ISPyB site report

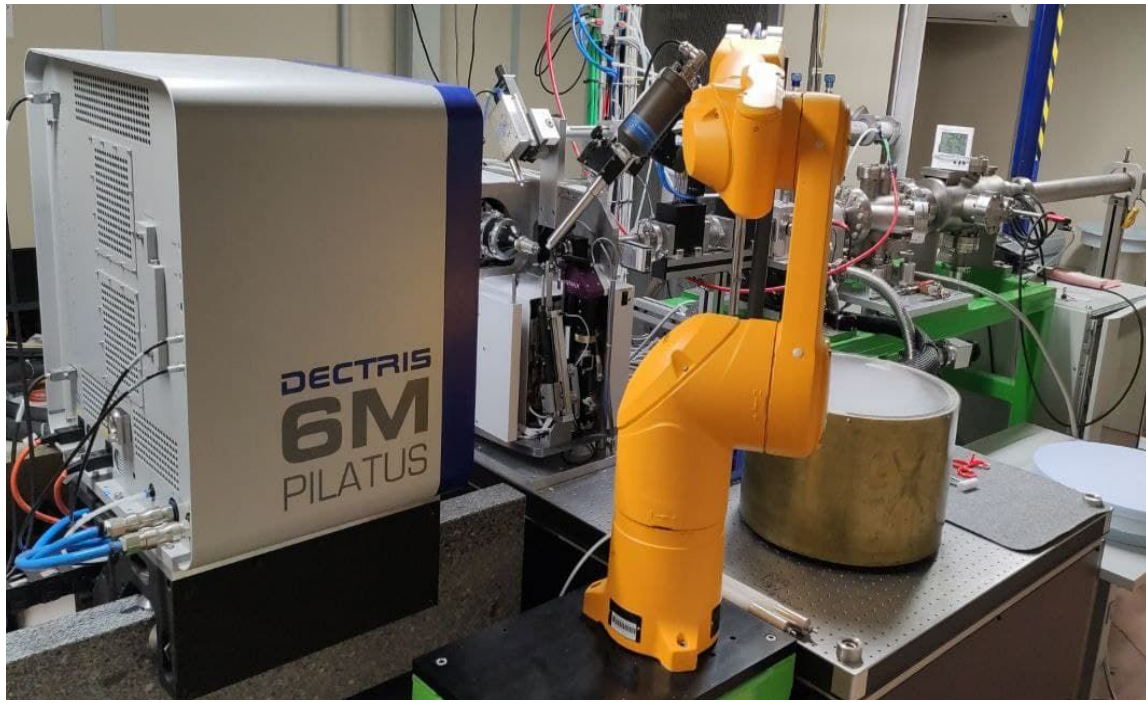
Elettra Sincrotrone Trieste

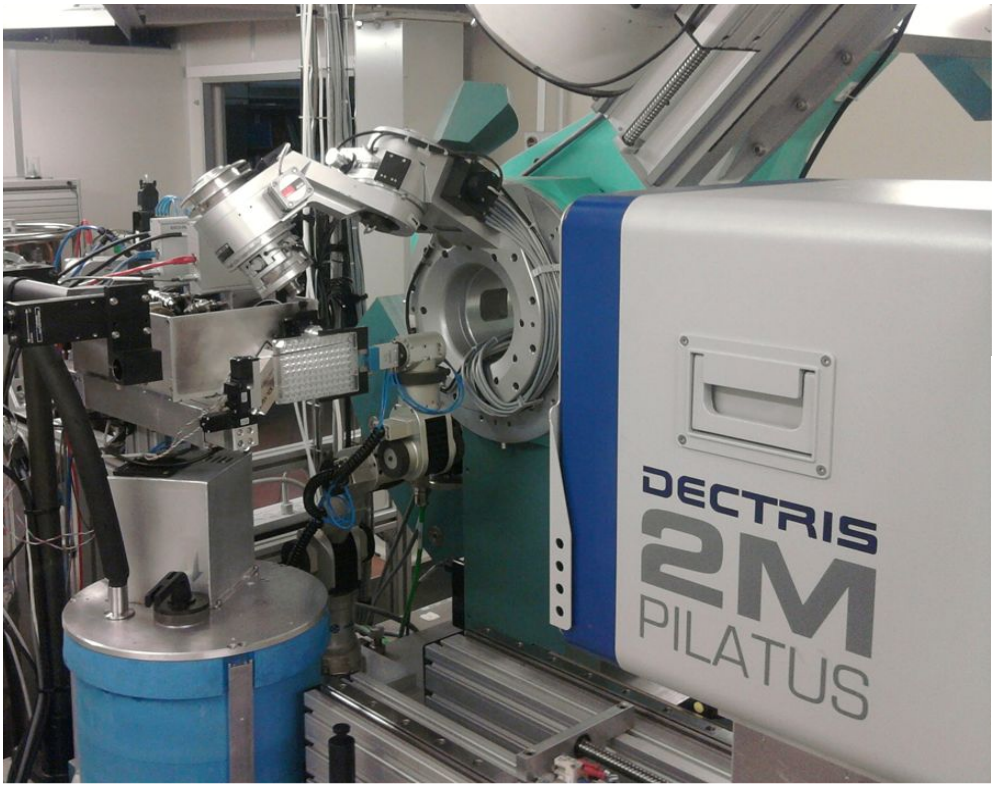
Brief beamlines summary

XRD2 (X-ray diffraction 2):

Focussed on MX - SPINE standard samples only

Surviving without a LIMS is impossible!



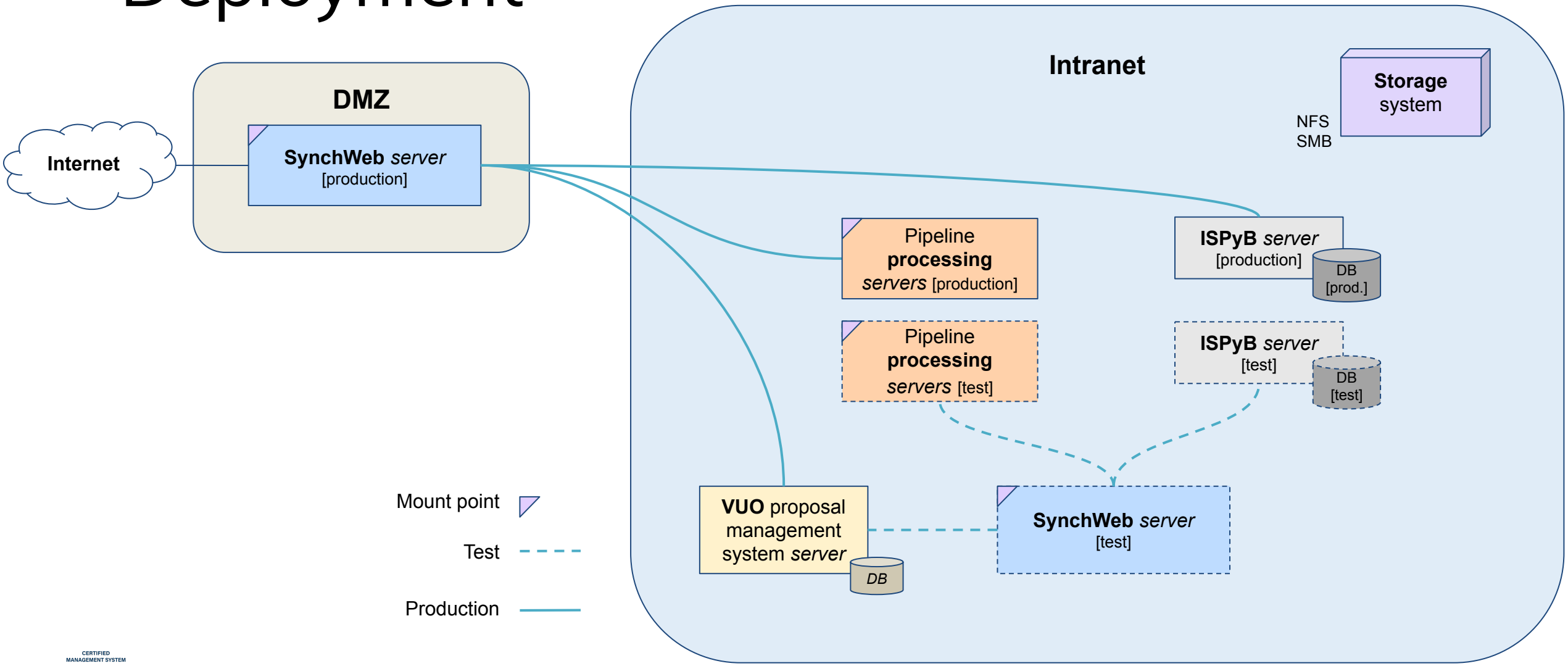


XRD1 (X-ray diffraction):

General purpose XRD - multiple supports accepted

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

Deployment


Intranet
DMZ
Internet
SynchWeb server
[production]
Storage
system
NFS
SMB
Pipeline
processing
servers [production]
ISPyB server
[production]
DB
[prod.]
Pipeline
processing
servers [test]
ISPyB server
[test]
DB
[test]
VUO proposal
management
system server
DB
SynchWeb server
[test]
Mount point
Test
Production

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:

- Synchweb 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

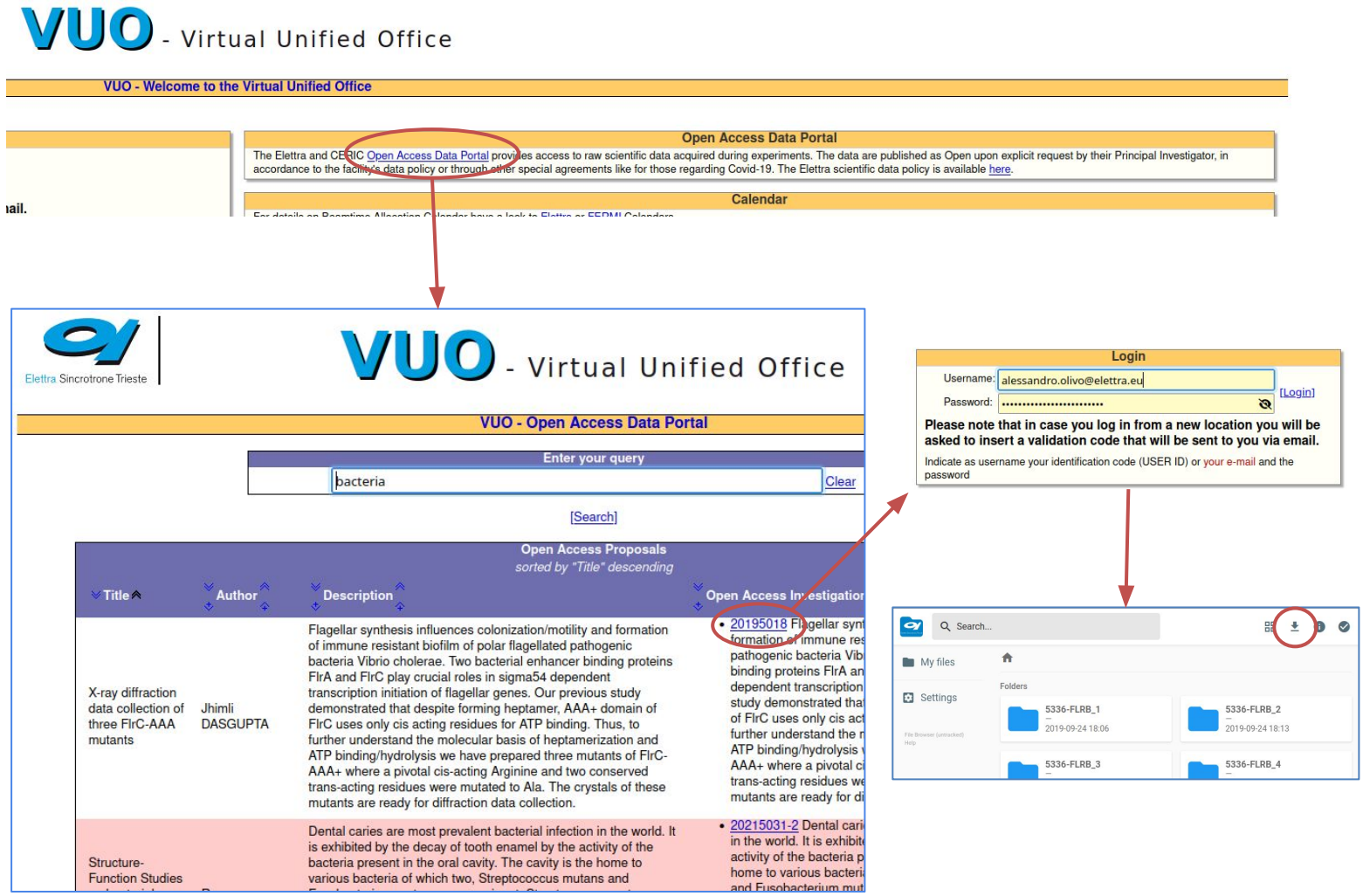
Development of is basically frozen due to:

- “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



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