

ISPyB site report

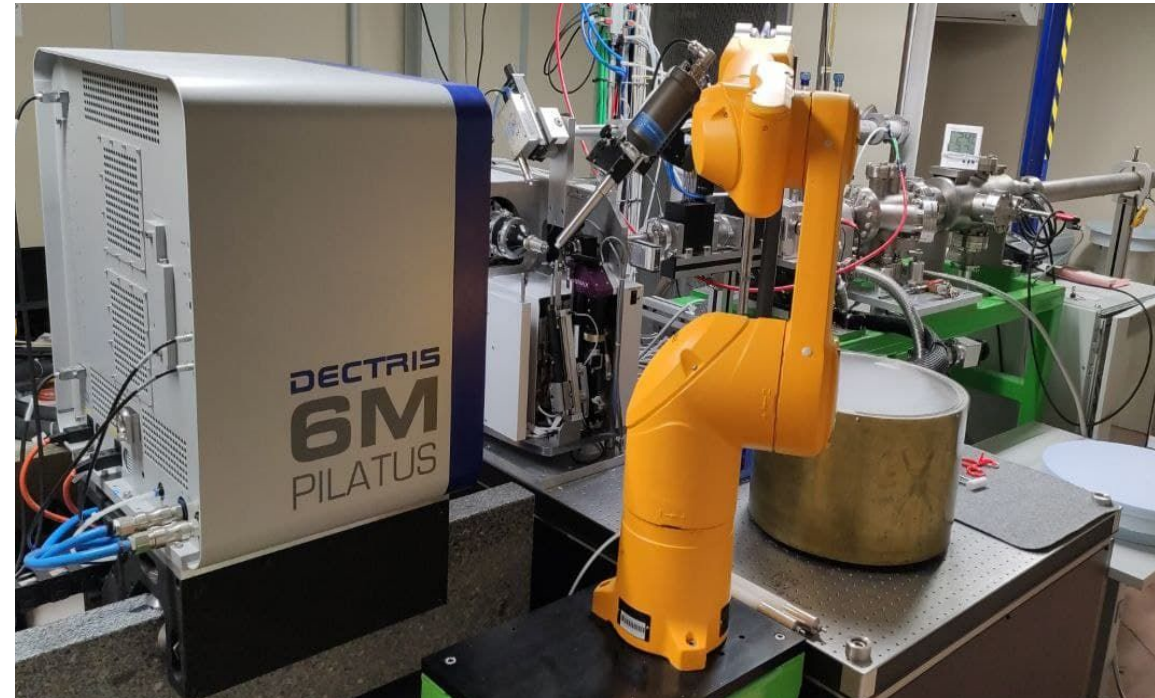
Elettra Sincrotrone Trieste

Brief beamlines summary

XRD2 (X-ray diffraction 2):

Focussed on MX - SPINE standard samples only

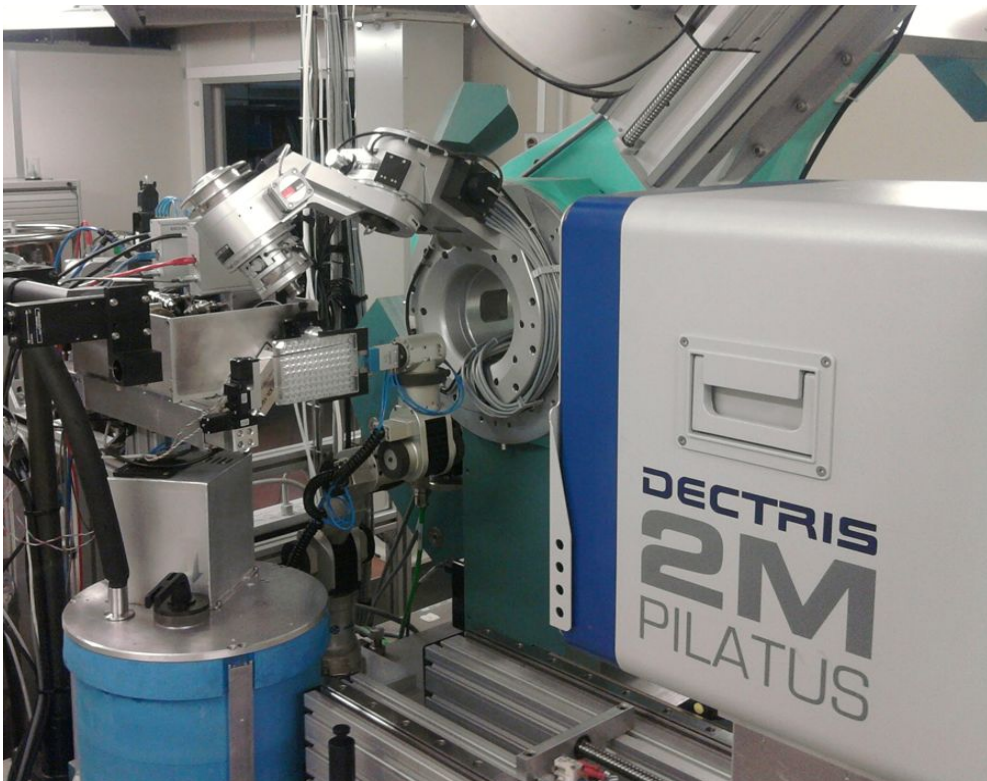
Surviving without a LIMS is impossible!



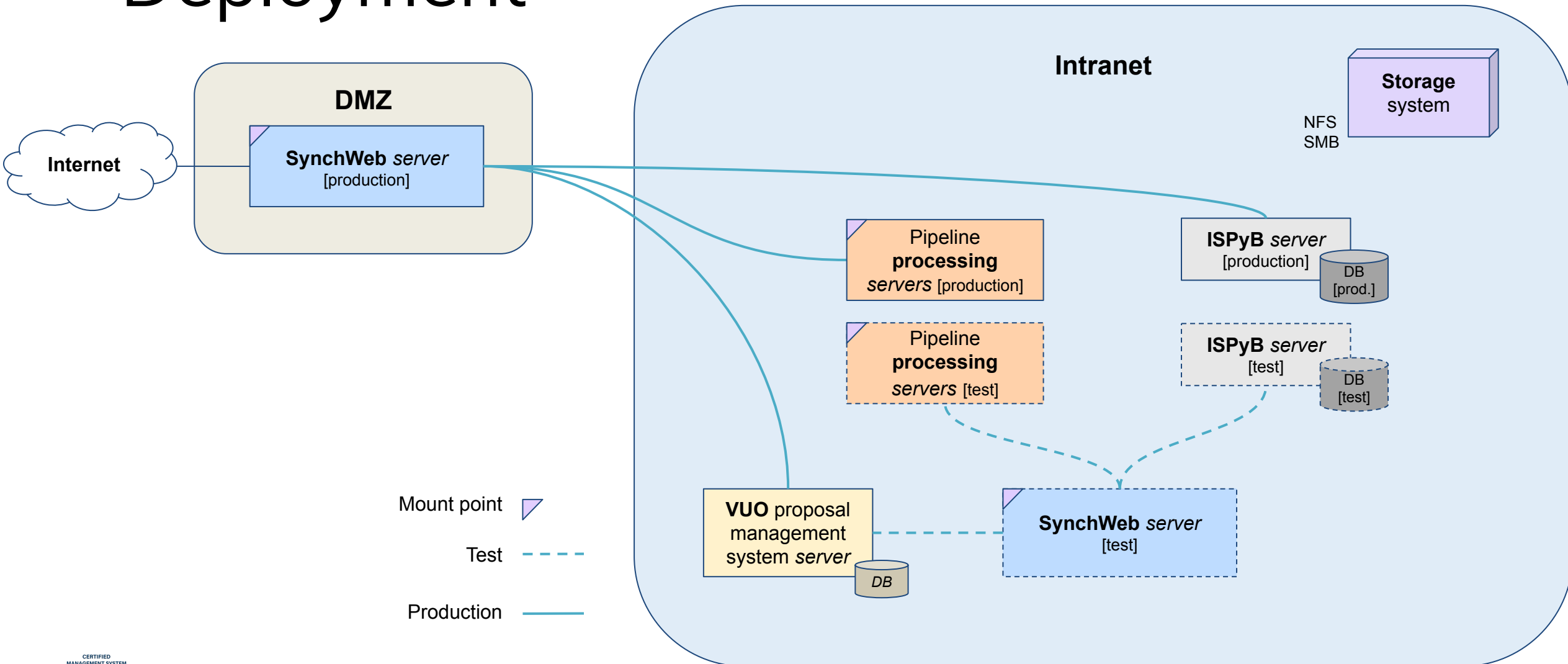
XRD1 (X-ray diffraction):

General purpose XRD - multiple supports accepted

Experiments other than SC-XRD are not asking for a LIMS (not high throughput anyway)



Deployment



ISPyB status (1)

Backend:

- Deployment at glance:
 - CentOS 7 with Apache in DMZ
 - Schema version **3.0.0**
 - Database version **10.4.12 MariaDB**
- DLS ISPyB <https://github.com/DiamondLightSource/ispyb-database>
- Updated to version 3 applied the changes

Frontend:

- Synchronise from php 5 to php 7
- Re-apply all the local changes and bug fixes

ISPyB status (2)

Tools:

- **ispyb-datasync**

Synchronization between VUO and the ISPyB database ingesting all the proposals, users and sessions

- Python3.6

- **ispyb-api**

Interface with ISPyB from python

- Version 9 (compatible with ISPyB v3.0.0)
- Migrating from stored procedure to SQLAlchemy (MXCuBE)

- **ispyb-database**

- It allows creating and updating the ISPyB schema

Plans for the next six months

- Fixing (random) folder permission problems
- (Optimistically) allow SynchWeb to relaunch pipelines using RunScriptWeb

Development of is basically frozen due to:

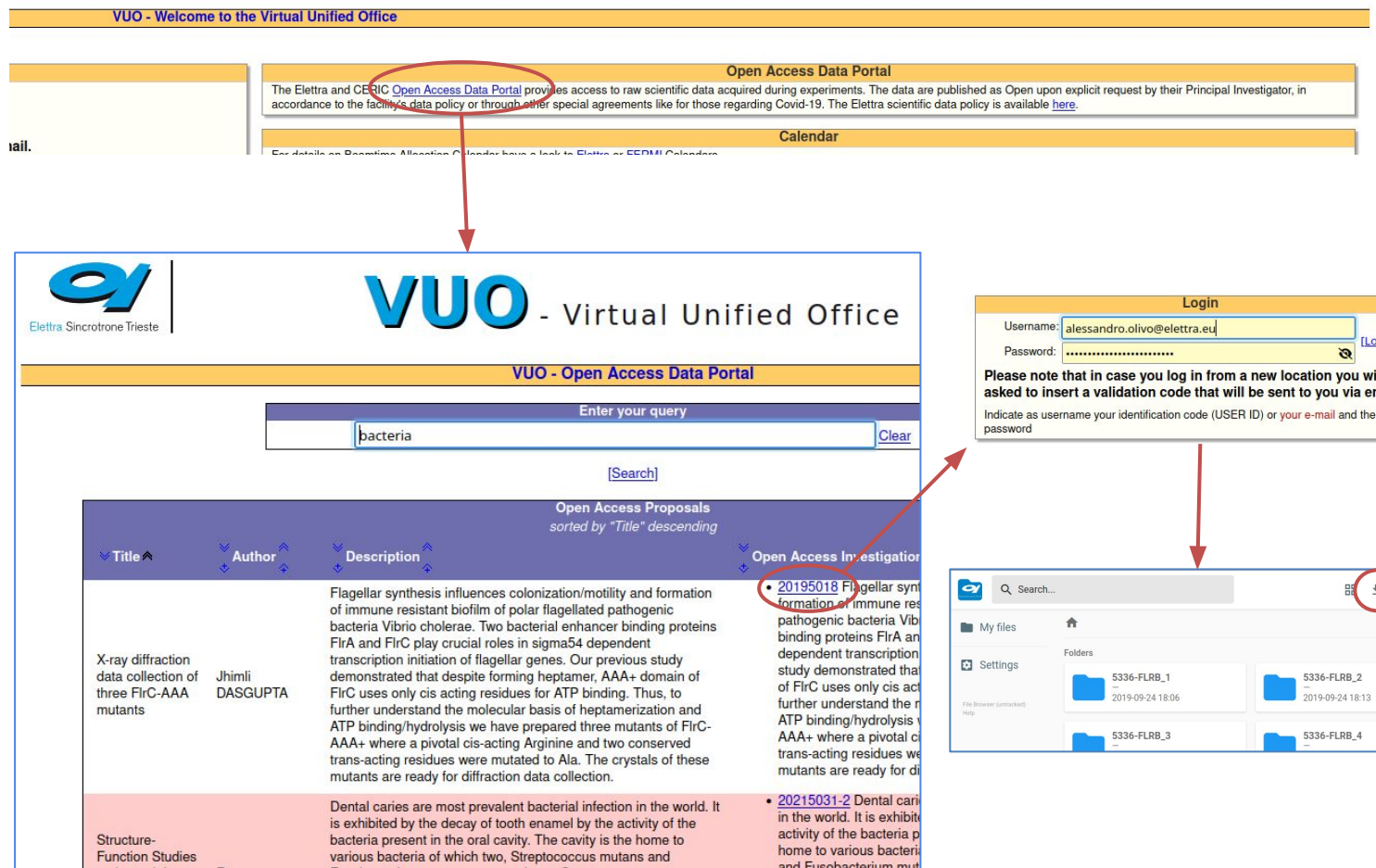
- “limited” Human Resources allocated (dark period coming in 2025)
- current “Elettra users needs” fit the db and SynchWeb interface works great (clean and intuitive)

Better performance for pipelines and more features needed with uXRD on Elettra 2.0 (Multi-crystal, time dependant experiments ...CryoEM support?)

Catalog

- Integrated in VUO
- Implementing the data policy for the opendata
- Public users can browse open investigations:
 - Simple filtering (name, title, description)
- Authenticated users can download investigation data

VUO - Virtual Unified Office



The screenshot shows the VUO - Virtual Unified Office interface. At the top, there is a navigation bar with "VUO - Welcome to the Virtual Unified Office" and "Open Access Data Portal". Below this, a text box explains the data policy: "The Elettra and CERiC Open Access Data Portal provides access to raw scientific data acquired during experiments. The data are published as Open upon explicit request by their Principal Investigator, in accordance to the facility's data policy or through other special agreements like for those regarding Covid-19. The Elettra scientific data policy is available [here](#)." A red circle highlights the "Open Access Data Portal" link in the text, with an arrow pointing to the main search interface.

The main search interface has a header "VUO - Virtual Unified Office" and "VUO - Open Access Data Portal". It features a search bar with the text "bacteria" and a "[Search]" button. Below the search bar, there is a table of "Open Access Proposals sorted by 'Title' descending". The table has columns for "Title", "Author", "Description", and "Open Access Investigation".

Title	Author	Description	Open Access Investigation
X-ray diffraction data collection of three FirC-AAA mutants	Jhimli DASGUPTA	Flagellar synthesis influences colonization/motility and formation of immune resistant biofilm of polar flagellated pathogenic bacteria Vibrio cholerae. Two bacterial enhancer binding proteins FirA and FirC play crucial roles in sigma54 dependent transcription initiation of flagellar genes. Our previous study demonstrated that despite forming heptamer, AAA+ domain of FirC uses only cis acting residues for ATP binding. Thus, to further understand the molecular basis of heptamerization and ATP binding/hydrolysis we have prepared three mutants of FirC-AAA+ where a pivotal cis-acting Arginine and two conserved trans-acting residues were mutated to Ala. The crystals of these mutants are ready for diffraction data collection.	20195018 Flagellar synthesis of immune resistant pathogenic bacteria Vibrio cholerae. Two bacterial enhancer binding proteins FirA and FirC play crucial roles in sigma54 dependent transcription initiation of flagellar genes. Our previous study demonstrated that despite forming heptamer, AAA+ domain of FirC uses only cis acting residues for ATP binding. Thus, to further understand the molecular basis of heptamerization and ATP binding/hydrolysis we have prepared three mutants of FirC-AAA+ where a pivotal cis-acting Arginine and two conserved trans-acting residues were mutated to Ala. The crystals of these mutants are ready for diffraction data collection.
Structure-Function Studies		Dental caries are most prevalent bacterial infection in the world. It is exhibited by the decay of tooth enamel by the activity of the bacteria present in the oral cavity. The cavity is the home to various bacteria of which two, Streptococcus mutans and E. coli are the most common.	20215031-2 Dental caries are most prevalent bacterial infection in the world. It is exhibited by the decay of tooth enamel by the activity of the bacteria present in the oral cavity. The cavity is the home to various bacteria of which two, Streptococcus mutans and E. coli are the most common.

On the right side of the screenshot, there is a "Login" window. It contains a "Username" field with the value "alessandro.olivo@elettra.eu" and a "Password" field. A "[Login]" button is next to the password field. Below the fields, there is a note: "Please note that in case you log in from a new location you will be asked to insert a validation code that will be sent to you via email. Indicate as username your identification code (USER ID) or your e-mail and the password". A red circle highlights the "[Login]" button, with an arrow pointing to a file browser window.

The file browser window shows a search bar and a list of folders under "My files". The folders are: "5336-FLRB_1" (created 2019-09-24 18:06), "5336-FLRB_2" (created 2019-09-24 18:13), "5336-FLRB_3", and "5336-FLRB_4". A red circle highlights the download icon in the top right corner of the file browser window.



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