



MXCuBE at MAX IV

Jie Nan On behalf of MX-group at MAX IV

Oct 30, 2019

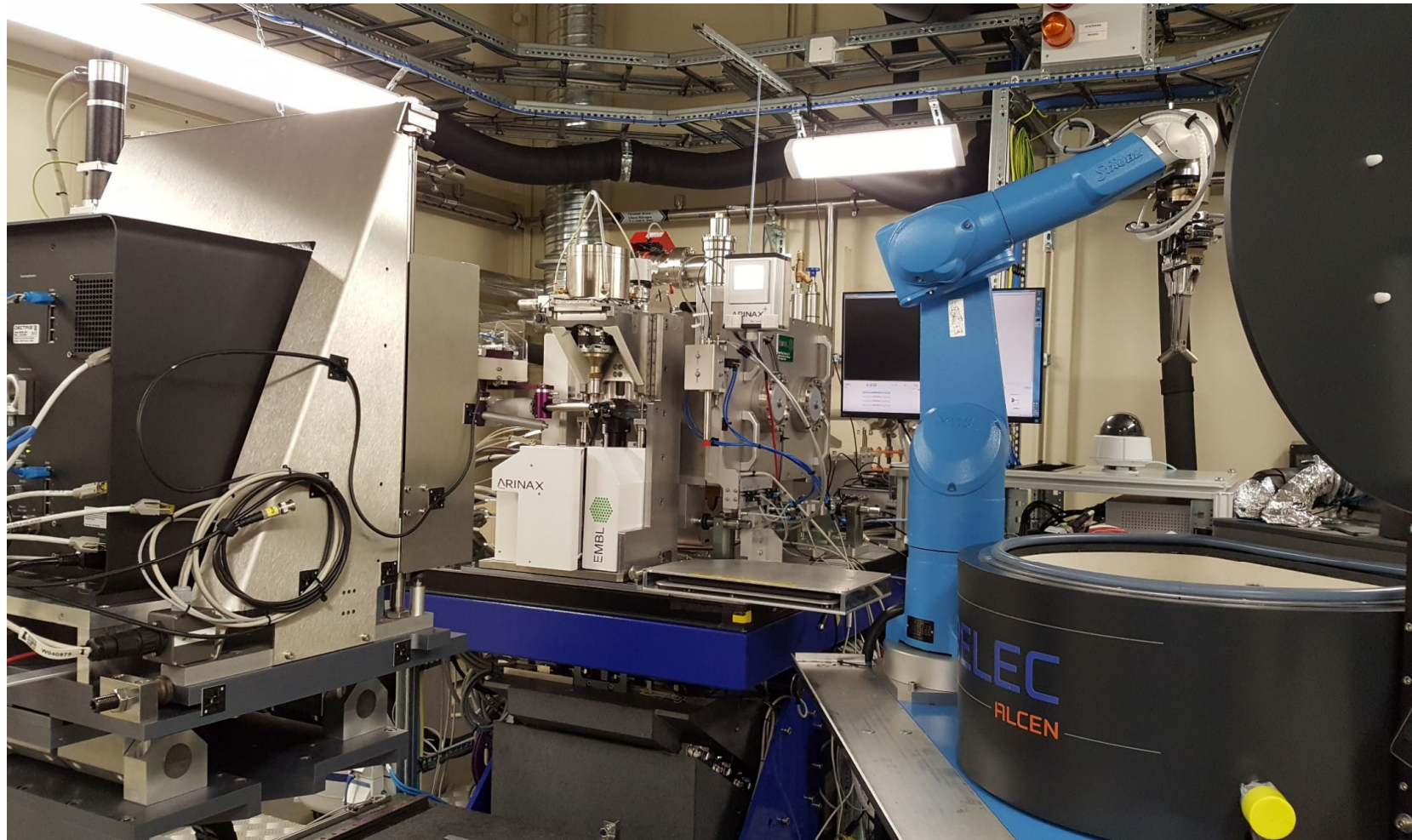
MAXIV

MX Beamlines at MAX IV

BioMAX

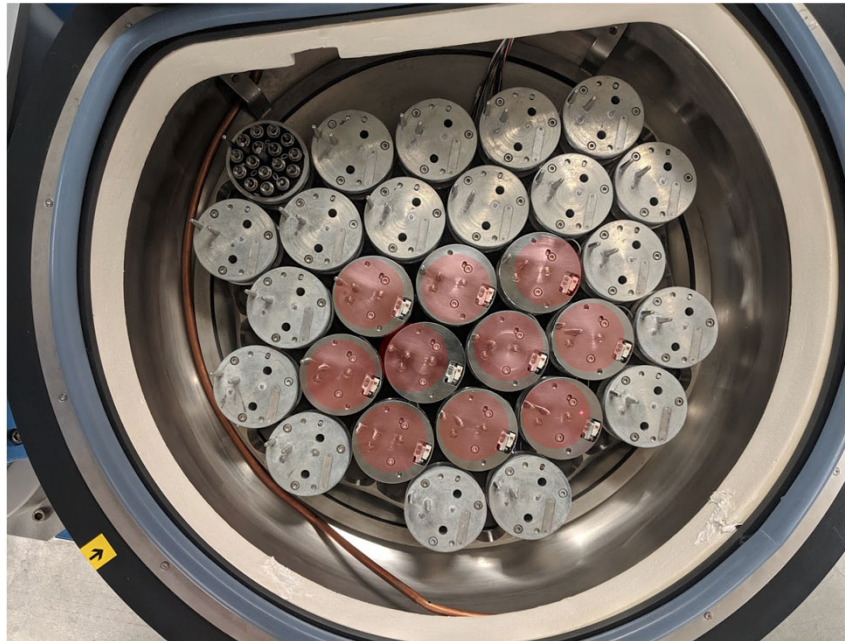
- In-vacuum undulator
- 5 – 25 keV
- 10^{13} ph/s @250mA
- BCU
- Cryojet5, HC-lab and REX
- Eiger16M
- ISARA sample changer
- MD3 Diffractometer
- Amptek fluorescence detector
- Roadrunner

MicroMAX



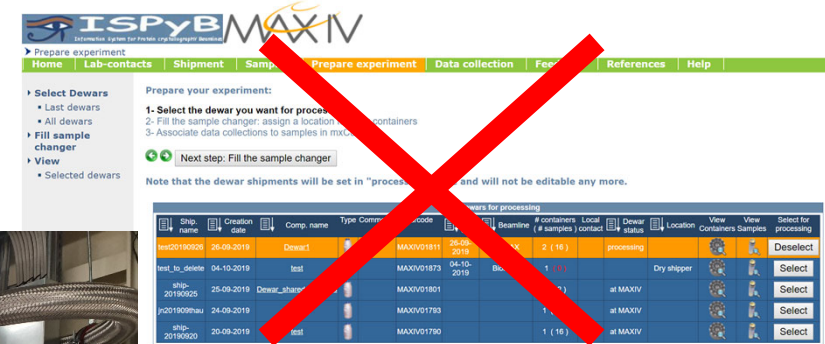
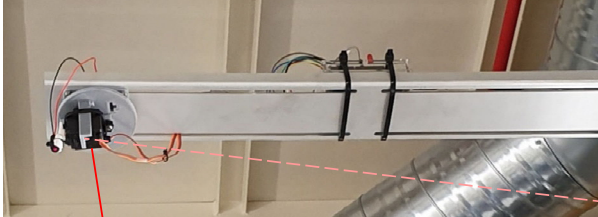
What's new - ISARA upgrade

- Upgrade of 10 new Unipuck positions and implementation within ISARA/MXCuBE
- Spare gripper tool

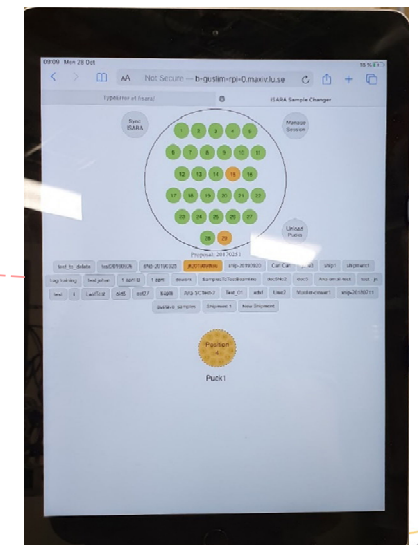


Uni-Puck support only, 29 positions = 464 samples

What's new - Puck loading app



Puck positions are automatically registered in ISPyB



What's new - MD3 upgrade

Problems

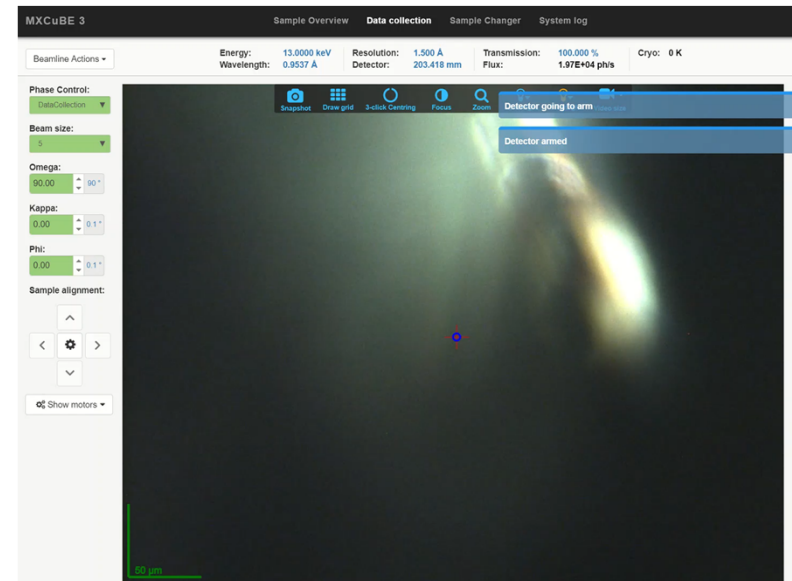
- Raster scan frequently failed due to “insufficient calculation time” error
- overhead > 1s for each turn
- *Raster, 50x50 cells, 2500 imgs, 10 ms per img*
25 s collection + >50 s overhead

Upgrade

- Turbo PMAC → Power PMAC (including PMAC program)
- New Server, 4U RAID1 Core i7-6700
- MD3 software from v2.4 to v3

Achieved

- no failure of “insufficient calculation time”
- reduced overhead **0.33 s per turn**
- *Raster, 50x50 cells, 2500 imgs, 10 ms per img*
25 s collection + 17s overhead



What's new – Minikappa upgrade



Minikappa upgraded, compatible with ISARA

MXCuBE 3

Beamline Actions ▾

Phase Control:
Transfer ▾

Beam size:
50 ▾

Omega:
360.00 ▴ ▾ 90°

Kappa:
90.00 ▴ ▾ 0.1°

Phi:
20.00 ▴ ▾ 0.1°

MXCuBE3 at BioMAX - 1

MXCuBE3 in production

- MXCuBE3, 3.0.1
- HardwareRepository, 2.2
- Same as spring

Deployed new features

- Lucid3
- Flux calculation
- Characterization analysis
- Performance improvement
- Remote operation, control handling

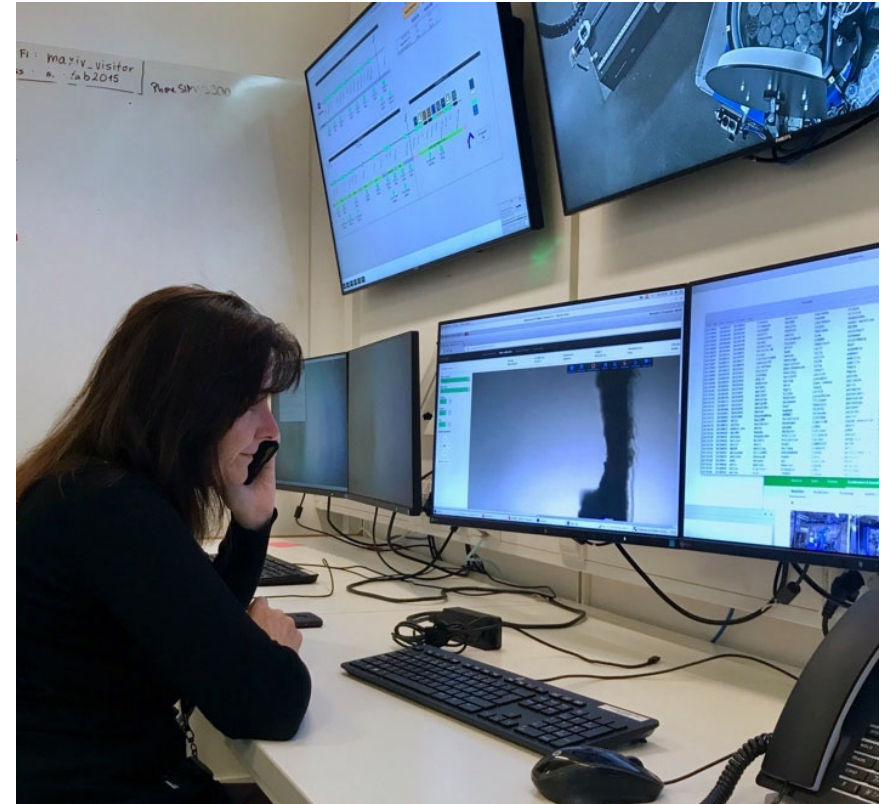
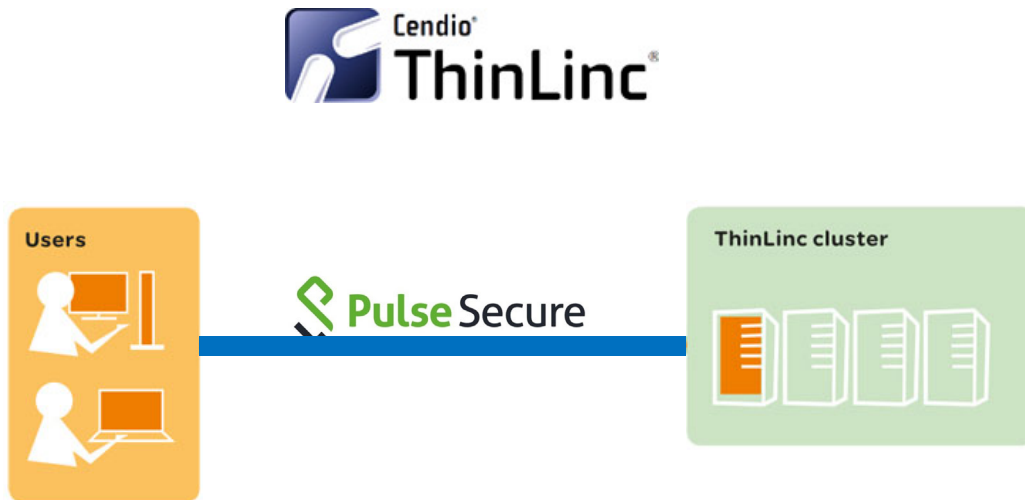
The screenshot displays the MXCuBE3 control interface. At the top, there are navigation tabs: Sample Overview, Data collection (active), Sample Changer, and System log. The top right corner includes Help, RA, and Sign out options. Below the navigation, there are status indicators for Sample Changer (READY), Safety Shutter (OPEN), and Ring Current (248.15). The main interface is divided into several sections:

- Beamline Actions:** A dropdown menu.
- Energy/Wavelength:** Energy: 13.0000 keV, Wavelength: 0.9537 Å.
- Resolution/Detector:** Resolution: 5.032 Å, Detector: 800.004 mm.
- Transmission/Flux:** Transmission: 100.000 %, Flux: 0 ph/s.
- Cryo:** 0 K.
- Phase Control:** Centring (selected), Beam size: 50, Omega: 360.00°, Kappa: 0.00°, Phi: 360.00°.
- Sample alignment:** A set of directional arrows and a 'Show motors' checkbox.
- Microscope View:** A central image showing a sample in a microscope. A blue circle highlights a 'Point-1' on the sample. A 50 µm scale bar is visible in the bottom left corner.
- Top Bar:** Snapshot, Draw grid, 3-click Centring, Focus, Zoom, Backlight, Frontlight, Video size.
- Right Panel:** Run Queue, Unmount, Settings. Below this, a table for 'Point-1: Data Collection' is shown.

Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
360.00	0.20	0.0110	1800	100.00	1.300	13.0000	0.00	0.00

Remote operation

- Remote access for commissioning users, success with two proposal groups
- Users run MXCuBE3 on remote desktop via ThinLinc



Ana Gonzalez is assisting remote users during data-collections

MXCuBE3 at BioMAX - 2

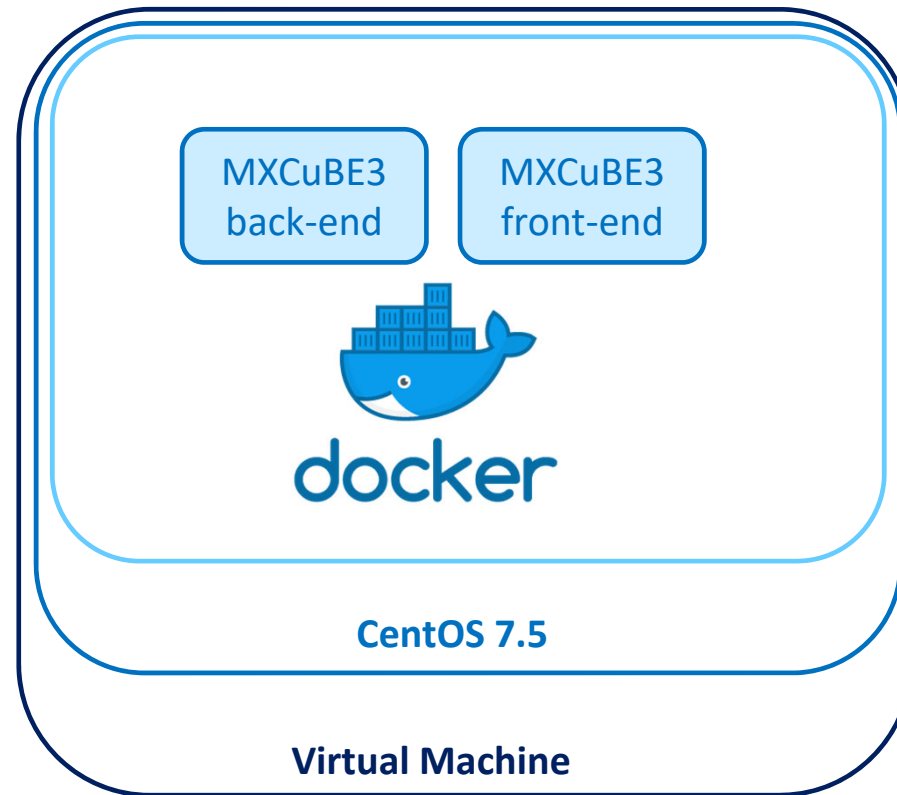
Ongoing

- Raster scan
- Multicast (tested)
- Beamline operation macros, i.e. Beam alignment
- Integration of Amptek to support for XRF, XANES

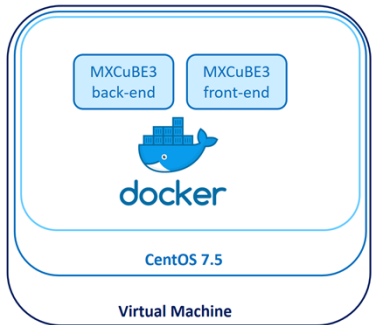
The screenshot displays the MXCuBE3 control interface. At the top, it shows the current state: Energy: 13.0000 keV, Wavelength: 0.9537 Å, Resolution: 5.032 Å, Detector: 800.004 mm, Transmission: 100.000 %, Flux: 0 ph/s, and Cryo: 0 K. The interface is divided into several sections:

- Phase Control:** Includes settings for Centring, Beam size (5), Omega (360.00), Kappa (0.00), and Phi (360.00).
- Sample alignment:** Features navigation buttons and a 'Show motors' option.
- Data collection table:** A table with columns for Name, V-Space, H-Space, Dim, Dim, #Cells, and Ω. It lists a grid with dimensions 140 x 28 x 33 (924 cells) and a rotation of 360.00°.
- Live Image:** A central image showing a sample with a green grid overlay. A 'Point-1' is marked on the grid, and a context menu is open with options: Mesh Scan, Centring Point on cell, and Delete.
- Right Panel:** Shows 'Sample: cau - cau' and 'Queued Samples (0)'. It includes a 'Run Queue' button and a 'Settings' dropdown.

How we run MXCuBE3 Server?



How we update MXCuBE3 Server?



Build docker images

28b007ae

Pipeline Jobs 3

Build

build_backend

build_frontend

a few minutes

Deployment by Ansible

39841 - mxcube-prod Playbook Run

STARTED 10/21/2019 10:26:19 AM FINISHED 10/21/2019 10:27:08 AM

LAUNCHED BY jjenan

JOB TEMPLATE mxcube-prod

INVENTORY IMS Inventory

PROJECT IMS Project

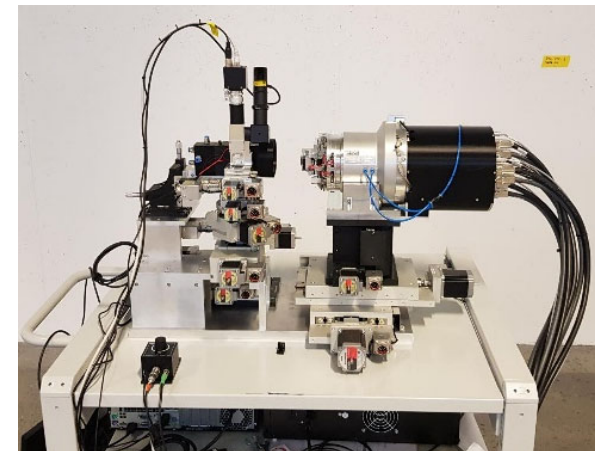
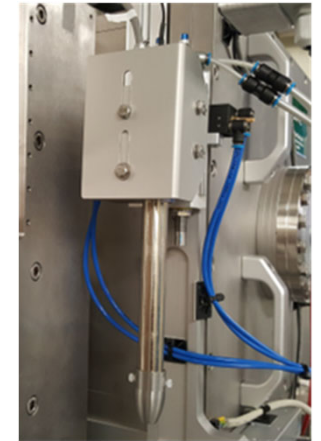
CREDENTIALS ims-user ims-vault

Relaunch using the same parameters

AWX

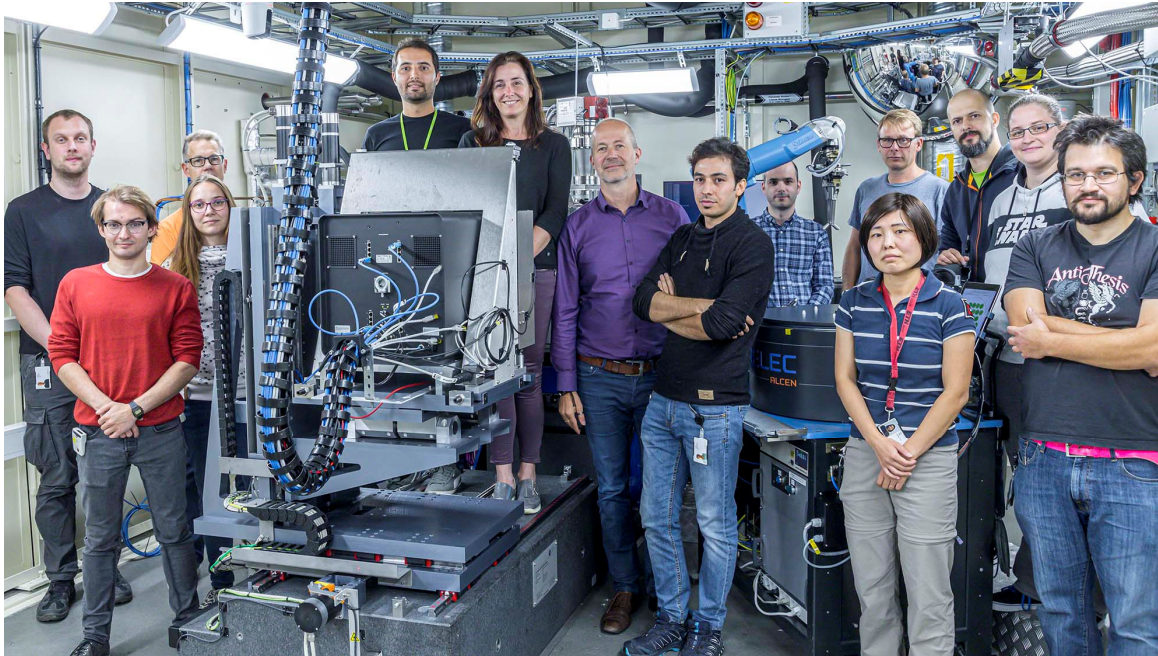
Ongoing and future work

- Upgrade MXCuBE3
- Raster scan
- MAD experiments
- Minikappa, visual or X-ray based re-orientation, strategy calculation
- Better support of SSX



Acknowledgement

The MX group



From left to right:

- Oskar Aurelius
- Vladimir Talibov
- Laila Benz
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- Gustavo Lima
- Ana Gonzalez
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- Vahid Haghghat
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- Jie Nan
- Johan Unge
- Mirko Milas
- Monika Bjelcic
- Elmir Jagudin

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- Many others from MAX IV and MXCuBE/ISPyB collaboration