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MXCuBE / ISPyB Meeting

Berlin, Germany



# Update Status ISPyB/SynchWeb at beamline XRD2

presented by Annie Héroux

**Roberto Borghes, Milan Prica, Fulvio Billè**

XRD2

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

XRD1

- Maurizio Polentarutti, Giorgio Bais



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## Why SynchWeb?

Installation Sept 2018:

Neil, James and Karl, Milan and Roberto  
Apache server  
ISPyB DLS version with SynchWeb

Login SynchWeb March 2019:

Rest authentication through ELETTRA VUO  
Sandboxes, explore the tables and SynchWeb

VUO-ISPyB

Modify synch scripts, adapt to our needs

Integrate MXCuBE July 2019

login , sessions  
scan sc

Expose Synchweb Elettra to the world

Add...

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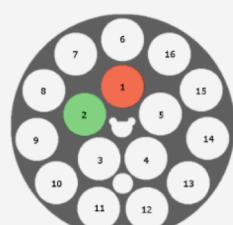
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This page shows the contents of the selected container. Samples can be added and edited by clicking the pencil icon, and removed by clicking the x

Shipment	dummy
Dewar	ELE-01-9999
Container Type	Puck
Container Name	welcome
Registered Container	-
Owner	Annie HEROUX [You] <input type="button" value="View"/>
Comments	Comment for the container:
just for show	



+ Clone from Last Sample

Location	Protein Acronym	Abundance	Components	Name	Spacegroup	Barcode	Comment	+ Extra Fields
1			Add:	W1				<input type="button" value="x"/>
2			Add:	WW1				<input type="button" value="x"/>
3			Add:					<input type="button" value="x"/>
4			Add:					<input type="button" value="x"/>
5			Add:					<input type="button" value="x"/>
6			Add:					<input type="button" value="x"/>
7			Add:					<input type="button" value="x"/>
8			Add:					<input type="button" value="x"/>
9			Add:					<input type="button" value="x"/>
10			Add:					<input type="button" value="x"/>
11			Add:					<input type="button" value="x"/>
12			Add:					<input type="button" value="x"/>
13			Add:					<input type="button" value="x"/>

# 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**
    - 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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synchweb.elettra.eu

Logout Elettra Sincrotrone Trieste

Login with your VUO account (email/password)

### Login

Username (email) peter.parker.elettra@gmail.com

Password (VUO) \*\*\*\*\*

Login

SynchWeb? What is This?

Proposals

This page lists all proposals available to you. Click on a row to select that proposal

Code	Number	Visits	Title
mx	20195568	1	test for ILO
mx	20199016	1	In-house Proposal
mx	20199015	1	In-house Proposal
mx	20195566	1	MF 20191017
mx	20195565	1	for DAn
mx	20195107	1	Structural and biochemical studies on the sanitation enzyme MutT1 from Mycobacterium smegmatis
mx	20195213	1	Bacterial proteins
mx	20190641	0	Structural and functional analysis of M. tuberculosis EccC+CFP10/ESAT6 complex from ESX-1 virulence factor secretion system
mx	20195561	3	Chemical crystallography on MOFs
mx	20195029	0	Structure and Function Studies of peptidoglycan recognition proteins from innate immune system
mx	20195026	0	Analysis of the crystals of a new potential hybrid antitumor agent complexed with human telomeric DNA

### Login SynchWeb:

- Rest authentication through Elettra VUO
- Details like changing logo, patterns for the fields (email address for login, hard coded DLS)
- Modifying the admin group for a full view of everything

Unclear what my superpowers are  
Peter.parker was needed

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### ISPyB → populate tables

Ispyb-propagation-master scripts to help us populate some tables from data in VUO

Brute force cron job, to query VUO, also python script for staff to trigger on-demand

Just one young beamline, not too much

- *Proposal*      —*investigation*—
- *Person*

*Role since we can't have more than one role- remove staff, beamline contact*

- *Blsession*

*Scheduling is not as flexible as we need.*

*One way street with VUO, I can modify start/end of session*

*Create in-house proposal*

- *Session\_has\_person* (*mxcube login, download of data*)

*At least everyone on the proposal,*

*Request access when users arrive, but what about remote?*



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### MISSION 1

### CONTAINERS MANAGEMENT

Flow difficult to figure out from the layout

**shipment → lab contact → dewar → container**

```
Select table_name, update_time from information_schema.tables order by update_time ;
```

#### SHIPMENT

Indian community are sending dewars here but most users bring their dewar and/or TRAYS

Even when they ship it here, Elettra deals with this via VUO  
solution create a dummy one

#### LAB CONTACT

solution create a dummy labid , add PI off proposal, proposal\_has\_person

#### DEWAR

solution create a dummy, again we have trays popping up

#### CONTAINER

solution create a dummy protein MP



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The screenshot shows the MXCuBE software interface for managing sample containers. On the left, there's a form for creating a new container:

- Owner: dummy
- Dewar: ELE-01-0999
- Container Type: Puck
- Container Name: welcome
- Registered Container: -
- Comments: Comment for the container: just for show

Below the form is a circular diagram representing a 16-well plate, with wells numbered 1 through 16. Wells 1 and 2 are highlighted: well 1 is orange (representing a funky character in the name), and well 2 is green.

At the bottom is a table for adding samples to the container:

Location	Protein Acronym	Abundance	Components	Name	Spacegroup	Barcode	Comment
1	mp		Add:	W1			
2	sabb		Add:	WW1			
3			Add:				
4			Add:				
5			Add:				
6			Add:				
7			Add:				
8			Add:				
9			Add:				
10			Add:				
11			Add:				
12			Add:				
13			Add:				

## MISSION 1

## CONTAINERS

Addressing issues such as  
having to fill them at every start of MXCuBE  
funky characters in name (orange)

when we first create the container, space are allowed  
in the name, the color changes to orange but at the  
end the container is saved, and MXCuBE doesn't care  
until you collect! Still progress.

If you edit, the behavior is different, the field are blank  
bad habits (meta data in name date, time, hopes)  
same name (**sampleid**) **OVERWRITING FRAMES**



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Help

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mx20199002 ▾

[View All Data](#)

Visits

Calendar

**Assign Containers**

Shipments

Registered Dewars

Registered Containers

Containers

Samples

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### MISSION 1

### ASSIGN CONTAINERS & use in MXCuBE

Assign / Unassign same container in both state problem with the name of beamline "X-RAY DIFFRACTION 2" XRD2

In MXCuBE when we scan containers, problem with unassigned assigned to position 0 in sc dewar

**ASSIGN CONTAINERS** two ways to reach this place and two behaviors

So far no cross check in sc dewar so no problem

The screenshot shows a web-based interface for managing beamline data. At the top, there's a navigation bar with links for 'Proposals', 'mx20199008 ▾', 'Projects', 'Unit Cell Search', 'Feedback', and 'Help'. Below this is a green login bar prompting 'Login with your VUO account (email/password)'. The main content area is titled 'Data Collections'. In the top right of this area, there's a horizontal bar with several colored segments: purple, red, blue, and grey. Below this bar is a menu with buttons for 'Assign Containers', 'Summary', 'Auto Processing', 'Visit Stats', 'Users', 'Dewars', 'Sample Changer', 'Reprocessing', and 'Beamline Status'. A red circle highlights the 'Assign Containers' button. Further down, there's a section titled 'XRD2 Webcams & Beamline Status' and a 'Log' section containing two entries: '16:44:52 - New data collection /net/online4xrd2/store//20199008/Arak1/1/rawdata/Arak1\_1\_#####.cbf' and '11:43:05 - New data collection /net/online4xrd2/store//20199008/oct11/2/rawdata/ref-oct11\_0\_2\_#####.cbf'. On the far right edge of the interface, there's a vertical scroll bar labeled 'Sample Changer'.

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MISSION 1

**UNASSIGN CONTAINERS & use in MXCuBE**

Login with your VUO account (email/password)

Container Allocation for mx20199008-1 on XRD2 at 19:27 07-10-2019

Assigned Containers: Sample Changer

1	2	3	4	5
6	7	8	9 Unipuck1	10
11	12			

Unassigned Containers

+ Add New Container

5 Page 《 < 1 > 》

How to remove from the view all the old containers?  
create a dumpster (poubelle) dewar and move the  
containers there

Still having some issues with assigning to the right  
visit. I need to create a dummy shipment for each  
visit .



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### MISSION 1

### ASSIGN CONTAINERS ..... and manual mount

#### MXCuBE CREATE SAMPLE

We use this frequently while troubleshooting something, just a loop on and bypass mounting with SC.

We also have, small molecules collected and local staff coming with very few crystals .

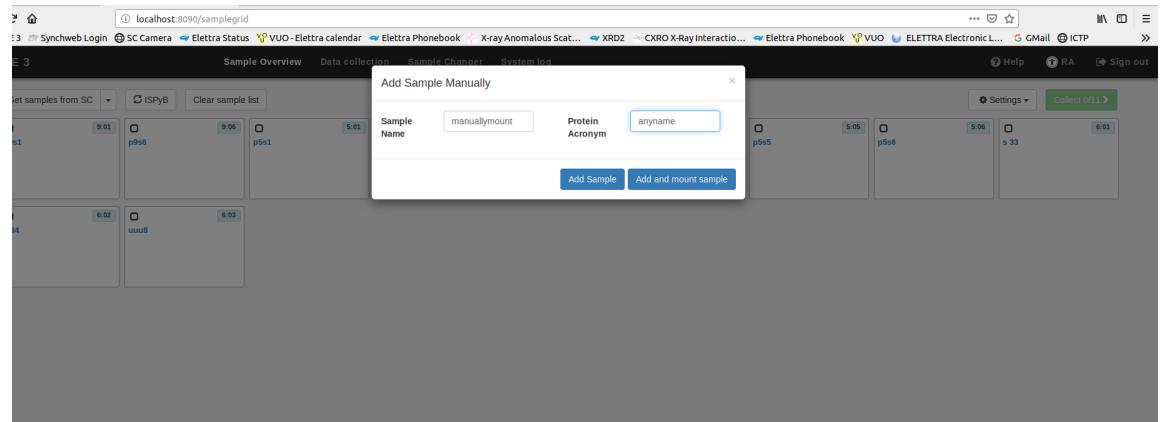
Protein is not something that we harvest from the proposal, in fact it's not a field per say in our form

Make my life easy and use MP (My Protein)

Then start generating

a crystalid

a blsampleid

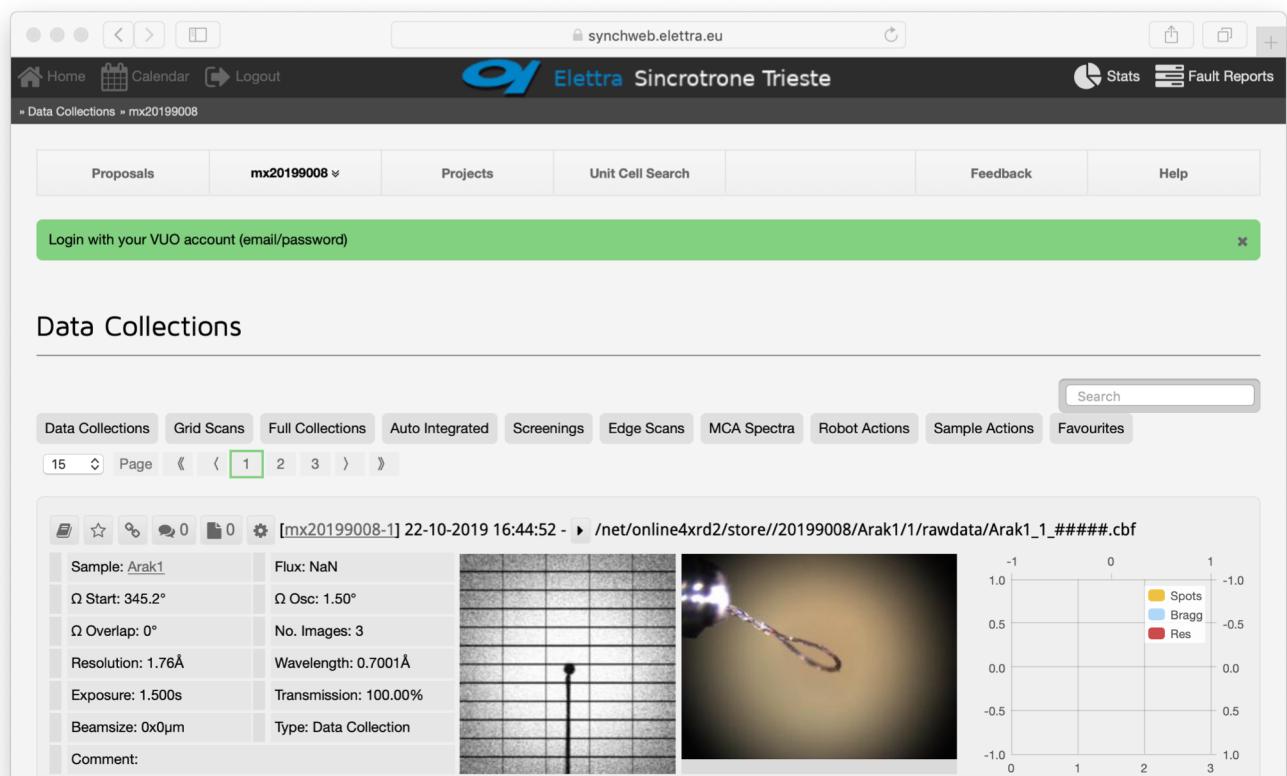




Crucial piece in place for remote, for “remote on-site” when collecting by someone from the group, a collaborator, mailin or really by someone off-site

### Presently WE USE IT

- Still have a mess for names because users are allowed to change it. Mostly there because we will overwrite data when we restart MXCuBE server
- Still early, and modification on how we handle visits, shipments impact what our , checks if files exists (thumbnail of diffraction was harder than it should be)





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### Future plans

- Having a better way to deal with shipment and the visit they are associated with.
- Filing out some of the parameters missing (flux etc..)
- Capturing the stopped / aborted data collections.
- Be able to add comments
- Adding some of the data processing

Visits for October 2019						
Schedule of visits for the currently selected proposal						
2018		September			November	
Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	Sunday
1	2	3	4	5	6	
	05:00 XRD2: mx20190622-1 (8h) - MANJASSETTY Babu Allampura		05:00 XRD2: mx20190634-1 (24h) - DEMITRI Nicola		05:00 XRD2: mx2019561-2 (8h) - HEROUX Annie	
7	8	9	10	11	12	13
17:00 XRD2: mx20199008-1 <span style="background-color: green;">1358.875555555555</span>	05:00 XRD2: mx20190636-2 (24h) - DEMITRI Nicola	05:00 XRD2: mx20190622-2 (8h) - MANJASSETTY Babu Allampura	13:00 XRD2: mx20190652-2 (24h) - MANJASSETTY Babu Allampura			05:00 XRD2: mx20195561-3 (24h) - HEROUX Annie
14	15	16	17	18	19	20
05:00 XRD2: mx20190617-1 (24h) - DEMITRI Nicola	05:00 XRD2: mx20195010-1 (24h) - POLENTARUTTI	05:00 XRD2: mx20195565-1 (24h) - HEROUX Annie	05:00 XRD2: mx20195566-1 (24h) - DEMITRI Nicola			
21	22	23	24	25	26	27
			12:00 XRD2: mx20199015-1 (1001h) 13:00			

### Wishlist

- Being able to modify a proposal from cool calendar
- Better handle on the shipment, VUO as a really unfriendly way.
- ....

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# Thanks

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And Roberto Borghes



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