



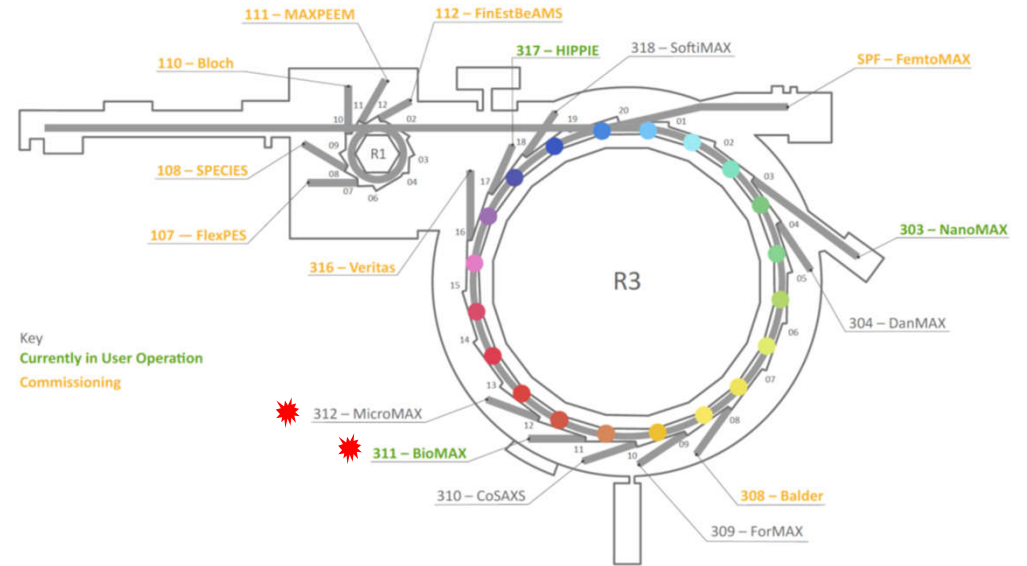
MXCuBE at MAX IV

Jie Nan On behalf of MX-group at MAX IV

Jun 29, 2020

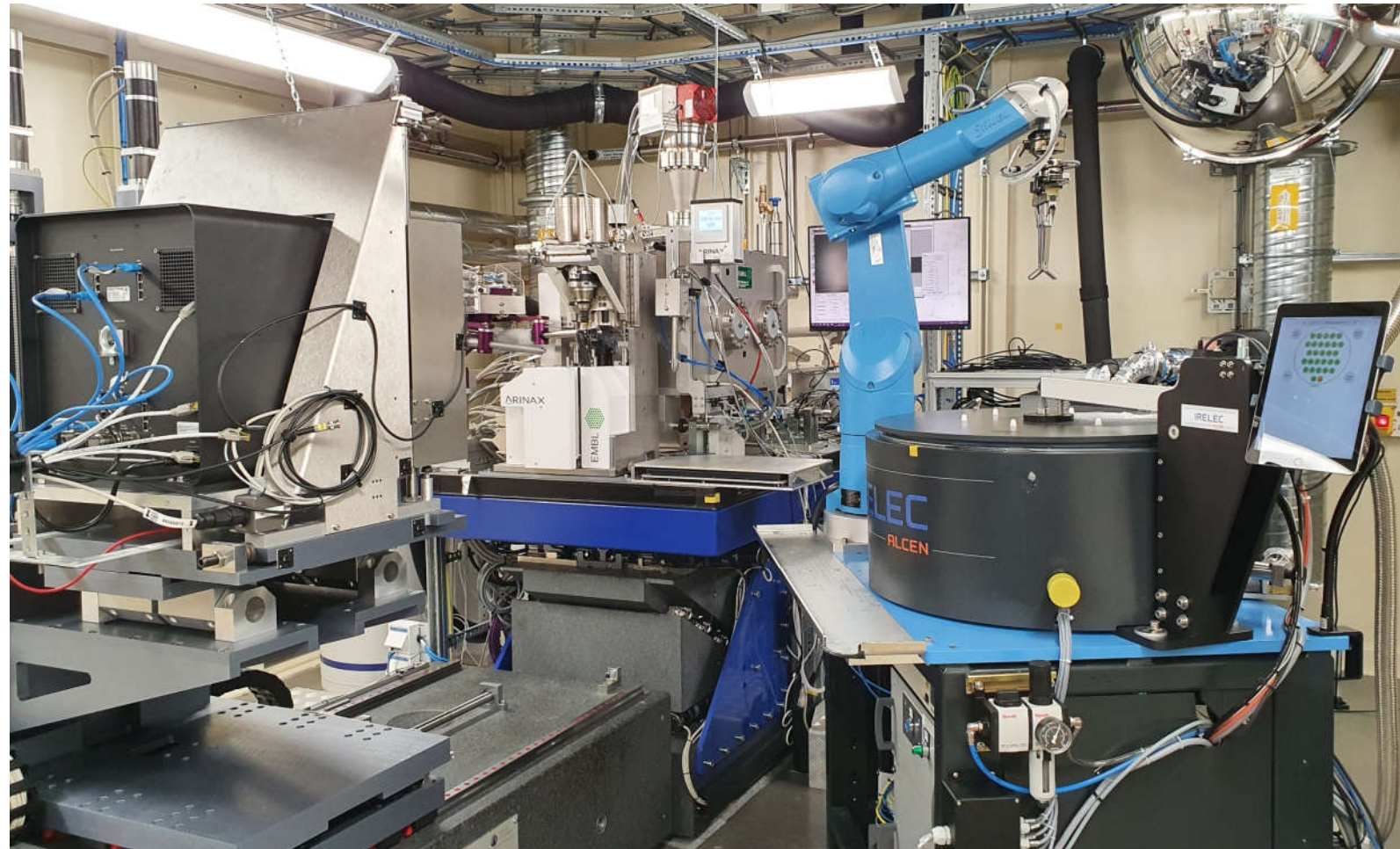
MAXIV

MX Beamlines at MAX IV



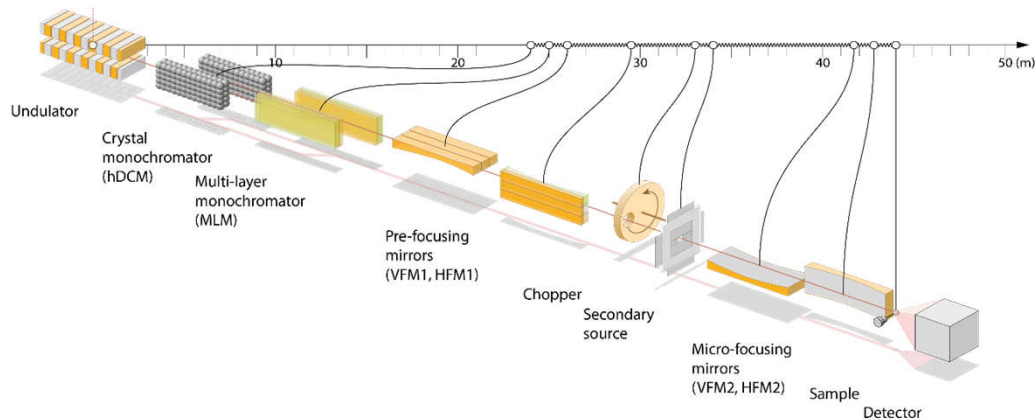
BioMAX – in operation

- In-vacuum undulator
- 5 – 25 keV
- 4×10^{12} ph/s @sample position
- BCU
- MD3 Diffractometer
- Cryojet5, HC-lab and REX
- Amptek fluorescence detector
- Eiger16M
- ISARA sample changer



MicroMAX – under construction

Scope	Serial crystallography; time-resolved study; standard rotation collection
Beam Size	Tunable between below 1 μm up to 10 μm
Energy Range	5–20 keV (option of higher energy)
Time Scales	Down to microseconds
User operation	2022



From Mirko Milas

MXCuBE3 at BioMAX - 1

MXCuBE3 in production

- MXCuBE3, 3.0.1
- HardwareRepository, 2.2
- Same as 2019 spring

Todo

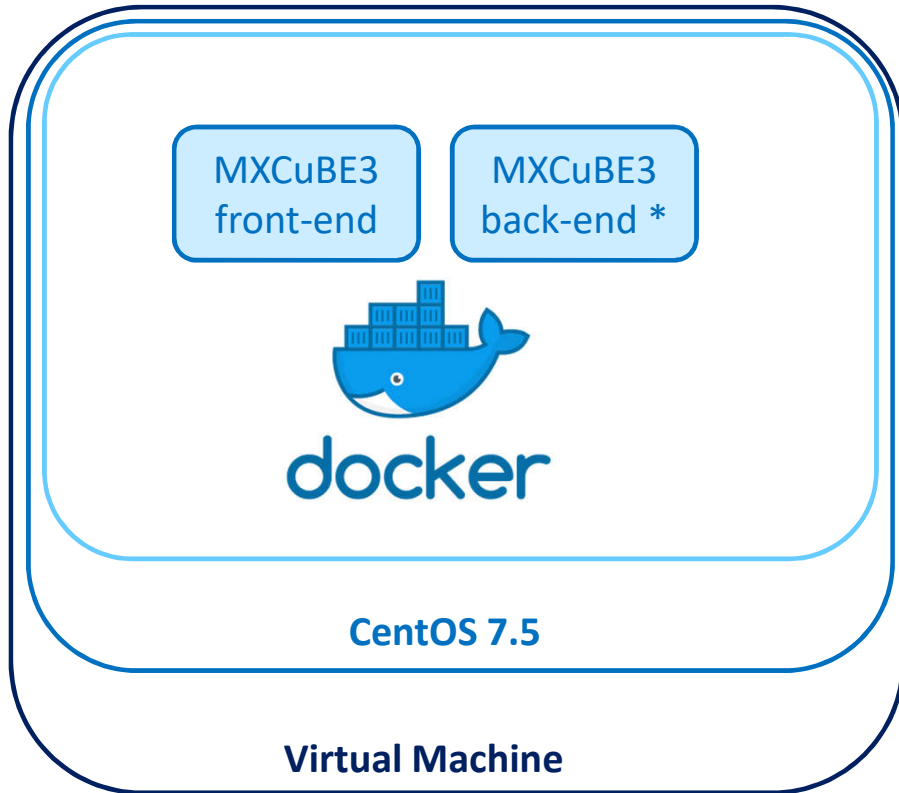
upgrade to the latest python3 version

New features / Improvements

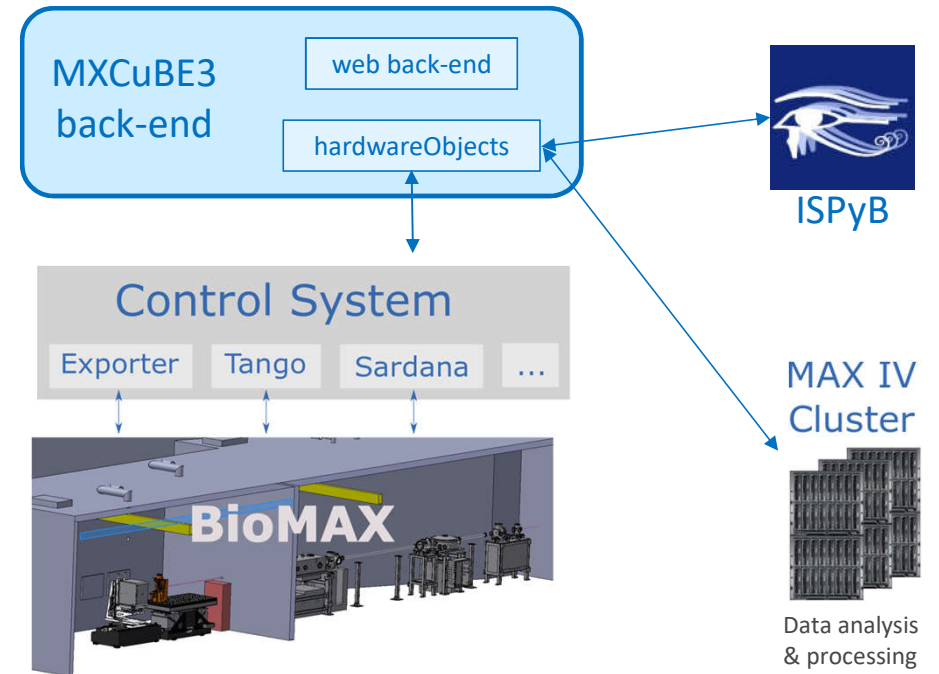
- Remote operation
- Enhanced SC operation
- XRF & Energy Scan
- Raster scan
- SSX

The screenshot displays the MXCuBE3 control interface. At the top, there are tabs for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. Below these, a status bar shows: Energy: 12.6998 keV, Wavelength: 0.9763 Å, Resolution: 1,500 Å, Detector: 196.838 mm, Transmission: 100.000 %, Flux: 2.75E+12 ph/s, and Cryo: 0 K. On the right, there are buttons for 'Sample Changer' (READY), 'Safety Shutter' (OPEN), and 'Ring Current' (249.62). The main area is divided into three sections: 1. Left sidebar: 'Phase Control' (Centring), 'Beam size' (50), 'Omega' (360.00 / 90°), 'Kappa' (0.00 / 0.1°), 'Phi' (0.00 / 0.1°), and 'Sample alignment' controls. 2. Center: A video feed showing a sample with a 'Point-1' marker. 3. Right sidebar: 'Sample: Sample-27:09', 'Queued Samples (0)', and a table for 'Point-1 : Characterisation'. The table has columns: Start, Osc., t (ms), # Img, T (%), Res. (Å), E (KeV), φ°, κ°. The table contains one row of data: 360.00, 0.50, 0.020, 4, 100.00, 1.500, 12.6998, 0.00, 0.00. At the bottom right, there is a 'Diffractometer' video window showing a live feed of the equipment with a timestamp 'BioMAX 2020-04-23 00:43:58'.

MXCuBE3 at BioMAX - 1



* User can restart from terminal

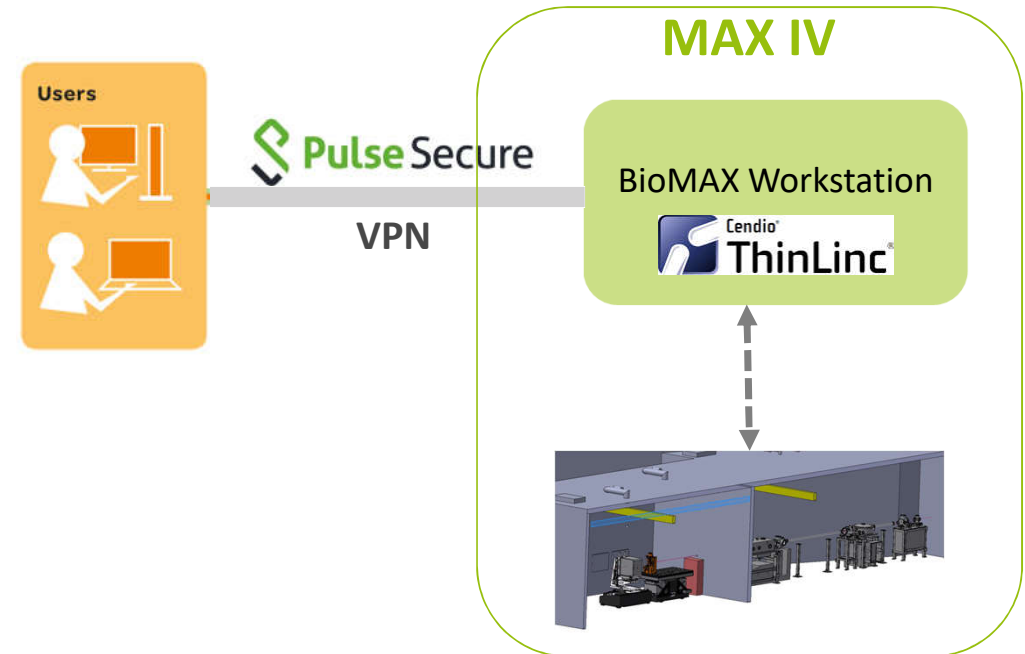


Remote operation

- Since 2019 October
- continue with ThinLinc with shadowing option
- Since Mid-march 2020, only remote operation due to Covid-19

Crucial that MXCuBE is stable and robust, but also important that users can handle some failures and errors remotely, e.x. empty sample mount, sample holder with long pin, beam recovery.

Improved throughput, ~1 puck (16 samples) per hour



Enhanced sample changer operation

Known issues:

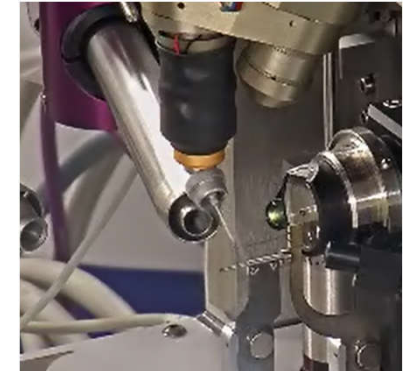
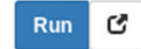
- Mount empty position (frequent)
Check sample ondiff
- Sample holder with too long pin (frequent)
Before unmount, check PhiY of last saved center position

MXCuBE – beamline actions

prepare_remove_long_pin

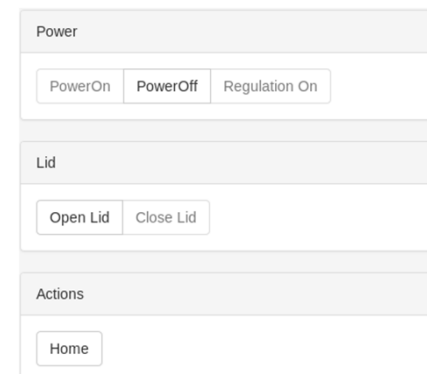
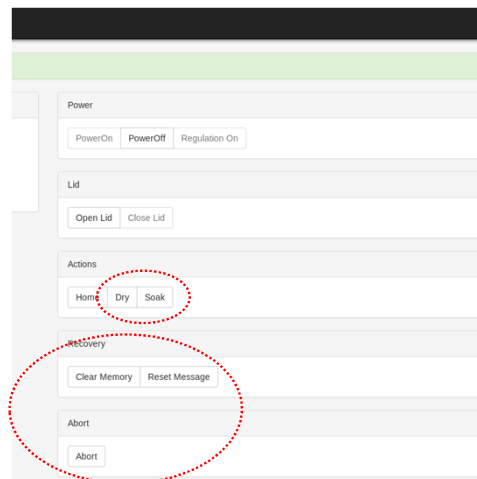
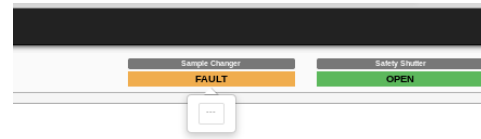


empty_sample_mounted

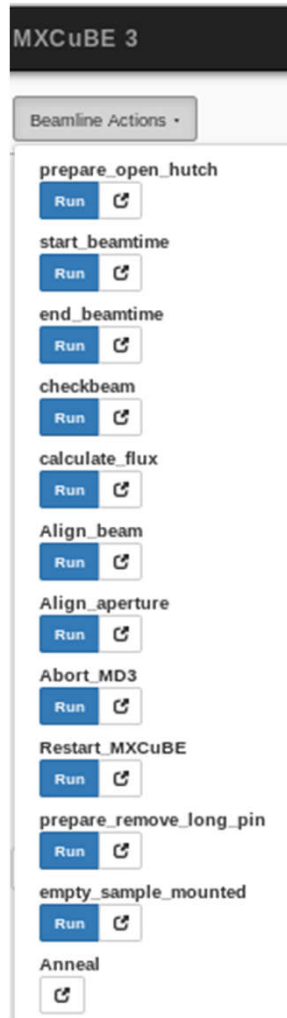


Sample holder with long pin

- Sample holder frozen to the unipuck base (new)



Growing beamline actions



Beam delivery

Software related

Sample changer

Todo →

- More interactive
- More organized, i.e. Troubleshooting Tab containing several sections

XRF and Energy Scan

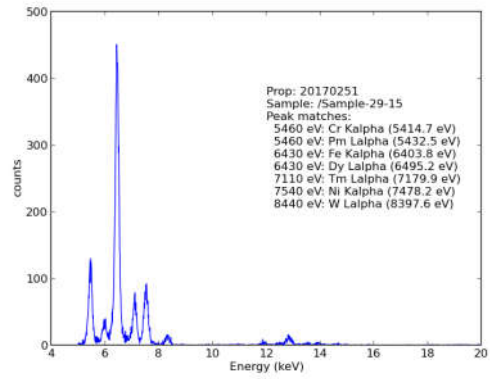
XRF ✕

Path: /data/visitors/biomax/20170251/20200624/raw/Sample-29-15/
 Filename:

Subdirectory:

Prefix:

Count time (s):



Energy Scan ✕

Path: /data/visitors/biomax/20170251/20200624/raw/Sample-29-15/
 Filename:

Subdirectory:

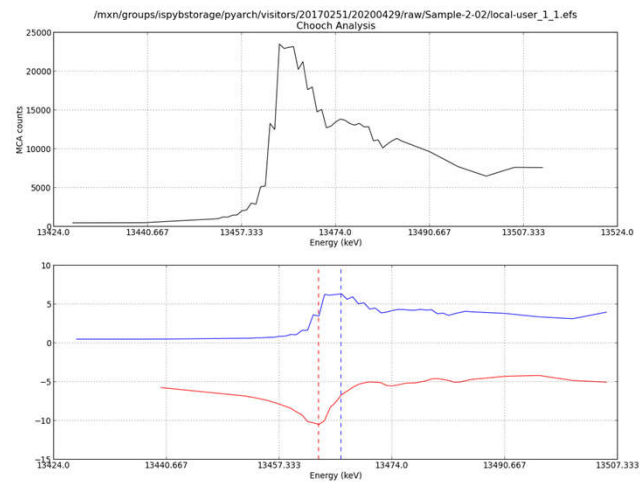
Prefix:

Element

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuq
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Element:

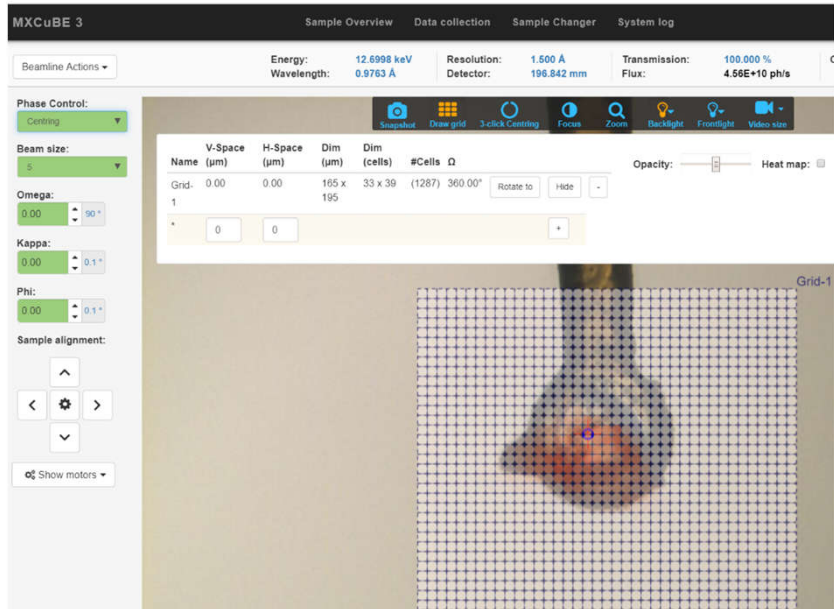
Edge:



Todo:

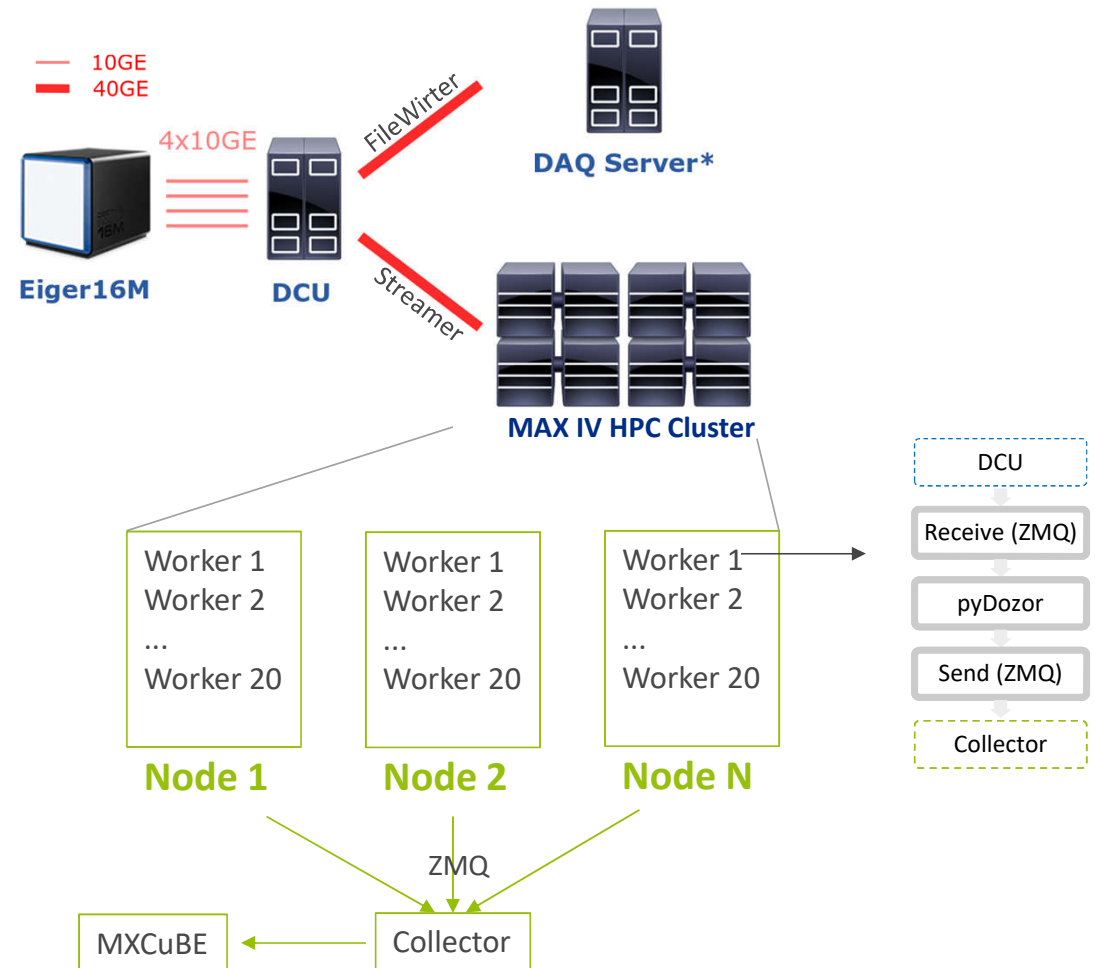
- Alive plot & results in MXCuBE3
- Interleave, how to handle Eiger data of multiple wedges, virtual dataset?

Raster Scan – on-the-fly spot finding with dozor



Todo:

- Improvement of usability and stability
- (auto) X-ray centering



What's new – SSX

Continuous liquid (i.e.HVE)

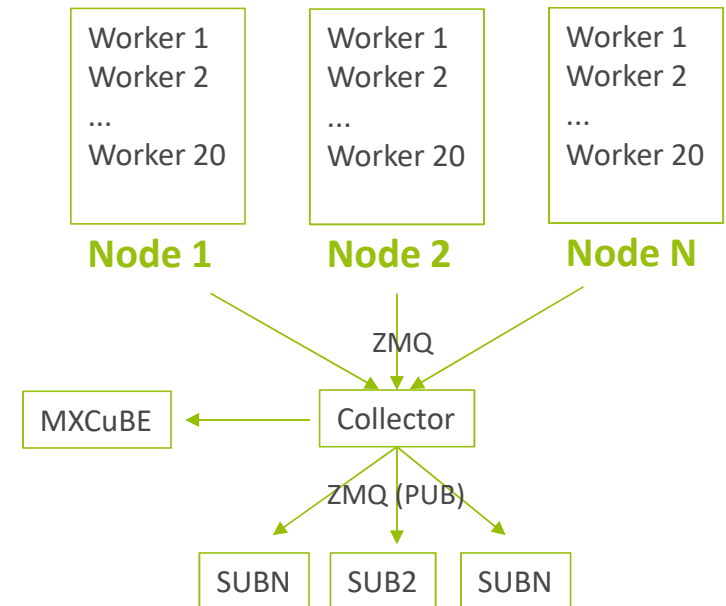
- MD3, different configs from MK3 setup, managed with git
- MXCuBE refactory
 - Past, using different installations using different hwobj branches
 - Now, same hwobj branch but different branches of config xmls

Fixed target

- Improve the performance of manipulating large mesh (ongoing)

Todo,

- Online feedback
- Towards MicroMAX requirements



Acknowledgement

MX group & many others from MAX IV

All BioMAX users

ESRF MXCuBE team

Gleb Bourenkov and Marina Nikolova

MXCuBE/ISPyB collaboration