



Elettra
Sincrotrone
Trieste

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



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

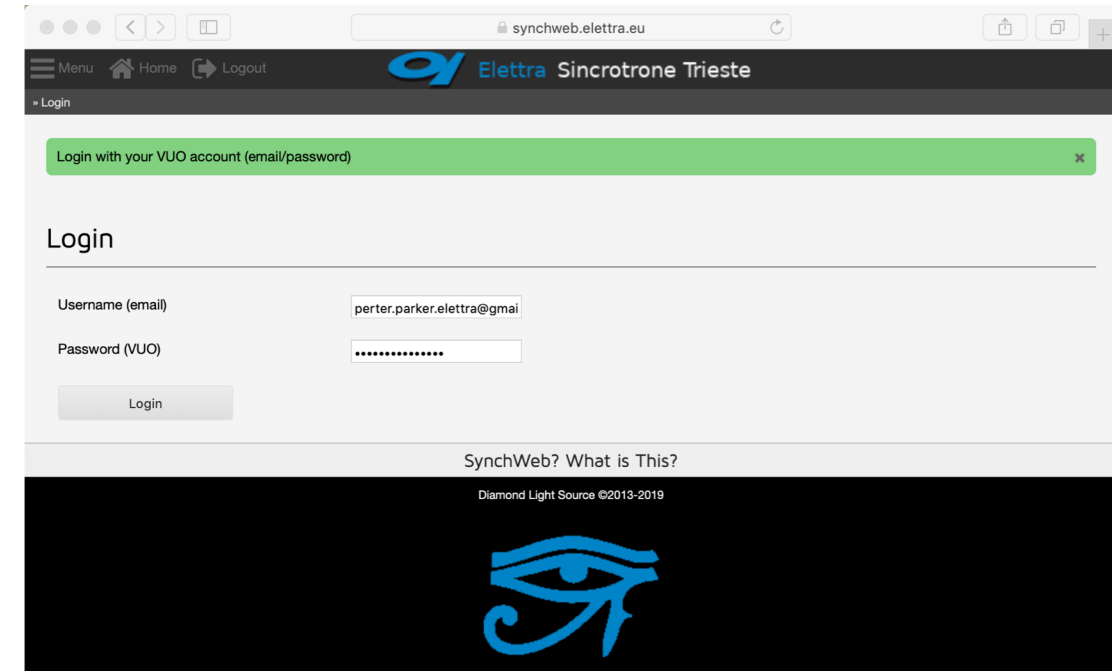
Integrate MXCuBE July 2019

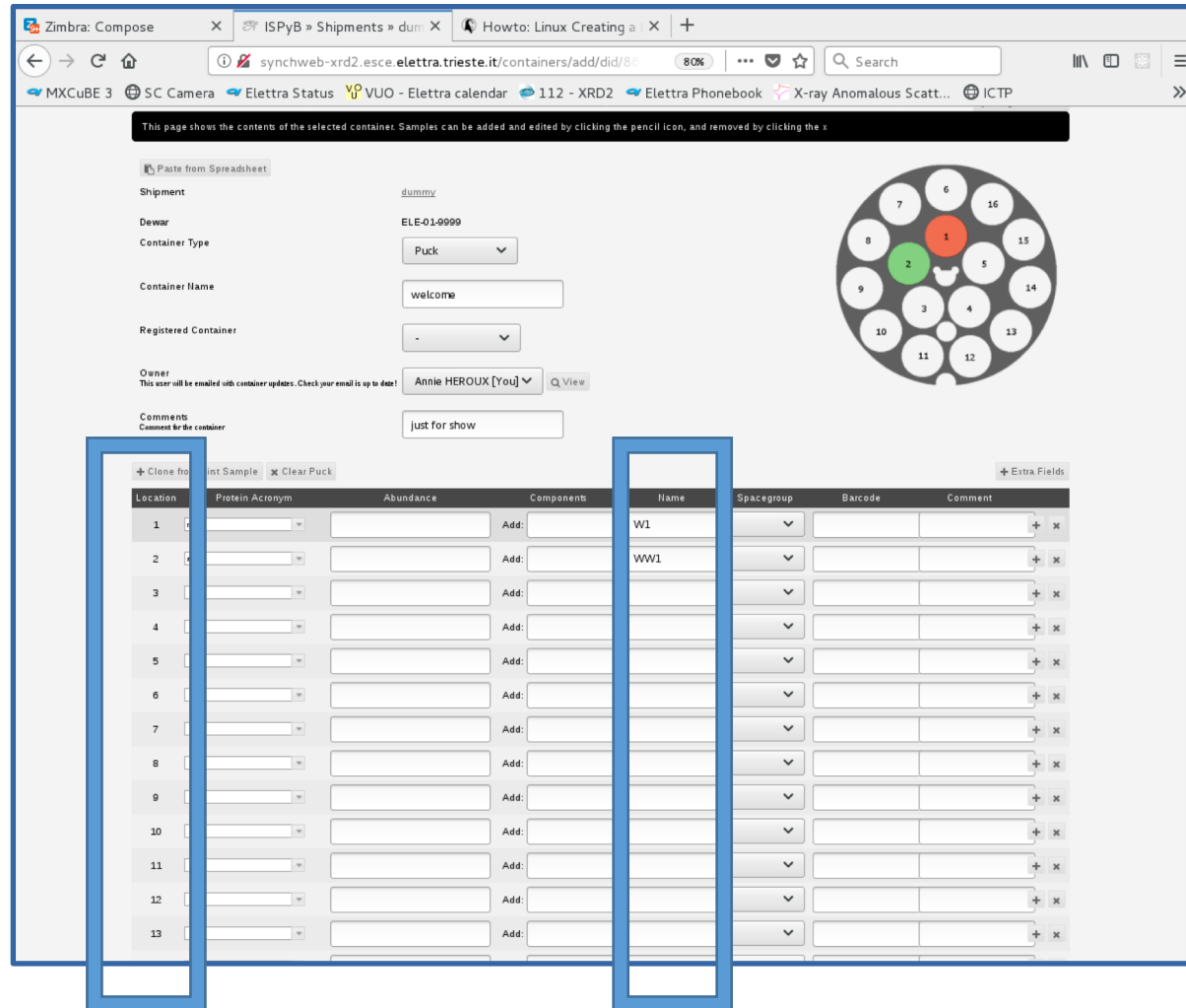
login , sessions

scan sc

Expose Synchweb Elettra to the world

Add...



The screenshot shows a web browser window with the URL `synchweb-xrd2.esce.elettra.trieste.it/containers/add/did/86`. The page displays a form for adding a container sample. The form includes fields for Shipment (dummy), Dewar (ELE-01-9999), Container Type (Puck), Container Name (welcome), Registered Container (-), Owner (Annie HEROUX [You]), and Comments (just for show). A circular diagram with 16 numbered positions is shown, with position 1 highlighted in red and position 2 in green. Below the form is a table with columns: Location, Protein Acronym, Abundance, Components, Name, Spacegroup, Barcode, and Comment. The table has 13 rows, with the first two rows containing data: W1 and WW1. Two blue rectangular boxes highlight the 'Location' and 'Name' columns.

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.



synchweb.elettra.eu

Logout  Elettra Sincrotrone Trieste

Login with your VUO account (email/password)

Login

Username (email)

peter.parker.elettra@gmail

Password (VUO)


.....

Login

SynchWeb? What is This?

ISPyB » Proposals

https://synchweb.elettra.eu/proposal

Home Logout  Elettra Sincrotrone Trieste

Proposals

Proposals No Proposal Feedback Help

Login with your VUO account (email/password)

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

29th Oct - 1st Nov 2019



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ISPyB → populate tables

Isipyb-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

» Shipments » Containers

Help

Tutorials

Feedback

Proposals

mx20199002 ▾

View All Data

Visits

Calendar

Assign Containers

Shipments

Registered Dewars

Registered Containers

Containers

Samples

29th Oct - 1st Nov 2019



MISSION 1

CONTAINERS

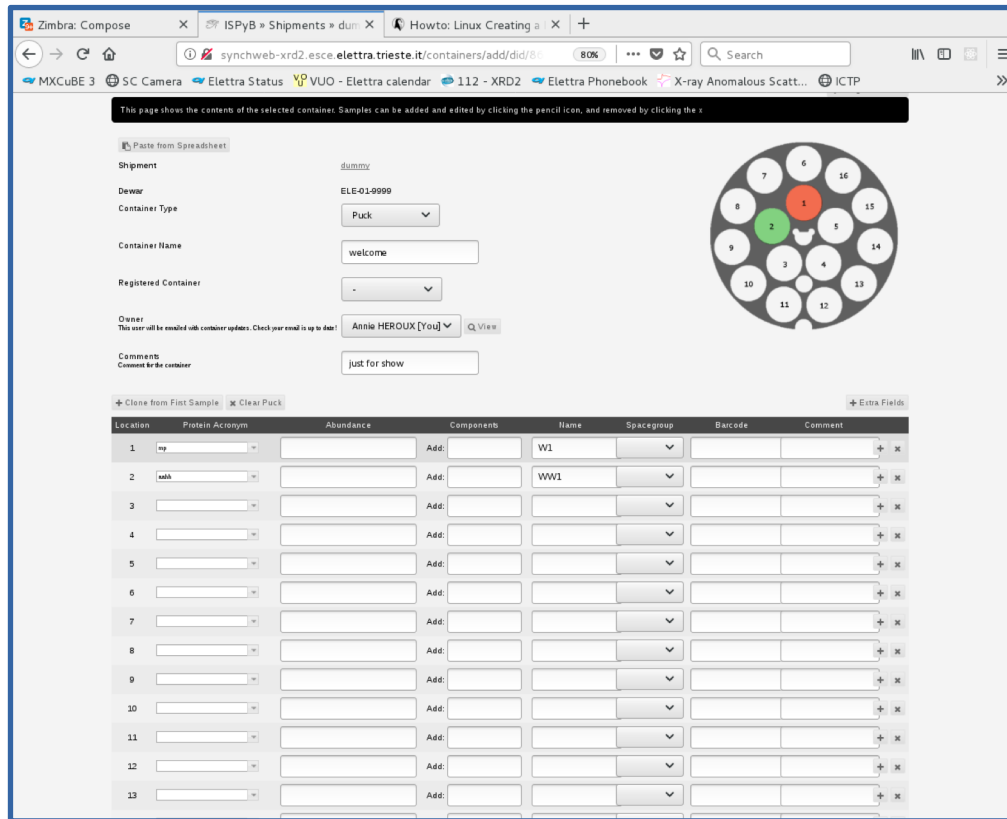
Addressing issues such as
~~having to fill them at every start of MXCuBE~~
funky characters in name (orange)

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



The screenshot shows the MXCuBE web interface. At the top, there's a browser window with the URL 'synchweb-xrd2.esce.elettra.trieste.it/containers/add/did/8'. Below the browser window, there's a form for adding a container. The form includes fields for 'Shipment' (dummy), 'Dewar' (ELE-01-9999), 'Container Type' (Puck), 'Container Name' (welcome), 'Registered Container' (-), 'Owner' (Annie HEROUX [You]), and 'Comments' (just for show). To the right of the form is a circular diagram with 16 numbered positions, where position 1 is orange and position 2 is green. Below the form is a table with columns: Location, Protein Acronym, Abundance, Components, Name, Spacegroup, Barcode, and Comment. The table has 13 rows, each with a dropdown menu for 'Location' and a text input for 'Protein Acronym'. The 'Name' column contains values like 'W1' and 'WW1'.



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MISSION 1

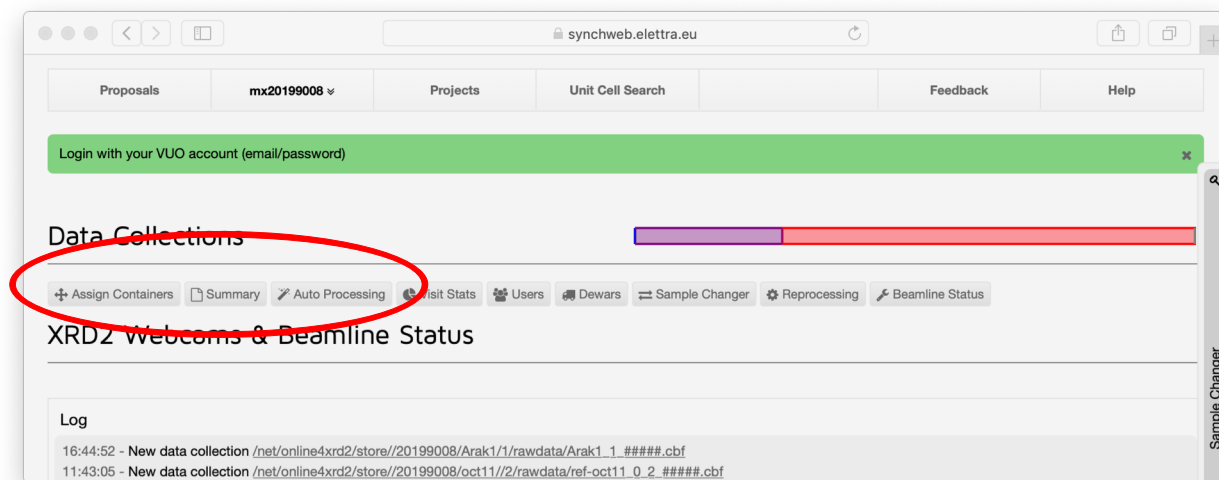
ASSIGN CONTAINERS & use in MXCuBE

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

ASSIGN CONTAINERS two ways to reach
this place and two behaviors

So far no cross check in sc dewar so no
problem

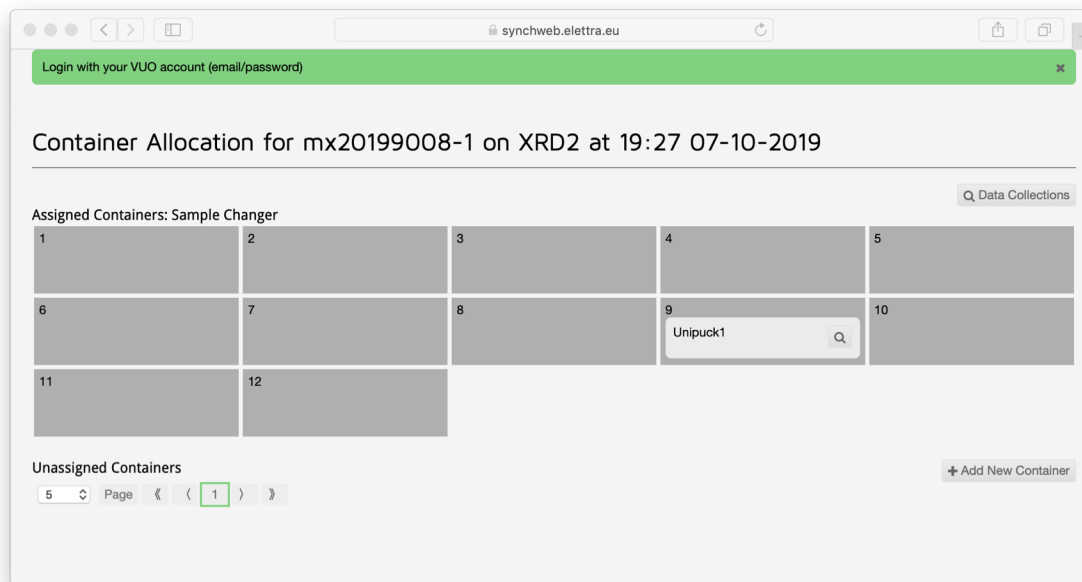
In MXCuBE when we scan containers,
problem with unassigned
assigned to position 0 in sc dewar





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UNASSIGN CONTAINERS & use in MXCuBE



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 .



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 .

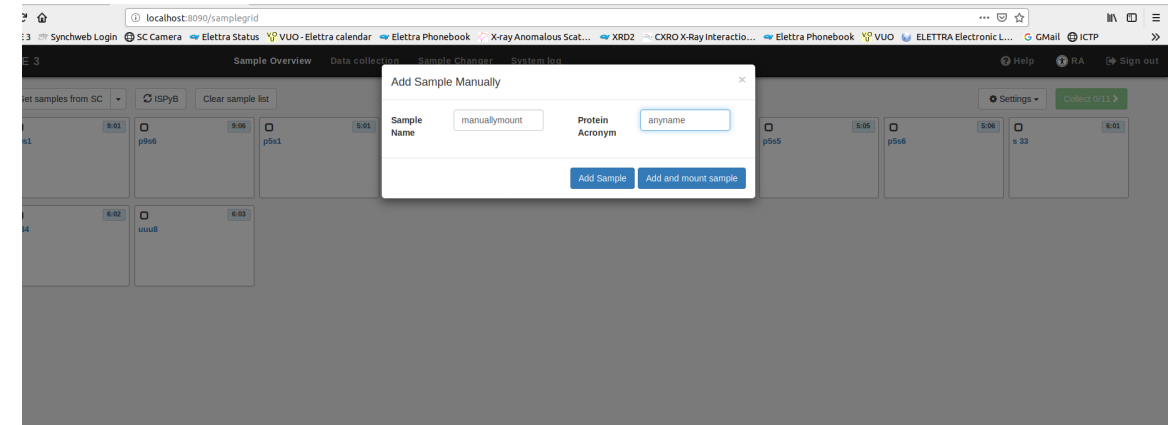
Protein is not something that we harvest from the proposal, in fact it's not a field per say in our form

Make my life easy and use MP (My Protein)

Then start generating

a crystalid

a blsampleid

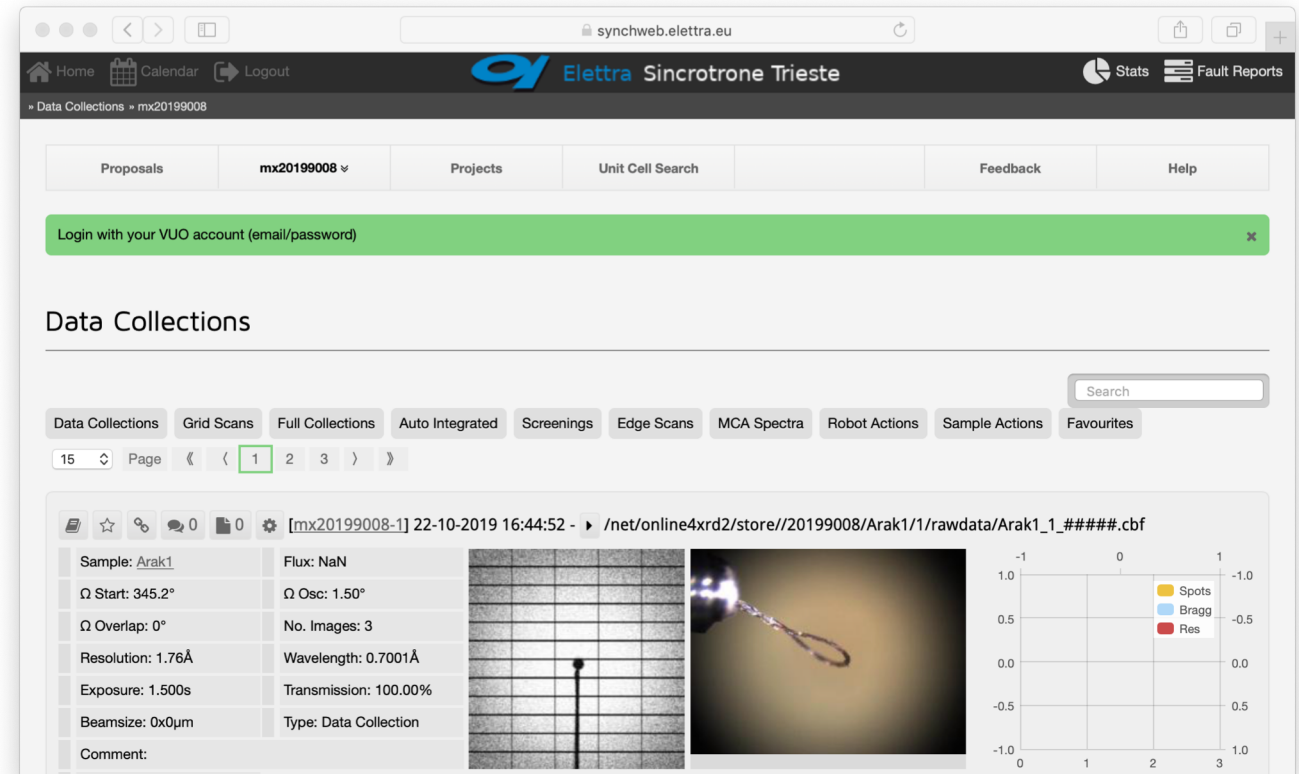




Crucial piece in place for remote, for “remote on-site” when collecting by someone from the group, a collaborator, mailin or really by someone off-site

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)



The screenshot shows the MXCuBE web interface. The top navigation bar includes links for Home, Calendar, Logout, and a search bar. The main content area displays a table of data collections for the sample 'Arak1'. The table has columns for Data Collections, Grid Scans, Full Collections, Auto Integrated, Screenings, Edge Scans, MCA Spectra, Robot Actions, Sample Actions, and Favourites. The 'Data Collections' column is highlighted, and a search bar is visible. Below the table, there is a detailed view of a specific data collection, showing a thumbnail of a diffraction pattern and a plot of intensity versus position. The plot shows a central peak with a tail, and the legend indicates 'Spots', 'Bragg', and 'Res'.



- 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

Wishlist

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

29th Oct - 1st Nov 2019



Thanks

Karl Levik

Neil Smith, James Hall

Fulvio Billè, Milan Prica , John Skinner (NSLS)

And Roberto Borghes



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