



Elettra
Sincrotrone
Trieste

MXCuBE / ISPyB Meeting

Berlin, Germany



Update Status MxCuBE3 at beamline XRD2

presented by Roberto Borghes

teams: Roberto Borghes, Milan Prica, Fulvio Billè

XRD2

- Nicola Demitri, Dan Dumitrescu, Babu Manjasetty, Annie Héroux

XRD1

- Maurizio Polentarutti, Giorgio Bais



In Operation since September 2019 (1 year) : Aim stability

Indian 35% - General User 35% **30% in-house/maintenance/Proprietary/Course**
Allocation of time: *all proposals are evaluated monthly,*
sometimes not fast enough, 8h shifts too long

Few new hardware implementation (lid for SC dewar):

Refining our model of operation:

~~ESRF pucks~~ ...

UNIPUCK onlyno more MD2 Capillary collision

New Capillary ...

more reliable to mount/unmount

Smartmagnet ...

new card with different with different magnetic field

Optimize beam ...

Move beam to center of camera

- No more moving the aperture/capillary
- Instead mono 2nd xtal roll/ mirror pitch

Problems ... Zoom (open loop), scintillator burn, conf files reset to non-working files

Computing environment

- Data collection simplify, kappa ... smartmagnet issues
- Data analysis barebone distl



March 2019

- Login :

- Rest authentication through ELETTRA VUO
- Logout **restart server every time**

- Data Collection Tab:

- Beamline Actions
 - Changing md2 phases
 - Robot actions
- Diffractometer (MD2):
 - *Lights (Tango)*
 - *Zoom (Tango)*
 - *Camera: MD2 JPG (Tango)*
 - *3 Click centring: MD2 command (Tango)*
 - *Automatic centring*

- Sample Changer Tab:

- XRD2 csv temporary solution -ISPyB

- Sample Overview Tab:

- Data Collection—Characterisation added
- MCA scans

October 2019

- Login :

- Rest authentication through ELETTRA VUO
- ISPyB
 - Connection with VUO, proposals, people
 - *Populating the table with persons on sessions for logins*
- Logout **restart server every time**

- Data Collection Tab:

- Beamline Actions
 - **Optimize beam, intensity,vert/horizontal positions, shape**
- Diffractometer (MD2):
 - Changing md2 phases moved to main menu
 - Automatic centring loop centering
 - Camera streaming
 - Better status of pin mounted/unmounted

- Sample Changer Tab:

- Fully integrated via SynchWeb-ISPyB
- Robot actions moves to SC

- Sample Overview Tab:

- MCA scans



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Since last meeting

Resolving issues other than MXCuBE

Data acquisition computer died (twice).... Two machines (dev machine)

Migrating to a new machine, different OS (Ubuntu 18.04), affecting everything not just MXCuBE

Mounting/unmounting undesired behavior ... pin over pin crash

When unmounting xtals sometimes we would have one pin umounted on an other.
Invested time at getting better status of the pin for different scenarios of failure to behave.

Add new standalone GUI for MCA

UnResolved issues

Overwriting the files! We have a database, we know what run each «name» has !?!

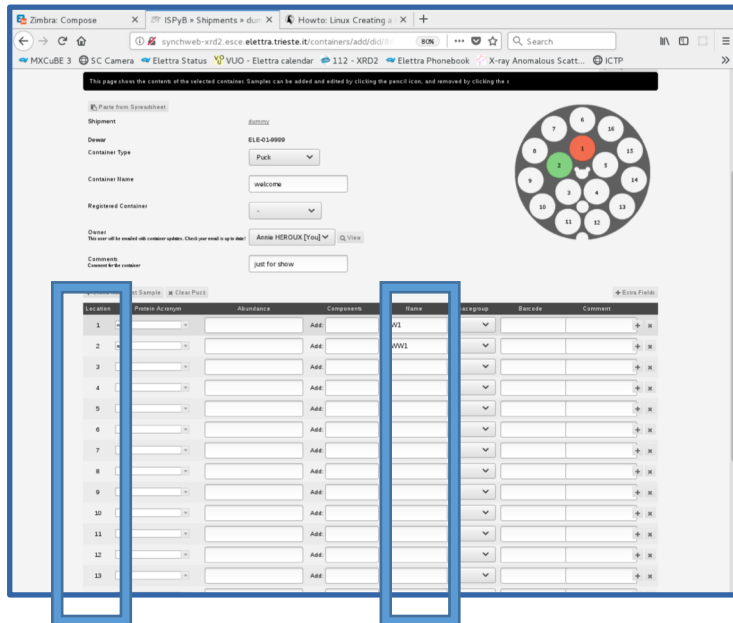
Login out



Main focus since last meeting

Integration of the database – MXCuBE

ISPyB (DLS version and SynchWeb)



MISSION 1

CONTAINERS MANAGEMENT

We were using CSV files. Despite having instructions and a template on the website, we had to modify it *every* time.

Addressing issues such as

1- having to re-fill them at every start of MXCuBE

Funky characters in name (space , %...)

Bad habits (meta data in name date, time, hopes...)

Same name (overwriting data)

Trays– freeze onsite

2- Users from India might or might not be synchronized with their dewars (Customs issues or Visa issues). The person having to deal with the data collections could be staff or a different user from India.



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Main focus during the last 6 months

Once the containers are done... why stop there?

- Login, Session
- In-house projects
- (unclear how mxcube in-house flag works)
- Harvesting the data collection parameters
- Displaying the snapshots of xtal and the diffraction pattern.
- Distl plot

The screenshot shows the ELETTRA web interface. The browser address bar is `synchweb.elettra.eu`. The page title is "Data Collections - mx20199008". The navigation bar includes "Home", "Calendar", "Logout", "Elettra Sincrotrone Trieste", "Stats", and "Fault Reports". The main content area is titled "Data Collections" and features a search bar and a list of tabs: "Data Collections", "Grid Scans", "Full Collections", "Auto Integrated", "Screenings", "Edge Scans", "MCA Spectra", "Robot Actions", "Sample Actions", and "Favourites". The "Data Collections" tab is active, showing a list of data collections. The selected collection is for sample "Arak1" on 22-10-2019 at 16:44:52. The details for this collection are:

Sample: Arak1	Flux: NaN
Ω Start: 345.2°	Ω Osc: 1.50°
Ω Overlap: 0°	No. Images: 3
Resolution: 1.76Å	Wavelength: 0.7001Å
Exposure: 1.500s	Transmission: 100.00%
Beamsize: 0x0µm	Type: Data Collection
Comment:	

Below the details are two images: a snapshot of the x-ray crystal (xtal) and a diffraction pattern. To the right of the diffraction pattern is a "Distl plot" showing a grid of data points. The plot has a legend with "Spots" (yellow), "Bragg" (blue), and "Res" (red). The x-axis ranges from 0 to 3, and the y-axis ranges from -1.0 to 1.0.



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Present focus : REMOTE tools and consolidating present user interfaces

VUO

- users need to register and added to proposal/investigations
- Dewar management
- Download data

MXCuBE3 Web version

Not ready but we have pressure to do a show and tell this month

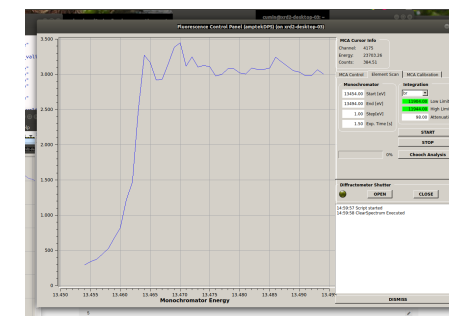
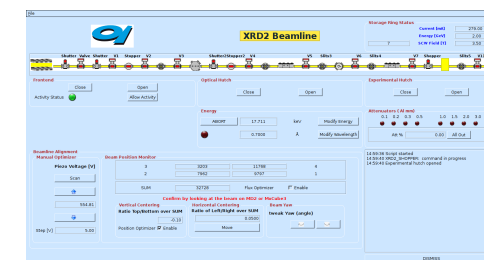
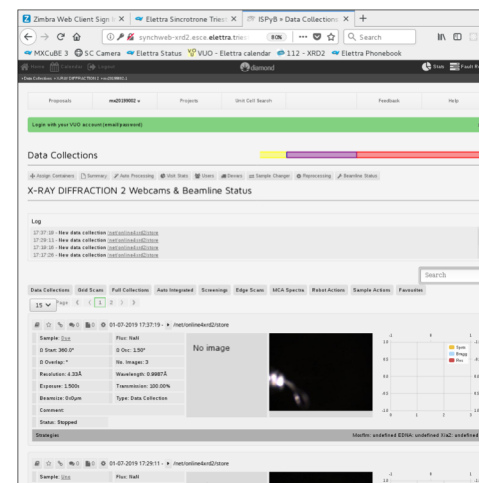
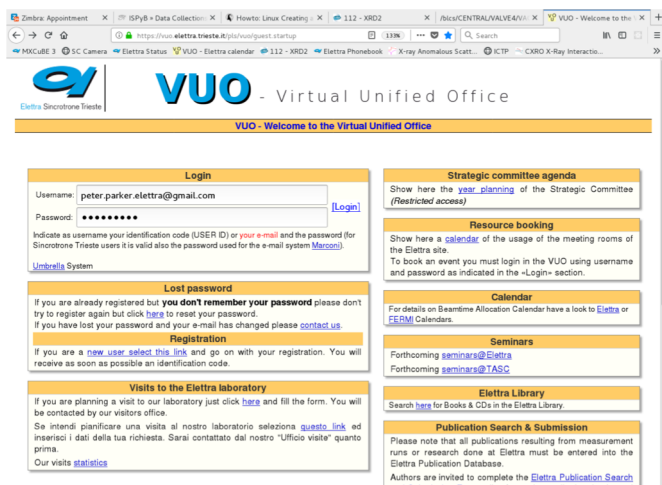
BRAGGY ???

Synchweb/ ISPyB

in place accessible to the world

Other UI

Beamline alignment
MCA





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Status Now and QUESTIONS **FRESH** from 2 days ago

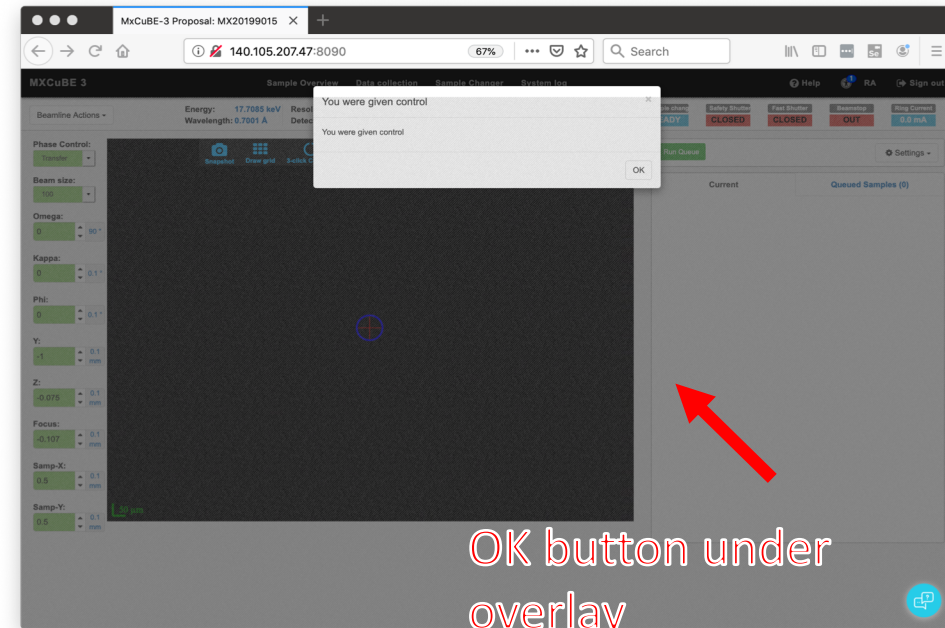
- Temporary solution in place to access the port on that daq machine
- Login same on master and observer,
- We can give control but can get it back. To regain control locally, kill server, overlay on top of buttons
- Observer can't log out, but re-login ok
- **How can the local staff monitor what is going ON?**
- Using Safari works *LESS*
- Braggy has a link in MXCuBE? How to authenticate?

Aiming for future

- Move to server on DMZ
- Individual Login , we know who should have access
- Control switch
- **We need to know what is going on**
- We need to add some beamline optimization
- We need to have a view of robot camera
- We need to see diffraction
- Add some pipeline for data analysis

Feedback

- Users in India very pleased
- Beamlines scientists terrified



OK button under
overlay



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