



MXCuBE at MAX IV

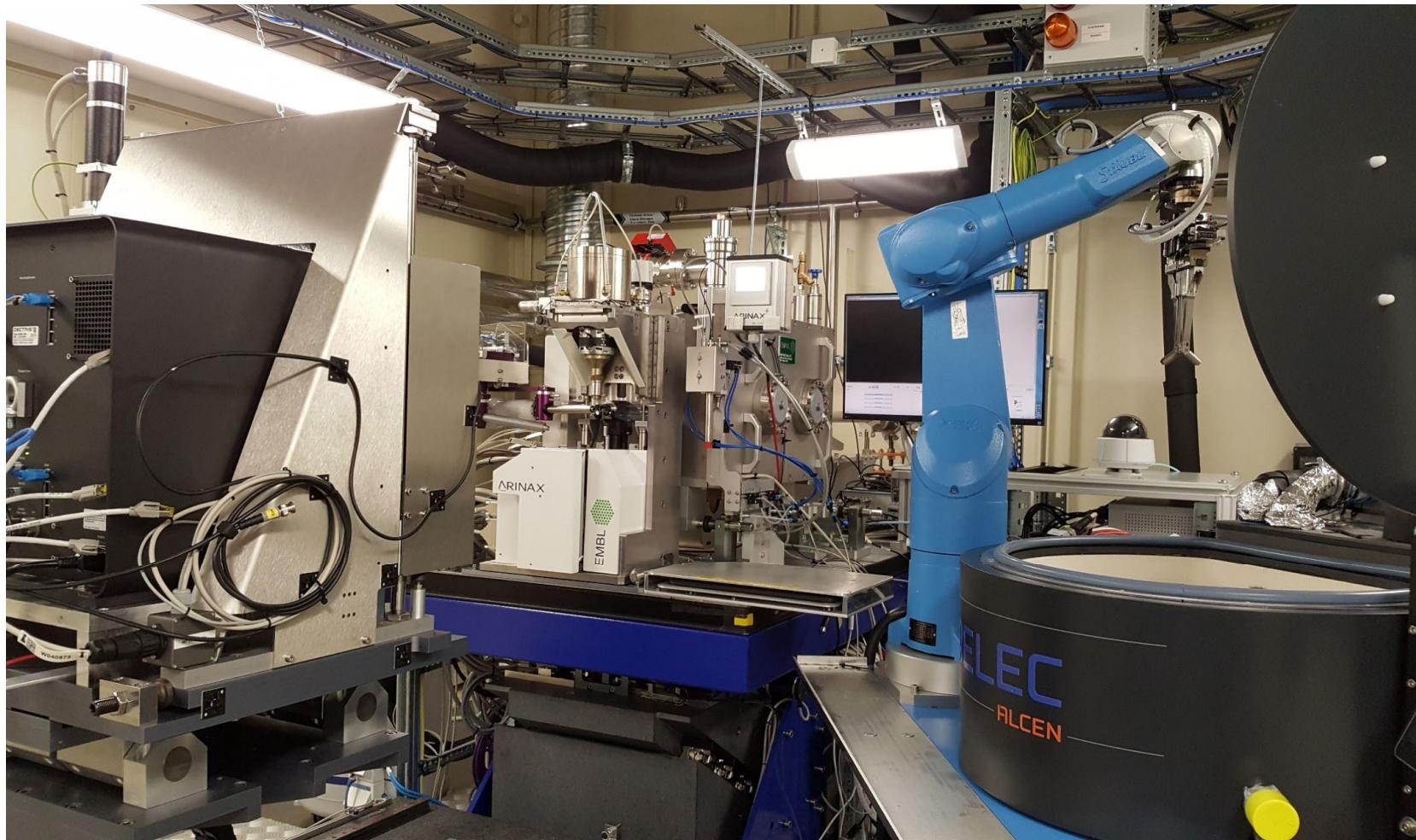
Jie Nan On behalf of MX-group at MAX IV

Oct 30, 2019

MX Beamlines at MAX IV

BioMAX

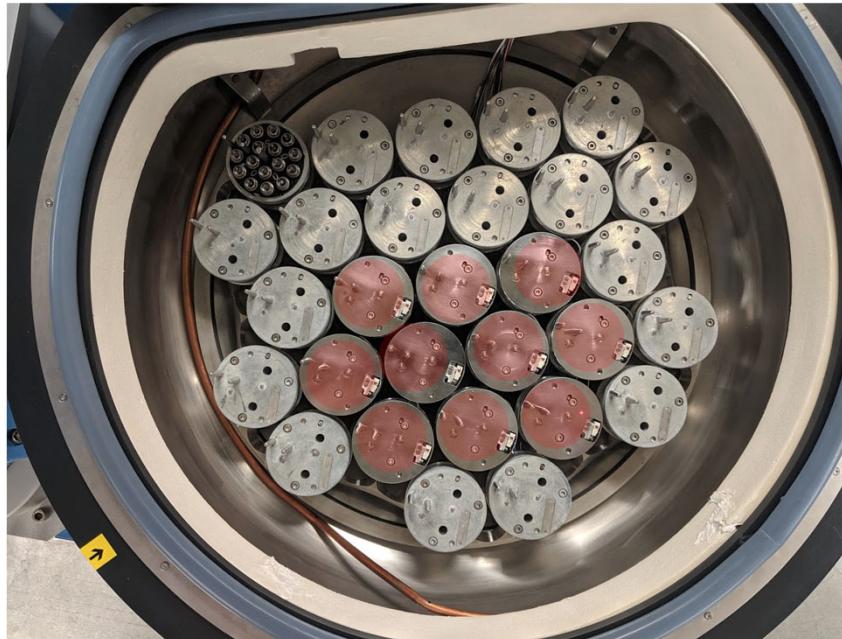
- In-vacuum undulator
- 5 – 25 keV
- 10^{13} ph/s @250mA
- BCU
- Cryojet5, HC-lab and REX
- Eiger16M
- ISARA sample changer
- MD3 Diffractometer
- Amptek fluorescence detector
- Roadrunner



MicroMAX

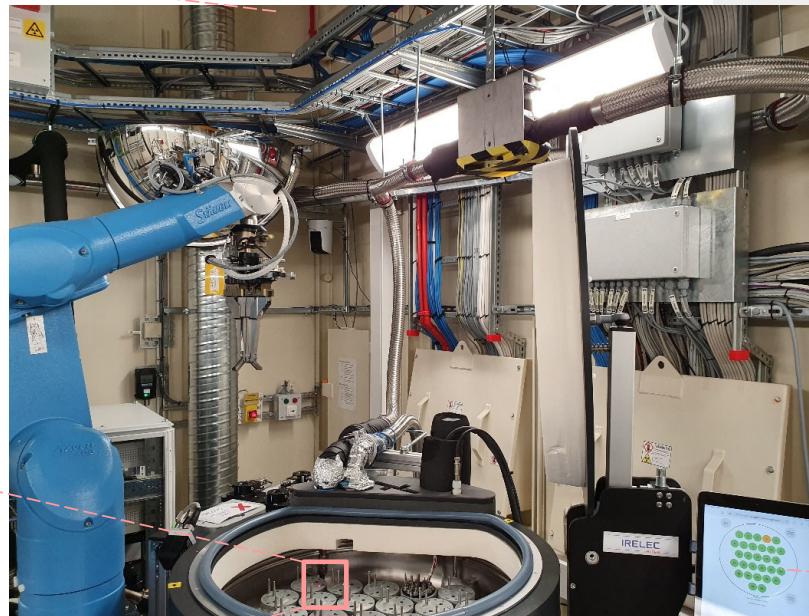
What's new - ISARA upgrade

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



Uni-Puck support only, 29 positions = 464 samples

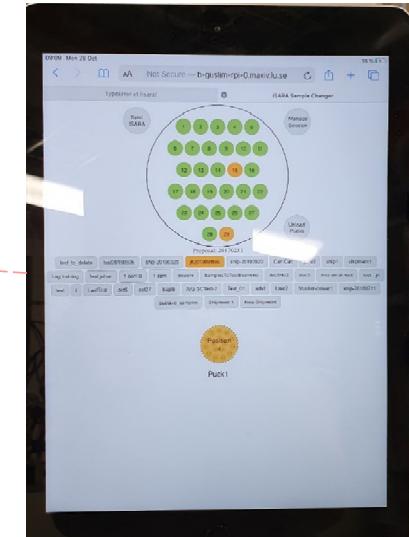
What's new - Puck loading app



The screenshot shows the ISPyB MAX IV software interface. At the top, there is a navigation bar with links like Home, Lab-contacts, Shipment, Sample, Prepare experiment, Data collection, Feedback, References, and Help. A large red 'X' is drawn over the right side of the screen. On the left, there is a sidebar with options: Select Dewars (Last dewars, All dewars), Fill sample changer, View (Selected dewars). The main area is titled 'Prepare your experiment:' with instructions: 1-Select the dewar you want for processing, 2-Fill the sample changer, assign a location, 3-Associate data collections to samples in mxdb. Below this is a button labeled 'Next step: Fill the sample changer'. A note says 'Note that the dewar shipments will be set in "processing" status and will not be editable any more.' A table lists 'Dewars for processing':

Ship name	Creation date	Comp. name	Type	Command	Beamline	# containers	Local	Dewar status	Location	View	Containers Samples	Select for processing
test20190909	26-09-2019	Dewar1			MAXIV01811	26-09-2019	X	2 (16)	processing			
test_to_delete	04-10-2019	test			MAXIV01874	04-10-2019		1 (0)		Dry shipper		
ship-20190925	25-09-2019	Dewar_sharer			MAXIV01801	25-09-2019		1 (0)		al MAXIV		
nc20190909au	24-09-2019				MAXIV01783	24-09-2019		1 (0)		al MAXIV		
ship-20190920	20-09-2019	test			MAXIV01790	20-09-2019		1 (16)		al MAXIV		

Puck positions are automatically registered in ISPyB



What's new - MD3 upgrade

Problems

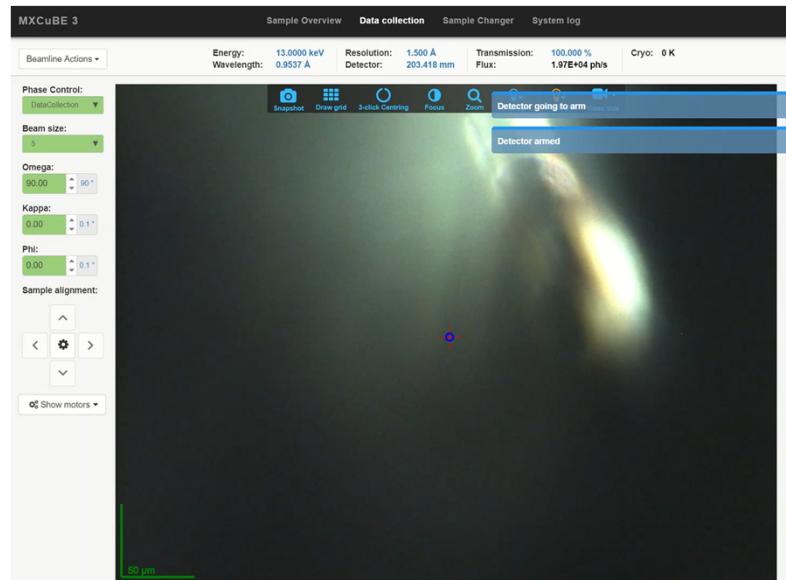
- Raster scan frequently failed due to “insufficient calculation time” error
- overhead **>1s for each turn**
- *Raster, 50x50 cells, 2500 imgs, 10 ms per img
25 s collection + >50 s overhead*

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*

Upgrade

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



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 °

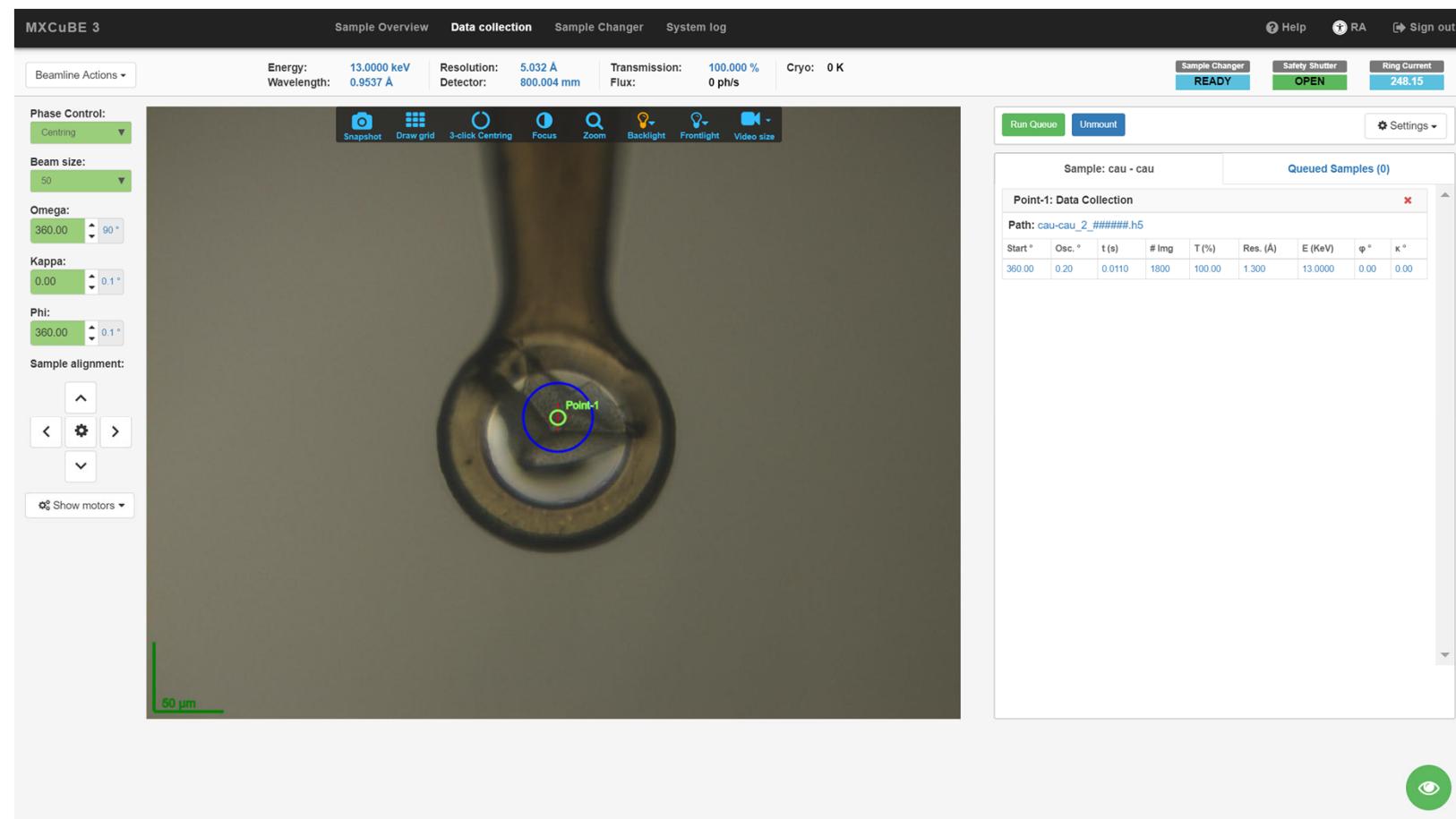
MXCuBE3 at BioMAX - 1

MXCuBE3 in production

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

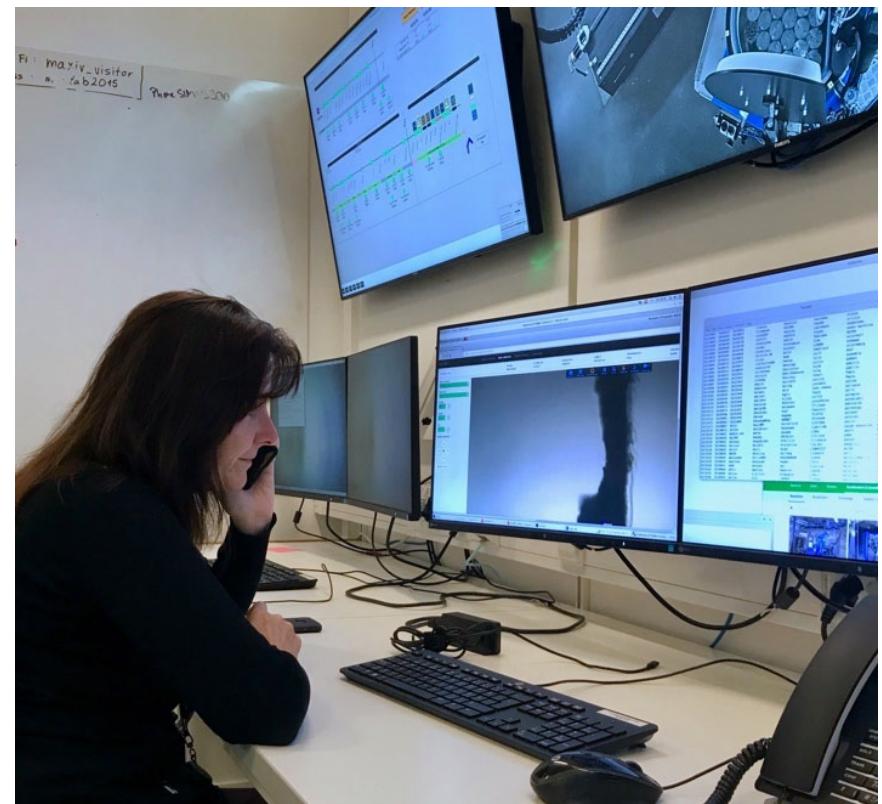
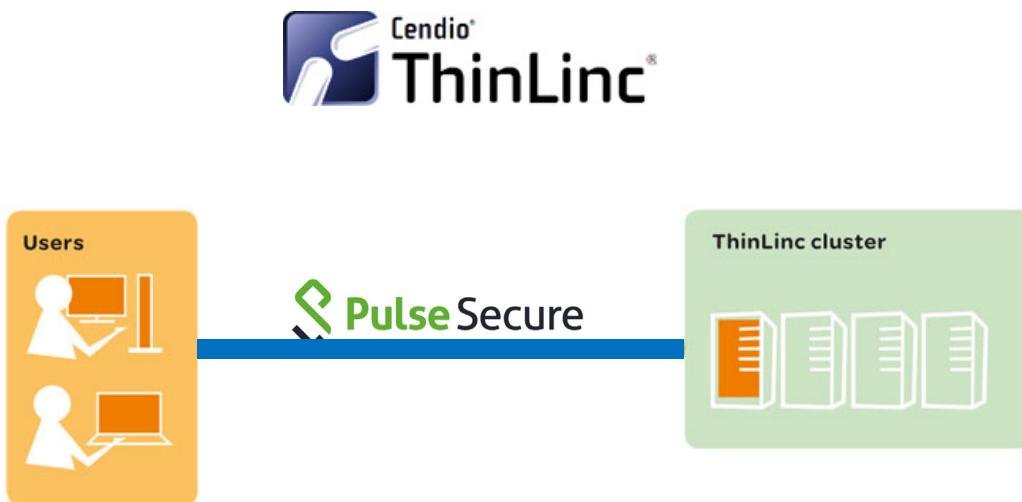
Deployed new features

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



Remote operation

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

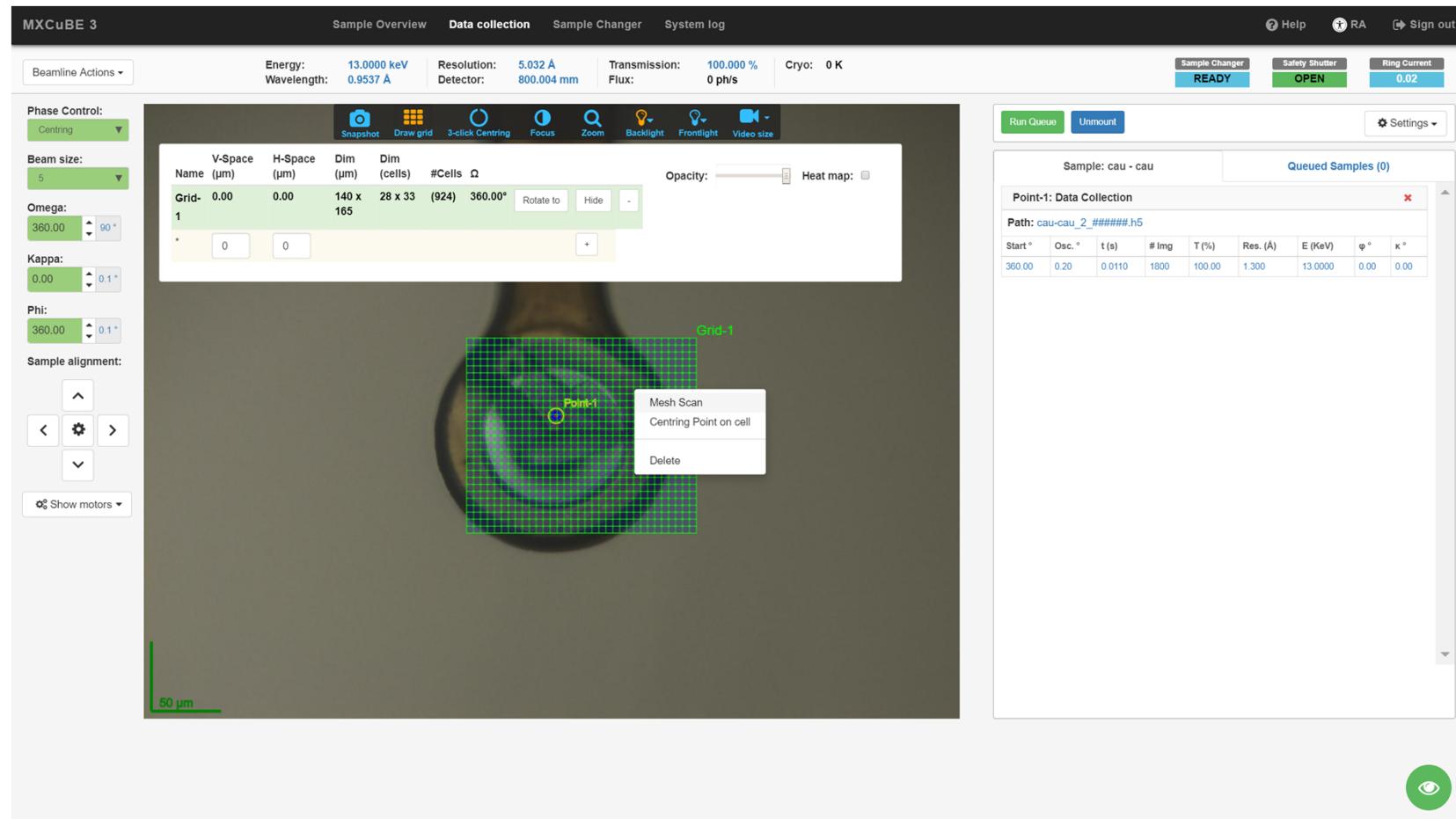


Ana Gonzalez is assisting remote users during data-collections

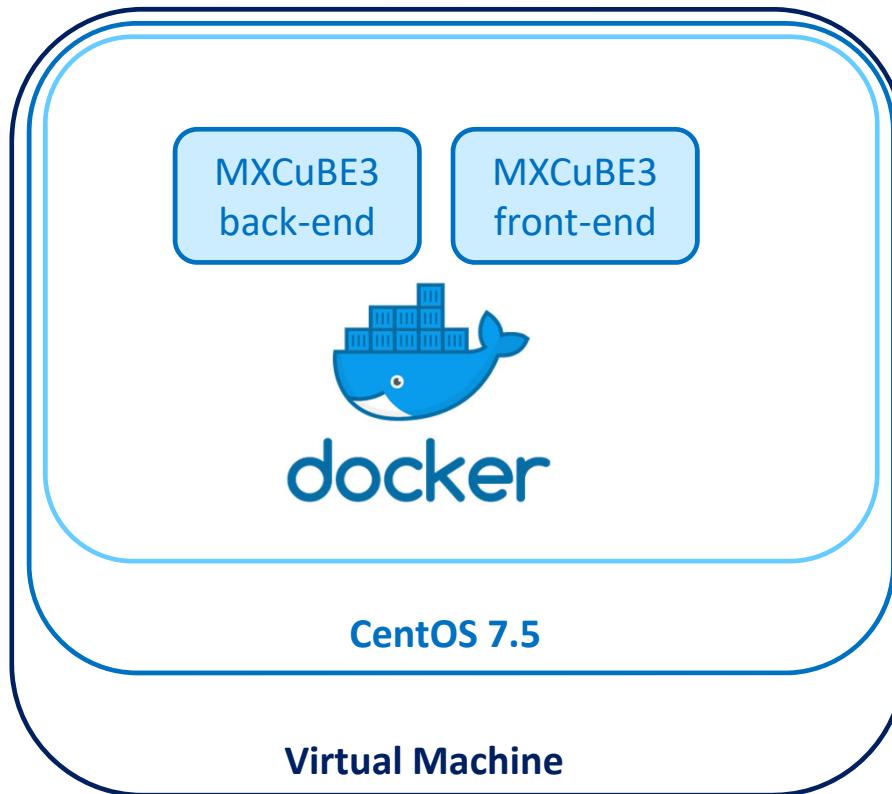
MXCuBE3 at BioMAX - 2

Ongoing

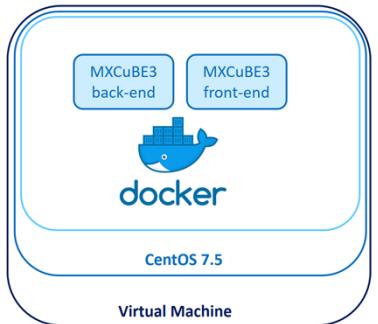
- Raster scan
- Multicast (tested)
- Beamline operation macros, i.e. Beam alignment
- Integration of Amptek to support for XRF, XANES



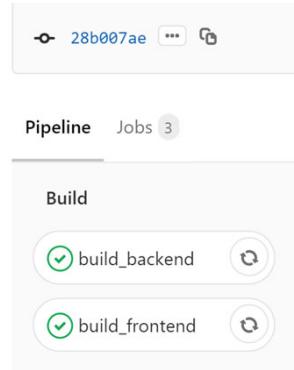
How we run MXCuBE3 Server?



How we update MXCuBE3 Server?



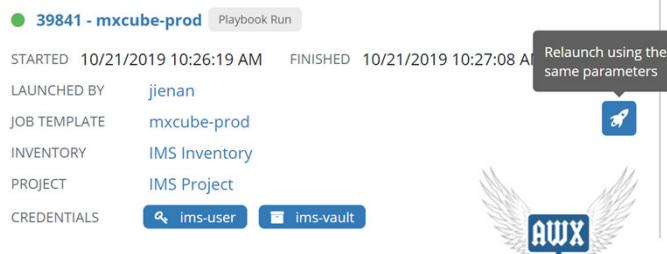
Build docker images



a few
minutes

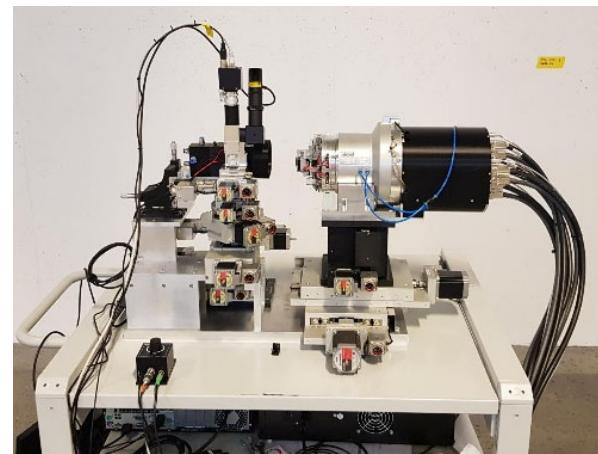


Deployment by Ansible



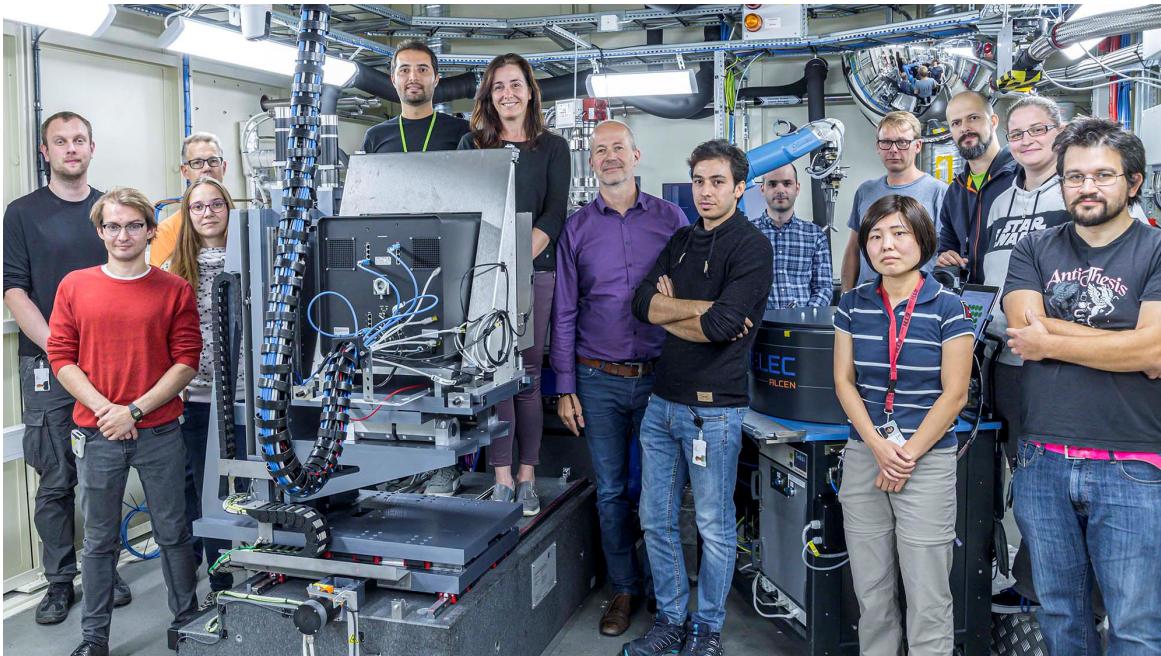
Ongoing and future work

- 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
- Thomas Ursby
- Gustavo Lima
- Ana Gonzalez
- Uwe Mueller
- Vahid Haghigat
- Mikel Eguiraun (KITS)
- Jie Nan
- Johan Unge
- Mirko Milas
- Monika Bjelcic
- Elmir Jagudin

- All BioMAX users
- Many others from MAX IV and MXCuBE/ISPyB collaboration