



MXCuBE at MAX IV

Jie Nan On behalf of MX-group at MAX IV

Mar. 12, 2019

MAXIV

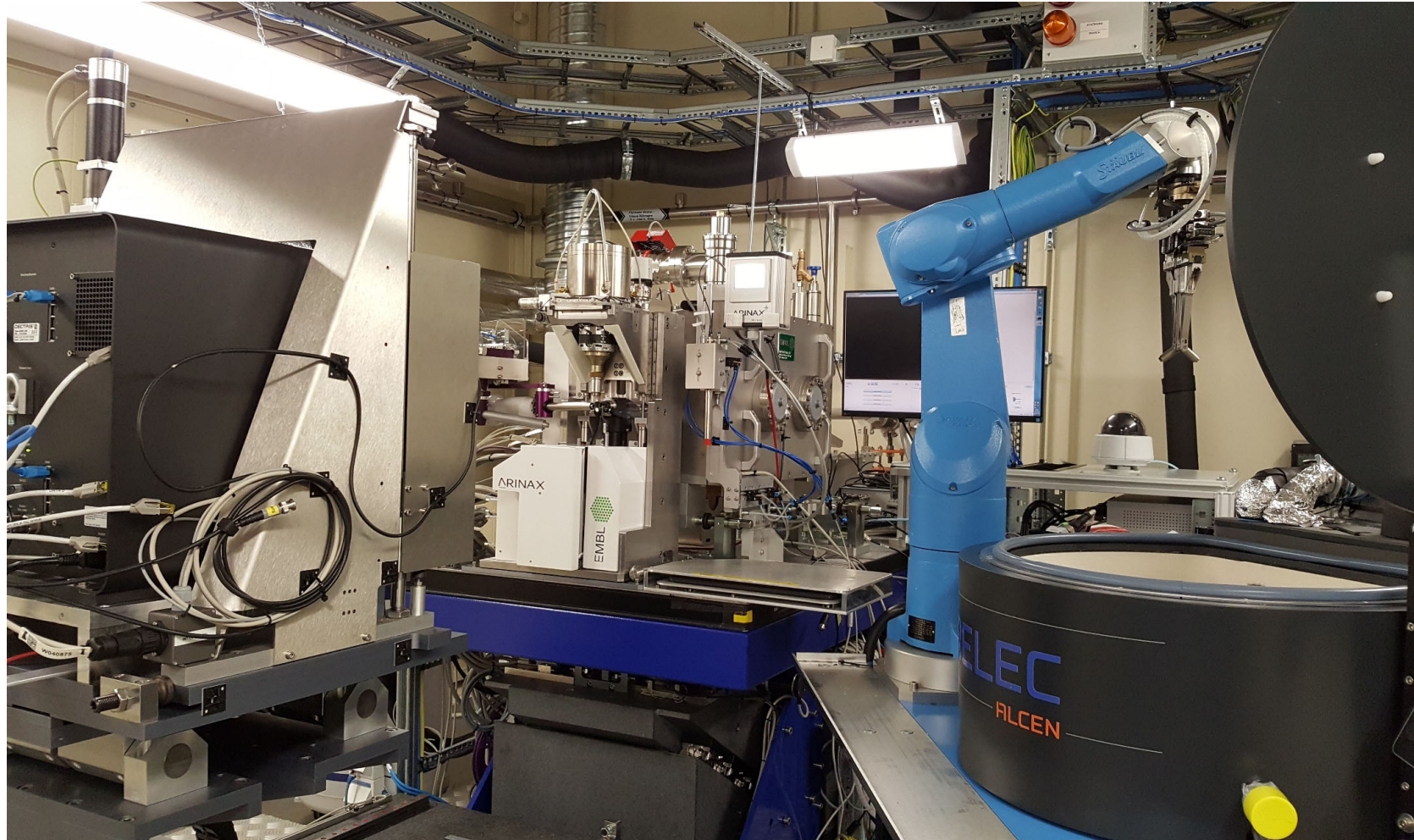
MX Beamlines at MAX IV

BioMAX

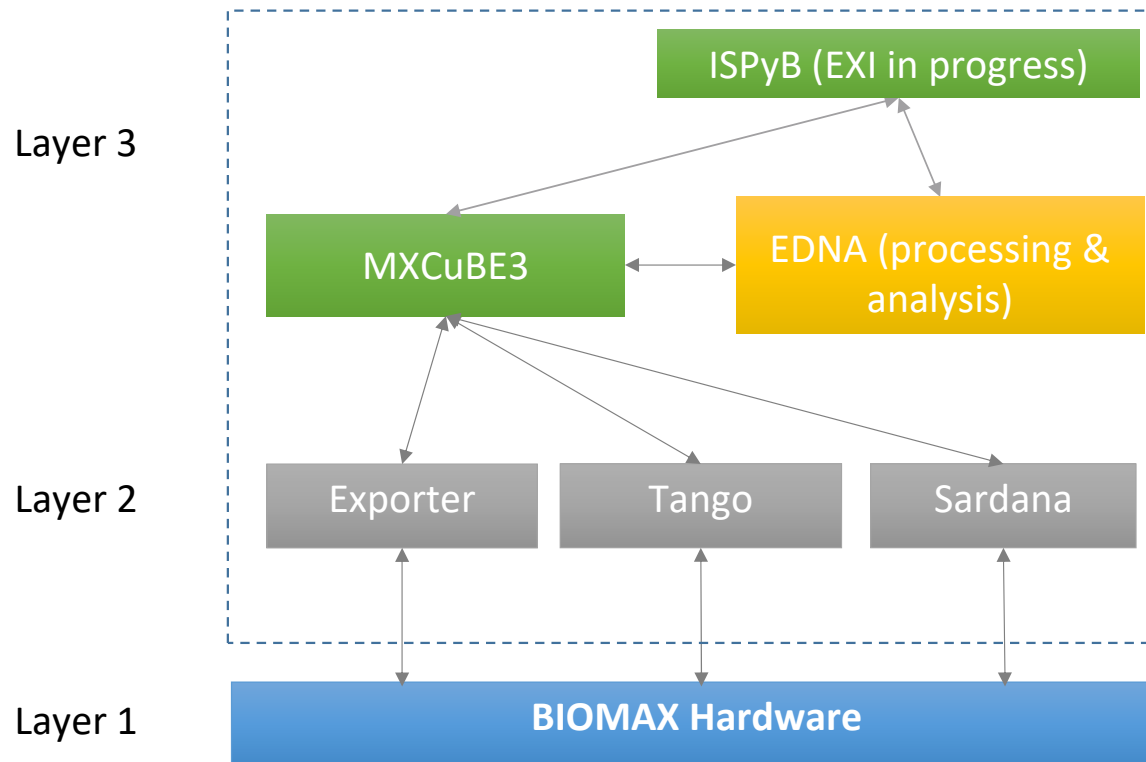
- In-vacuum undulator
- 5 – 25 keV
- 10^{13} ph/s @250mA
- BCU
- MD3 Diffractometer
- Cryojet5, HClab and REX
- Eiger16M
- ISARA sample changer
- Amptek fluorescence detector

MicroMAX

- DDR review last week, successfully passed



BioMAX Software Overview



MXCuBE3 at BioMAX

Production MXCuBE

- MXCuBE3, 3.0.1
- HardwareRepository, 2.2

What's new?

- Sample Changer operation, improved efficiency
- Stability, enhanced exception handling and motor limit check
- New macros of BL operation
- webCam (ongoing)
- SciCat

The screenshot displays the MXCuBE3 control interface. At the top, the browser address bar shows the URL `b-v-biomax-web-0.8081/datacollection`. The interface includes a navigation bar with tabs for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. A status bar at the top right shows 'Sample changer: DISABLED', 'Safety Shutter: OPEN', and 'Ring Current: 246.93'. The main control area features a central video feed of a sample, with a 'Point-1' label and a blue circle indicating the current position. To the left of the video are control panels for 'Phase Control' (Centring), 'Beam size' (50), 'Omega' (1.03), 'Kappa' (0), and 'Phi' (0). Below these are 'Sample alignment' controls and a 'Show motors' option. To the right of the video is a 'Run Queue' section with 'Run Queue' and 'Unmount' buttons, and a 'Settings' dropdown. Below the queue, the sample is identified as 'thau - thau7' and 'Queued Samples (0)'. A table shows the data collection path and parameters:

Start*	Osc.*	t [s]	#img	T [%]	Res. [Å]	E [keV]	ϕ^*	κ^*
360.00	0.10	0.0110	3600	9.92	1.580	13.5000	0.00	0.00

A 'View Results' link is provided below the table. A green 'Run' button is visible at the bottom right of the interface.

Sample changer operation in MXCuBE3

Sample changer (READY)

Contents

Refresh Scan all containers

CATS

Power

PowerOn PowerOff Regulation On

Lid

Open Lid Close Lid

Actions

Home Dry Soak

Recovery

Clear Memory Reset Message

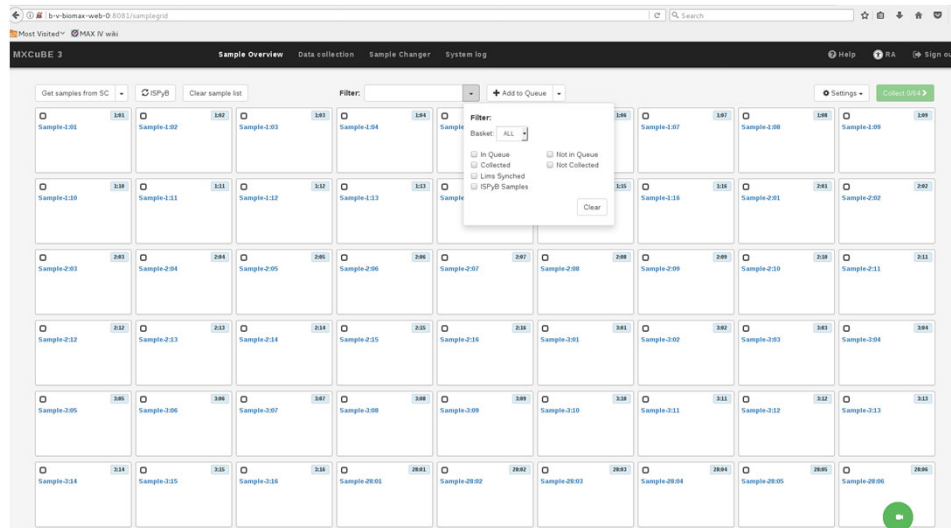
Abort

Abort

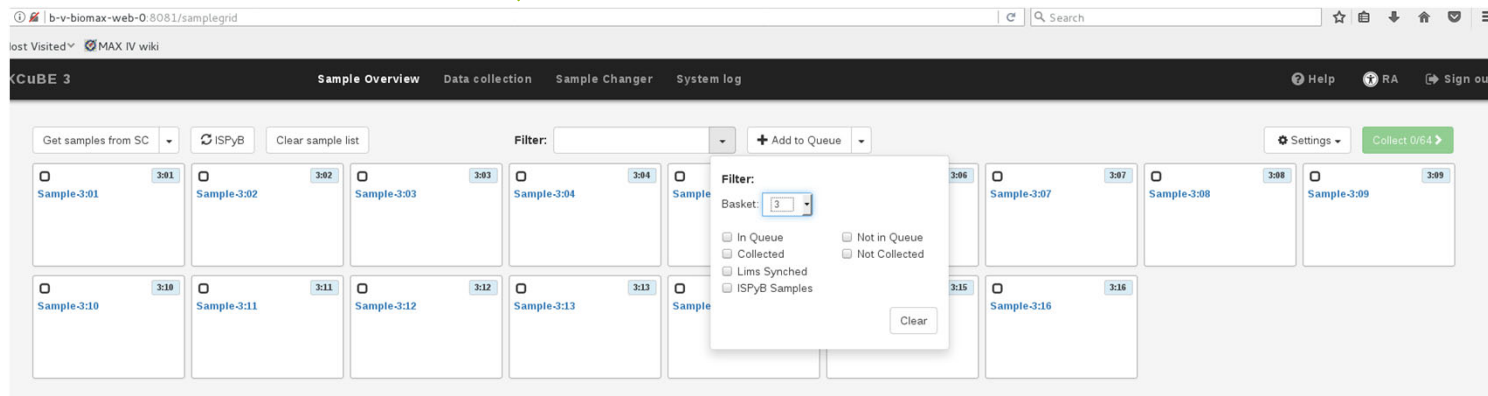
Status message

Mainly used by beamline staff

Sample changer operation in MXCuBE3 from user's perspective



Use filter function to select a group of samples to work with



MXCuBE3 - Sample changer operation from user's perspective

The screenshot displays the MXCuBE3 web interface in the 'Data collection' view. The top navigation bar includes 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. The status bar at the top right shows 'Sample changer: READY', 'Safety Shutter: CLOSED', and 'Ring Current: 263.94'. The main area is divided into a left sidebar with controls for Phase Control, Beam size, Omega, Kappa, Phi, and Sample alignment. The central panel shows a dark image with a yellow line labeled 'Line-1' connecting 'Point-1' and 'Point-2'. A scale bar indicates 50 μm. The right sidebar shows a 'Run Queue' and a list of 'Queued Samples (16)' from 3:01 to 3:15, each with a 'Mount' button.

Stay in the DataCollection view during the measurement of the list of samples

WebCam in MXCuBE3 (ongoing)

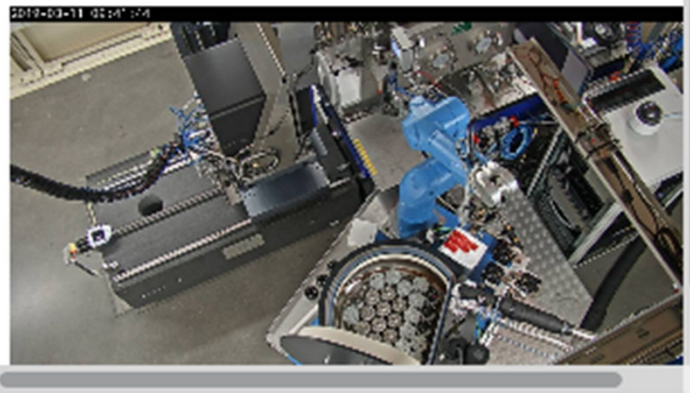
The screenshot shows the MXCuBE3 web interface. The top navigation bar includes 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. The main area displays a log of collection steps, such as 'Collection: Preparing to collect', 'Collection started', and 'Collection: Setting resolution to 1.400'. A table of parameters is visible, including Start, Stop, Time, Flux, Resolution, Energy, and Phi. A small video window in the bottom right corner shows a live feed of the diffractometer, with a red box highlighting a green 'ON' button.

Start	Stop	Time	Flux	Res. (Å)	E (keV)	Phi	Chi
300.00	0.00	0.0110	3000	10.00	1.000	13.5000	0.00

Diffractometer ▼



Experimental Hutch ▼



SciCat at MAX IV

SciCat MAX IV

Datasets / Maxiv/93f8576e-fb7c-4196-8d5b-0a8008f6bc2b /

Details Datafiles Attachments Admin Export to CSV

About the data

- Name:** thau/thau-thau
- Owner:** Ana Gonzalez
- PID:** maxiv/93f8576e-fb7c-4196-8d5b-0a8008f6bc2b
- Source Folder:** /data/visitors/biomax/20170251/20190310/raw/thau/thau-thau

Structural information

- Type:** raw
- Version:** 2.9.1
- Proposal:** 20170251

Administrative information

- Creation Time:** 2019/03/10 20:58
- Principal Investigator:** Ana.Gonzalez@maxiv.lu.se
- Creation Location:** BioMAX
- Owner Group:** 20170251-group
- Contact Email:** Ana.Gonzalez@maxiv.lu.se

Scientific Metadata

```
{
  "comment": "",
  "energy": 13.5,
  "motors": {
    "samps": 0.06393173262720867,
    "sampsy": -0.24534984430645366,
    "phi": 359.9988000000012,
    "zoom": null,
    "focus": -0.2723925781250003,
    "phi2": 0.21008917571176783,
    "phi3": -0.22599446405739166
  },
  "take_snapshots": 1,
  "shape": "p2",
  "in_interleave": false,
  "ybeam": 2130.3018601355157,
  "wavelength": 0.9184002510980636,
  "fileinfo": {
    "run_number": 3,
    "suffix": "h5",
    "filename": "/data/visitors/biomax/20170251/20190310/raw/thau/thau-thau-thau-thau_3_master.h5",
    "num_files": 1,
    "prefix": "thau-thau",
    "template": "thau-thau_3_06d.h5",
    "archive_directory": "/mxn/groups/ispystorage/pyarch/visitors/20170251/20190310/raw/thau/thau-thau/",
    "directory": "/data/visitors/biomax/20170251/20190310/raw/thau/thau-thau/",
    "process_directory": "/data/visitors/biomax/20170251/20190310/process/thau/thau-thau/"
  }
}
```

- SciCat stands for Scientific Catalog
- Hwobj, BIOMAXKafka.py

SciCat MAX IV

Filter Results Clear

Text Search

Location: BioMAX

Group: 20170251-group

Type

Keywords

Select a date range

MAR 2019

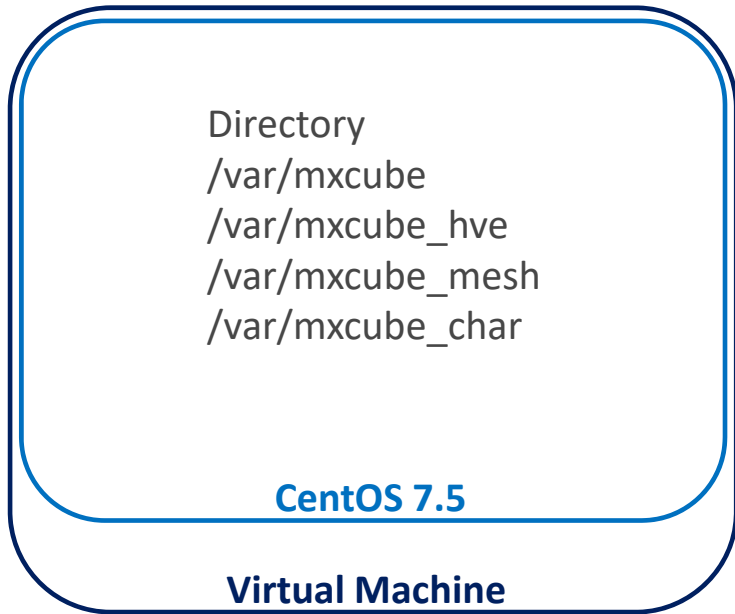
Source Folder	Size	Start Time	Type
/data/visitors/biomax/20170251/20190311/raw/msg/msg-msg	2 GB	2019/03/11 Mon 09:41	raw
/data/visitors/biomax/20170251/20190311/raw/msg/msg-msg	350 MB	2019/03/11 Mon 09:40	raw
/data/visitors/biomax/20170251/20190311/raw/msg/msg-msg	350 MB	2019/03/11 Mon 09:39	raw
/data/visitors/biomax/20170251/20190310/raw/thau/thau-thau	0 B	2019/03/10 Sun 20:58	raw
/data/visitors/biomax/20170251/20190310/raw/thau/thau-thau	2 GB	2019/03/10 Sun 20:56	raw
/data/visitors/biomax/20170251/20190309/delete/delete-delete	865 MB	2019/03/09 Sat 13:31	raw
/data/visitors/biomax/20170251/20190309/delete/delete-delete	1 GB	2019/03/09 Sat 13:30	raw
/data/visitors/biomax/20170251/20190309/delete/delete-delete	353 MB	2019/03/09 Sat 12:03	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	5 GB	2019/03/04 Mon 14:29	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04 Mon 14:28	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04 Mon 14:26	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04 Mon 14:25	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04 Mon 14:24	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04 Mon 14:23	raw
/data/visitors/biomax/20170251/20190304/raw/thau/thau-thau14	7 GB	2019/03/04	raw

Other MXCuBE3 branches

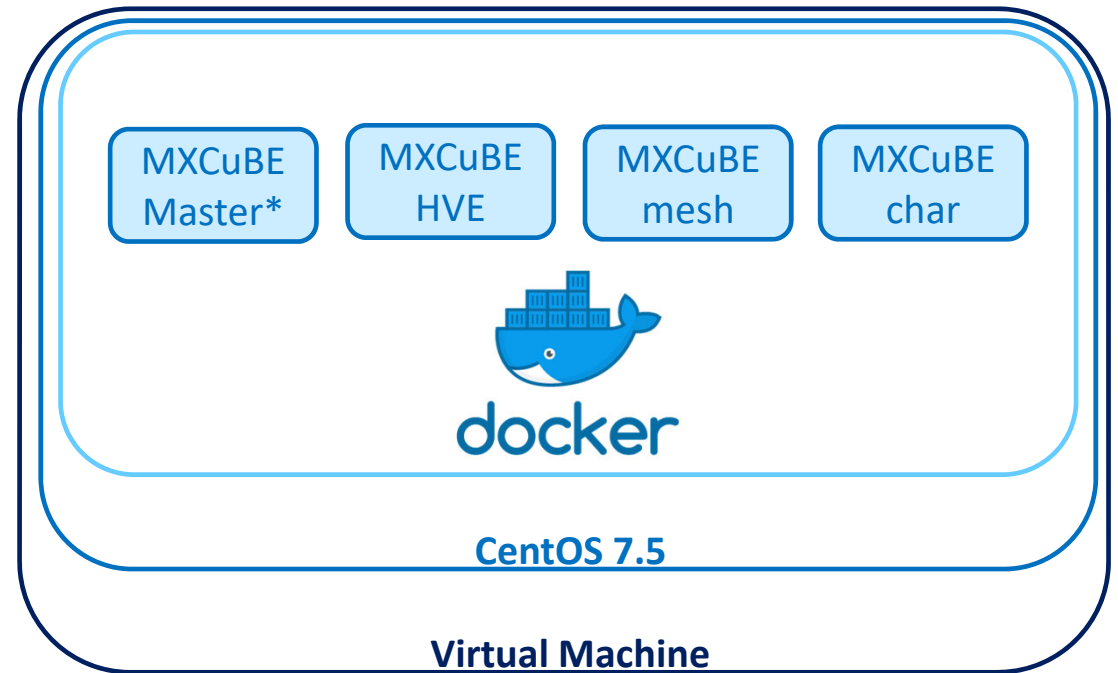
- MXCuBE_HVE
 - High Viscosity Extrusion, SSX
 - One year old, to be synchronized with master
- MXCuBE_mesh
 - X-ray centering & SSX
 - Under development
- MXCuBE_Char
 - Eiger Stream interface + EDNA_characterization
 - Finished, to be merged into master (only hwobj)
- MXCuBE_XRF

Remote Operation
(Ana Gonzalez)

How we run MXCuBE Server?



Now



Coming soon

Easy to start / stop different branches (for staff)




















Container list 
Containers

 Portainer support  biomax-user
[my account](#) [log out](#)

Containers Columns Settings

Start Stop Kill Restart Pause Resume Remove + Add container

Search...

<input type="checkbox"/> Name	State  Filter 	Quick actions	Stack	Image	Created	IP Address	Published Ports	Ownership
<input type="checkbox"/> mxcube	running	   	webmaxivmxcube3docker	docker.maxiv.lu.se/mxcube3	2019-01-04 13:42:43	-	-	 restricted
<input type="checkbox"/> mxcube_mesh	stopped	 	webmaxivmxcube3docker	docker.maxiv.lu.se/mxcube3	2019-01-04 13:30:40	-	-	 restricted
<input type="checkbox"/> mxcube_hve	stopped	 	webmaxivmxcube3docker	docker.maxiv.lu.se/mxcube3	2019-01-04 13:30:24	-	-	 restricted
<input type="checkbox"/> mxcube_char	stopped	 	webmaxivmxcube3docker	docker.maxiv.lu.se/mxcube3	2019-01-04 13:27:55	-	-	 restricted
<input type="checkbox"/> mxcube_frontend	stopped	 	webmaxivmxcube3docker	docker.maxiv.lu.se/mxcube-frontend	2019-01-04 13:23:08	-	-	 restricted

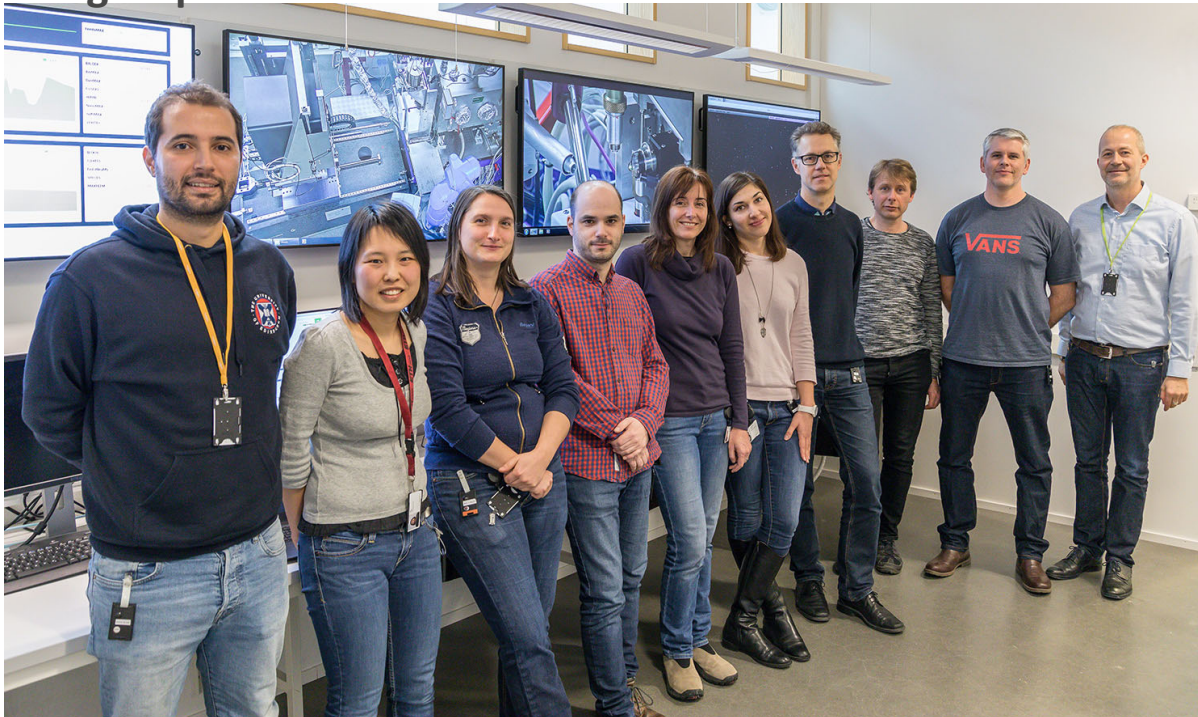
Items per page: 10

Near future work

- Hardware integration
 - Fluorescence detector
 - Roadrunner
- Experiments
 - EDXRF & XANES
 - Mesh scan
 - SSX
- Remote operation

Acknowledgement

MX-group



Many others from MAX IV and MXCuBE collaboration