



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



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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):

~~ESRF pucks~~ ...

New Capillary ...

Smartmagnet ...

Optimize beam ...

- 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
- Data analysis

simplify, kappa ... smartmagnet issues  
barebone distl

Refining our model of operation:

UNIPUCK only ....no more MD2 Capillary collision

more reliable to mount/unmount

new card with different with different magnetic field

Move beam to center of camera



## March 2019

- Login :

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

- Data Collection Tab:

- Beamline Actions
  - Changing md2 phases
  - Robot actions
- Diffractomer (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
- Diffractomer (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



## 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**

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

**Login out**



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### 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*.

The screenshot shows a web-based interface for managing sample containers. At the top, there's a header bar with various links. Below it is a form for creating a new shipment, including fields for Dewar, Container Type (set to Puck), Container Name (welcome), and Registered Container. A message about email notifications is present. On the right, there's a circular icon representing a container with numbered slots (1-16). Below the form is a table with columns: Location, Protein Acronym, Abundance, Component, Name, Subgroup, Barcode, and Comment. The first row has a value 'WW1' in the Name column. The entire interface is framed by a blue border.

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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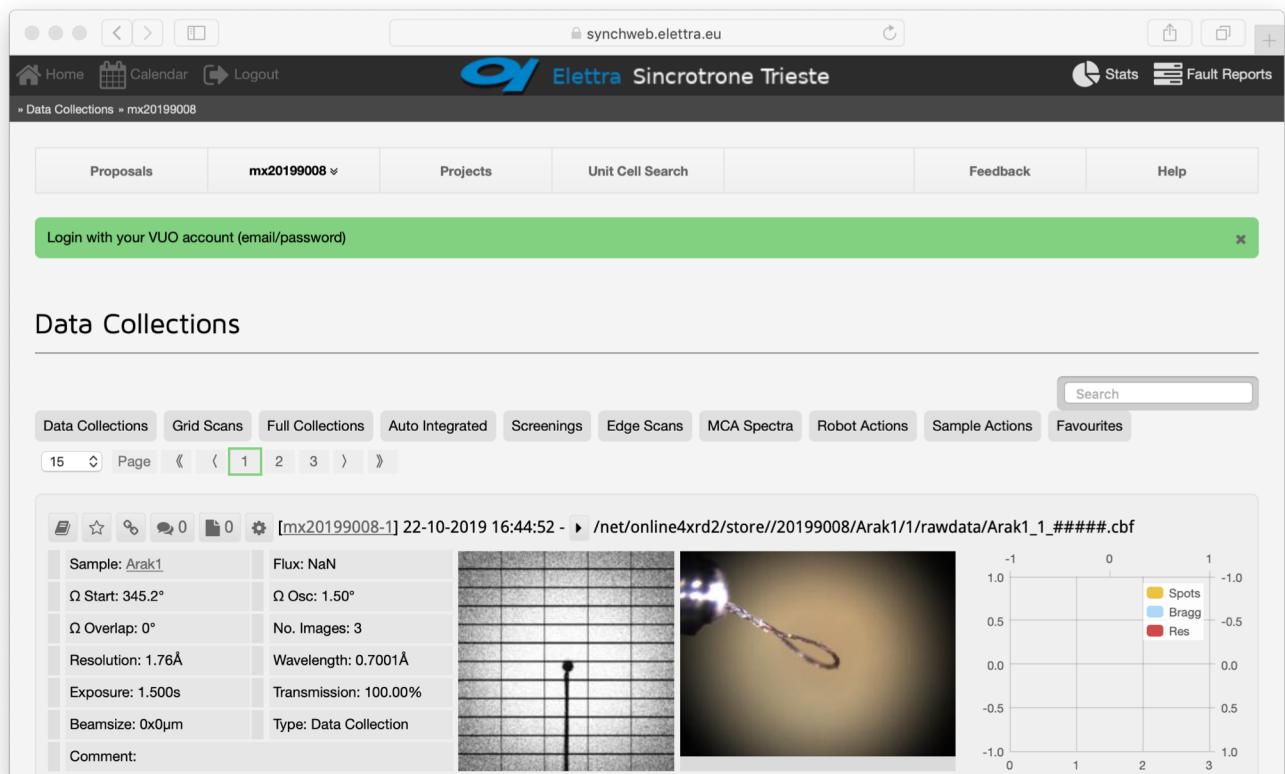
Berlin, Germany



### 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



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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

**VUO - Virtual Unified Office**

**Login**  
Username: peter.parker.elettra@gmail.com  
Password: \*\*\*\*\*  
Indicate as username your identification code (USER ID) or your e-mail and the password (for Sincrotrone Trieste users it is valid also the password used for the e-mail system **Macron**).  
**Umbrella System**  
If you are already registered but you don't remember your password please don't try to register again but click [here](#) to reset your password.  
If you have lost your password and your e-mail has changed please [contact us](#).  
**Registration**  
If you are a [new User](#) select [this link](#) and go on with your registration. You will receive as soon as possible an identification code.  
**Visits to the Elettra laboratory**  
If you are planning a visit to our laboratory just click [here](#) and fill the form. You will be contacted by our visitors office.  
Se intendi pianificare una visita al nostro laboratorio seleziona [questo link](#) ed inserisci i dati della tua richiesta. Sarai contattato dal nostro "Ufficio visita" quanto prima.  
Our visits [statistics](#)

**Strategic committee agenda**  
Show here the [year planning](#) of the Strategic Committee (Restricted access)

**Resource booking**  
Show here a [calendar](#) of the usage of the meeting rooms of the Elettra site. To book an event you must login in the VUO using username and password as indicated in the <Login> section.

**Calendar**  
For details on Beamline Allocation Calendar have a look to [Elettra](#) or [Fermi](#) Calendars.

**Seminars**  
Forthcoming [seminars@Elettra](#)  
Forthcoming [seminars@TASC](#)

**Elettra Library**  
Search [here](#) for Books & CDs in the Elettra Library.

**Publication Search & Submission**  
Please note that all publications resulting from measurement runs or research done at Elettra must be entered into the Elettra Publication Database.  
Authors are invited to complete the [Elettra Publication Search](#)

### MXCuBE3 Web version

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

**MXCuBE 3**

annie.heroux@elettra.eu

Sign in

### Synchweb/ ISPyB

in place accessible to the world

**Data Collections**

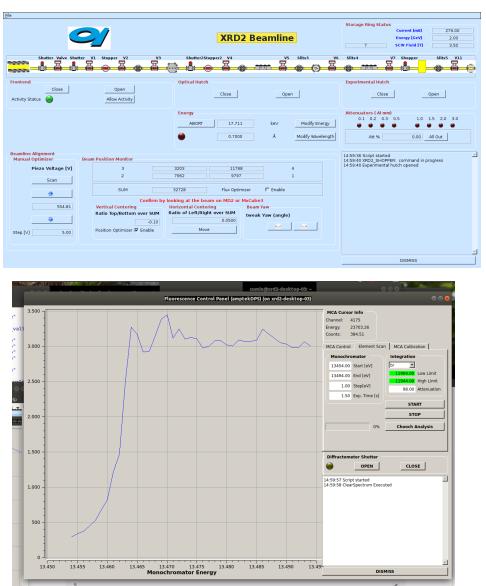
Log	Sample	Beamline	Comments
17/07/19 - New data collection	Instrumentation	MX	
17/07/19 - New data collection	Instrumentation	MX	
17/07/19 - New data collection	Instrumentation	MX	
17/07/19 - New data collection	Instrumentation	MX	

**Sample Actions**

Action	Sample	Beamline	Comments
Scan	MX	MX	
Auto	MX	MX	
Screening	MX	MX	
Edge Scan	MX	MX	
MCA Spectra	MX	MX	
PakActions	MX	MX	
Sample Actions	MX	MX	
File Actions	MX	MX	

### Other UI

Beamline alignment  
MCA





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

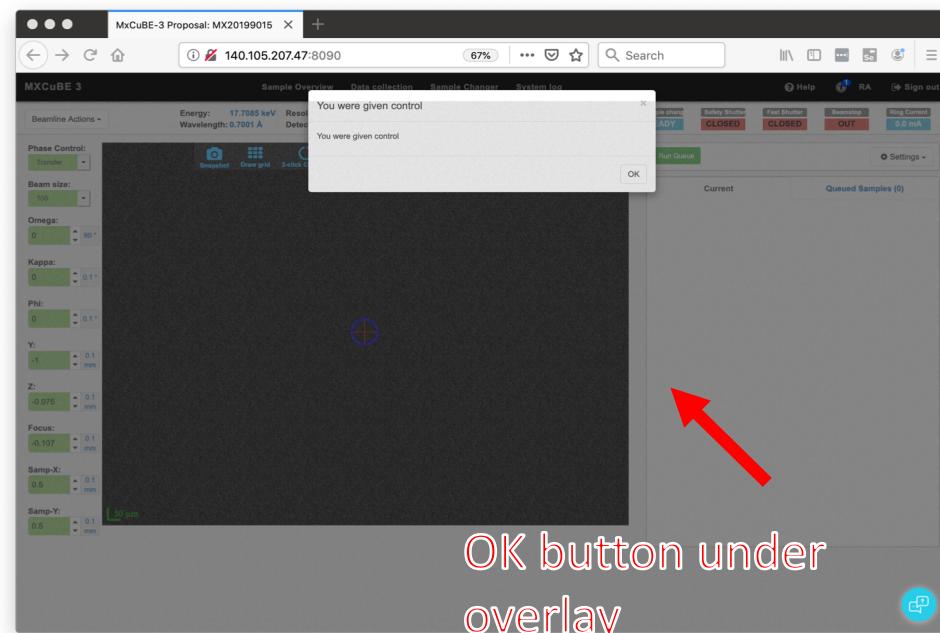
- Temporary solution in place to access the port on that daq machine
- Login same on master and observer,
- We can give control but can get it back. To regain control locally, kill server, overlay on top of buttons
- Observer can't log out, but re-login ok
- **How can the local staff monitor what is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





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