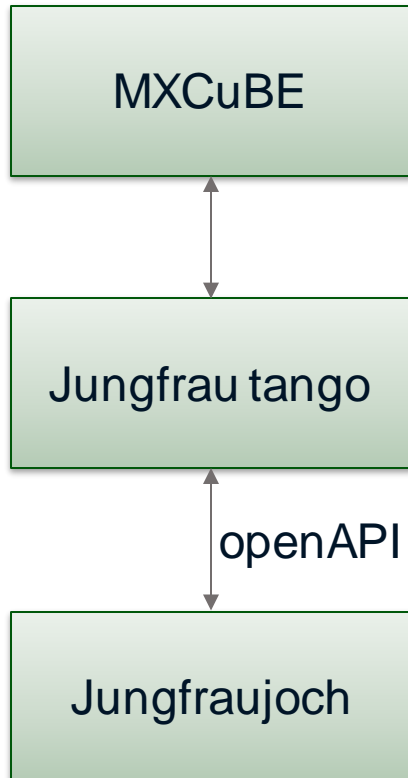
Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (keV)
264.26	0.10	0.000500	500000	10.00	2.200	12.9925

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)

# Jungfrau detector

DCU

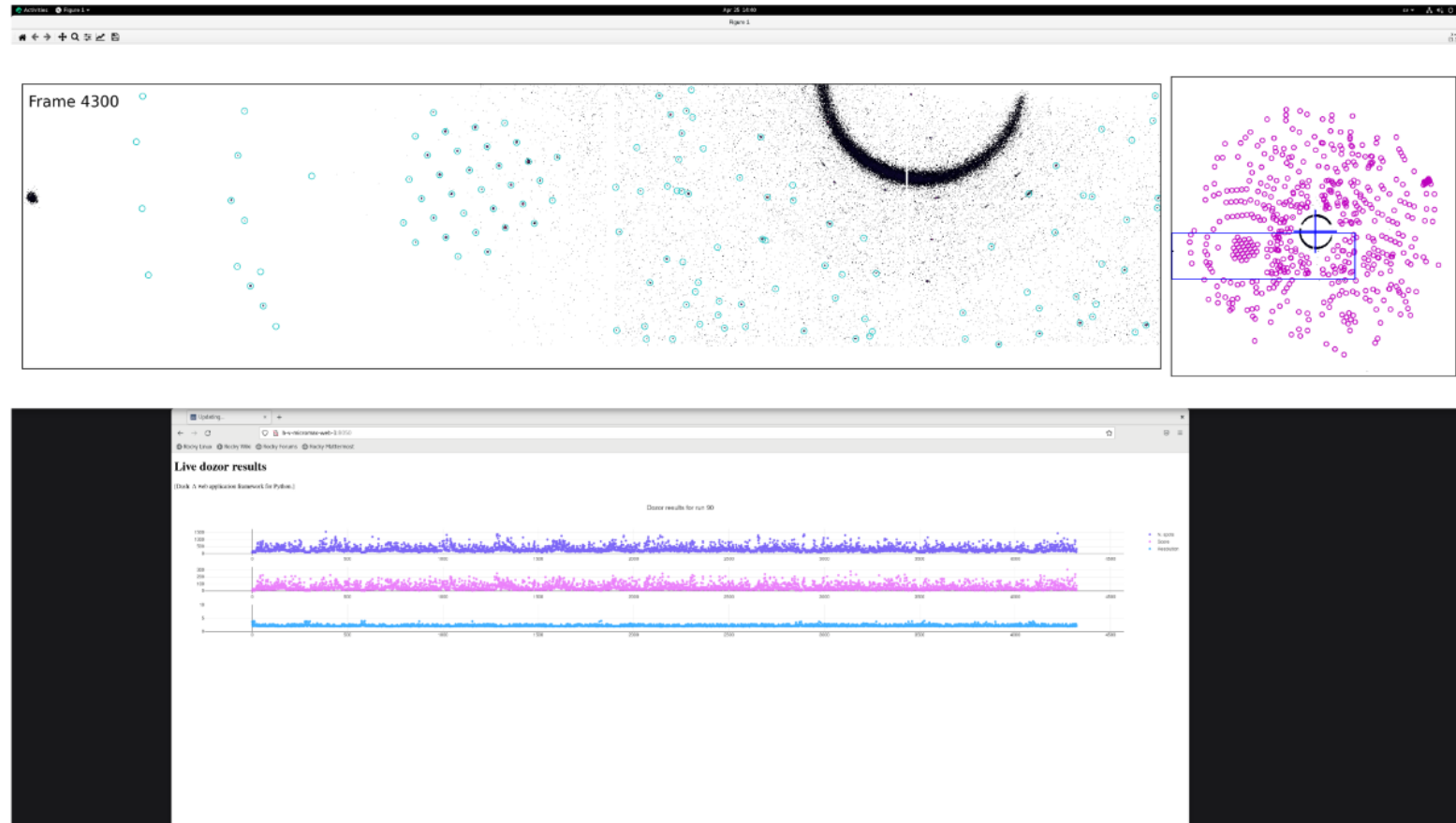




# MXSuite - ongoing

- Slurm job per collection → Service
- Stream for all types of collections
- Results to ISPyB
- web-based Live Viewer

Live spotting and viewer

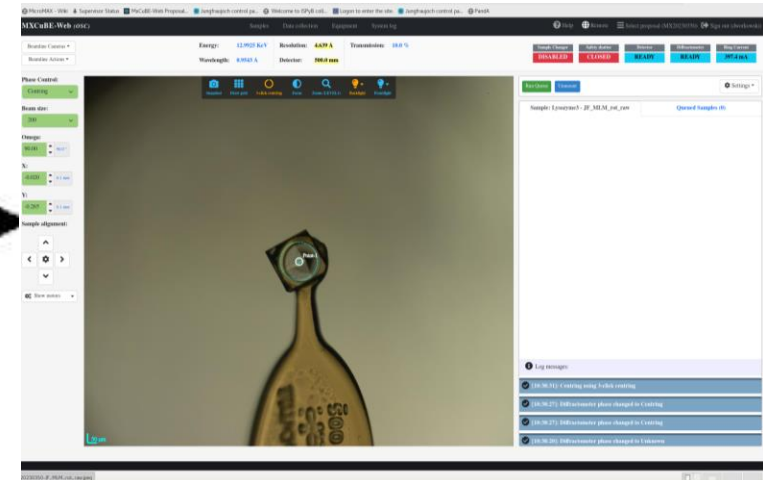
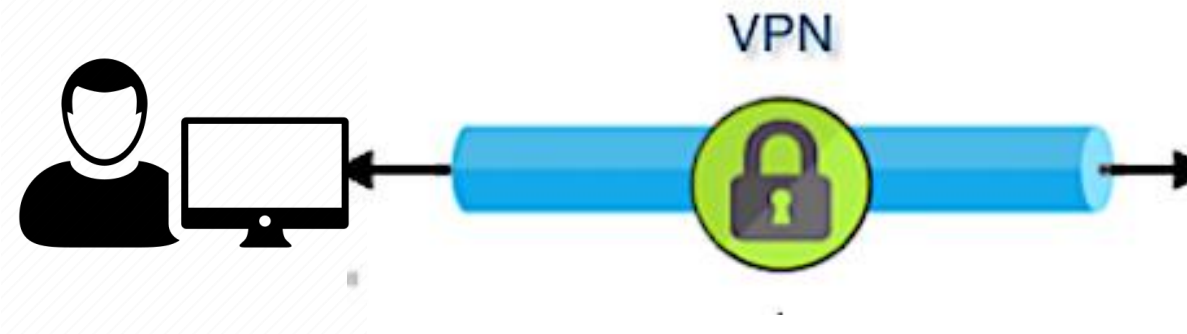


Cecilia Casadei

- Number of spots vs. frame number
- Dozor score vs. frame number
- Resolution [Å] vs. frame number

# Multi Factor Authentication

- All external access to MAX IV resources requires 2-factor authentication
- Time-Based one-time password (TOTP)
- mobile application, no SMS since 2024-01-15



# Plans for the next six months

- mxubecore / mxcube web at BioMAX
  - Include all features in mxcube3
  - Integrate Global Phasing workflow
- Same mxcube version at both BioMAX and MicroMAX
- Continue to develop the SSX features at MicroMAX
- Fast and easy switch between different setups, including detectors

# Acknowledgements

## **MAX IV**

- MX group
- Software group
  - Mikel Eguiraun
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- Peter Keller

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