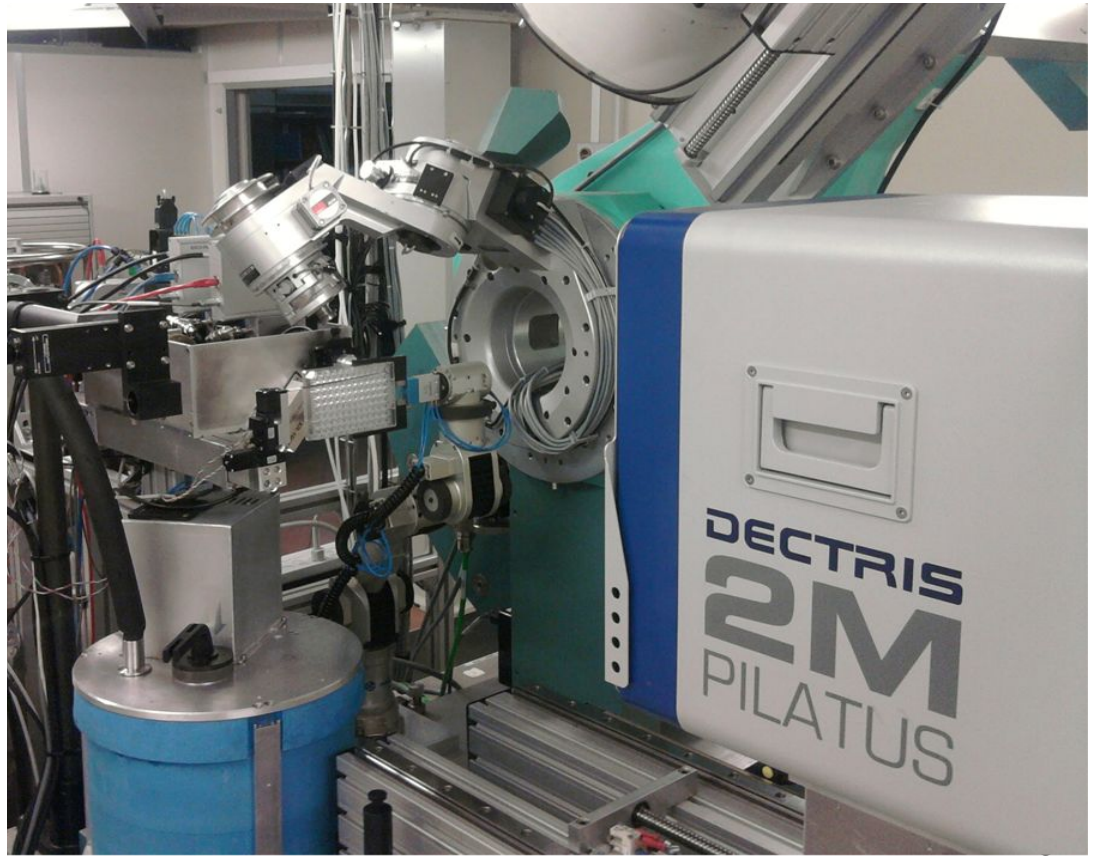
Elettra Sincrotrone Trieste

MXCuBE site report

Elettra-Sincrotrone Trieste

Brief beamlines summary (1)

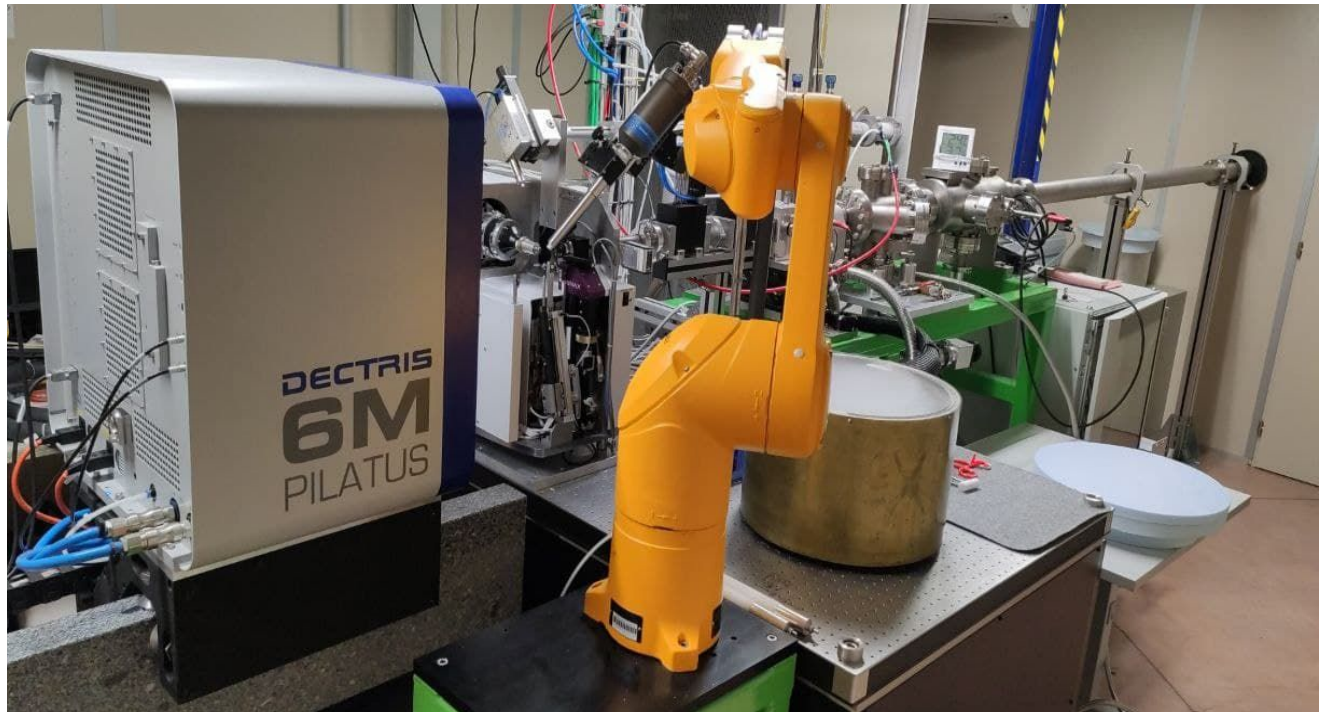
- **XRD1** (X-ray diffraction):
  General purpose XRD - multiple sample supports accepted
  - Huber Kappa Goniometer
  - Pilatus 2M
  - Arinax BZoom
  - Custom sample changer for SPINE (Neuronics Katana on internally developed 5 ESRF pucks dewar and in-house developed Galil code)



Brief beamlines summary (2)

- **XRD2** (X-ray diffraction 2):

  Focussed on MX - SPINE standard samples only
  - Arinax MD2s
  - Pilatus 6M
  - Arinax BZoom
  - Custom sample changer (Staubli TX60L on internally developed 12 Unipucks dewar and in-house developed Val3 code)



MXCuBE status (1)

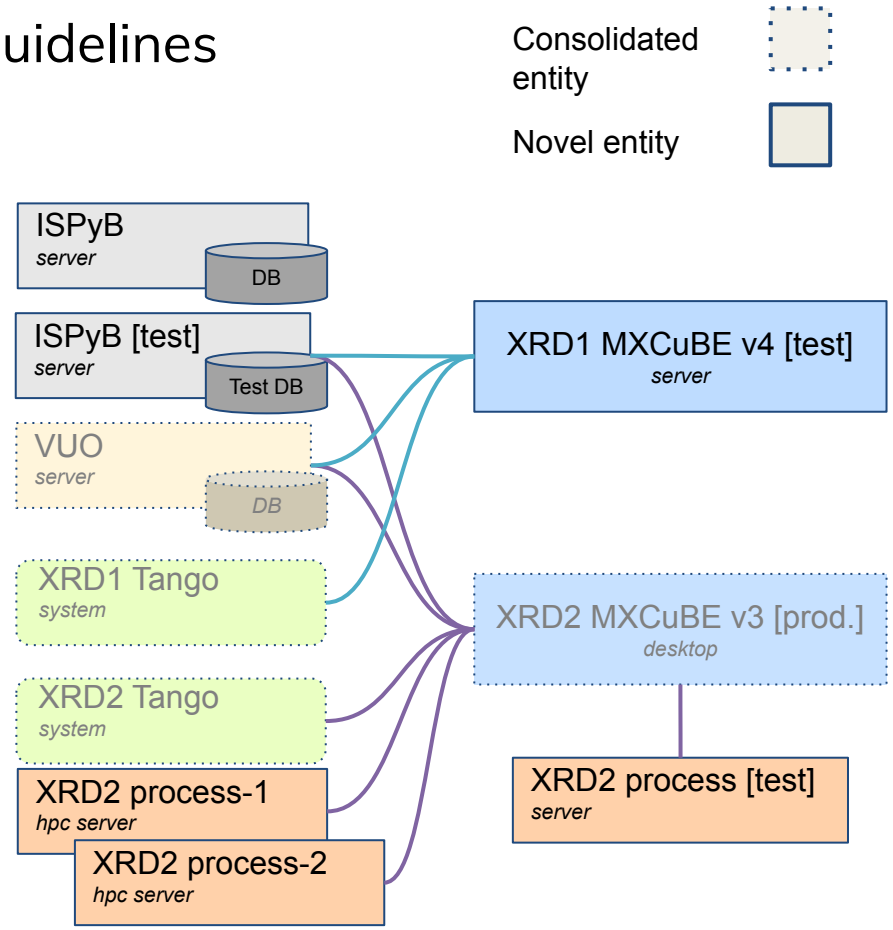
- **XRD1**
  - Developing on the following versions:
    - mxcubecore **v1.71.0-48-g945e3116c** commit **33958b91** (Mar 2024) + local changes committed in separated branches
    - mxcubeweb **v4.27.0-2-g3ae25970** commit **26fdad84** (Feb 2024) + local changes committed in separated branches
    - Deployed on a Rocky Linux 9 (*test server*), accessible only on intranet
    - Python 3.9.18 (python virtual environment), installed with pip

MXCuBE status (2)

- **XRD2**
  - Production version:
    - mxcube3: **v3.0.0-beta.1-100-g19640781** commit **b79f2fd8** (Feb 2018)
    - local changes committed on master
    - Deployed on an Ubuntu 18.04.4 LTS (*production desktop*), accessible from the internet during beamtime (behind firewall)
    - Python 2.7 without conda environment
  - Other deployments
    - 2 HPC nodes used for the data processing pipeline e.g. fastdp, autoproc, etc.

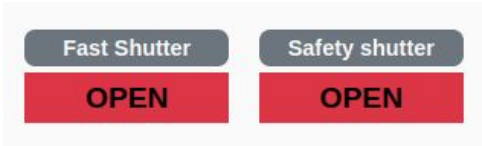
Developments since last meeting (1)

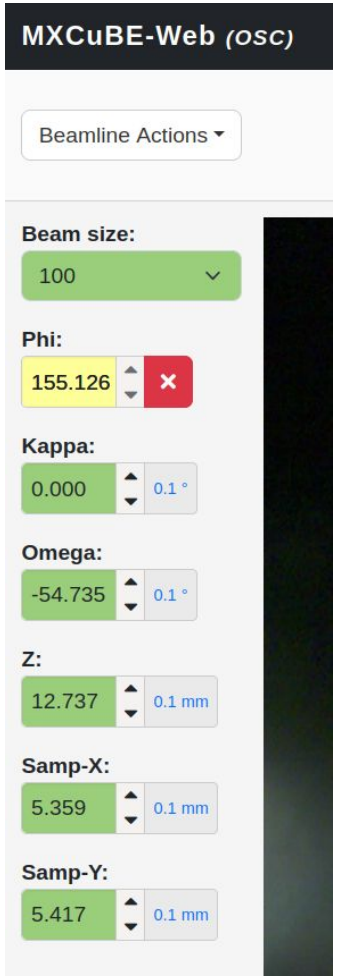
- Upgrade code base, mxcubecore (1.36.0 → 1.71.0) and mxcubeweb (1.89.0 → 4.27.0) following the contributing guidelines
- Reorganization of the MXCuBE ecosystem (see the schema)
- Refactoring (code cleanup) of the synchronization system between ISPyB and VUO proposals DB
- Development of a service called RunScriptWeb installed in the new HPCs for live data processing on XRD2 beamline, which allows remote scripts execution (fastdp, autoproc, dimple) Prioritization is under discussion (slurm queue?)



Developments since last meeting (2)

- Development of MXCuBE 4 (XRD1)
  - Refactoring of the “lims” HWO using SQL Alchemy and minor refactoring for others HWOs
  - Features development: “YAML GUI switches” (some examples):
    - Invert background color of the InOutSwitches,
    - Allow to hide phase control
    - Make left-side motors “customizable”
    - Make the name of the manual centering procedure customizable
  - Fixes applied (some examples):
    - Restore the emission of Tango signals after a “read attribute” error
    - Aperture status background color changing
    - Prevent negative clicks counting





Developments since last meeting (3)

- Development of MXCuBE 3 (XRD2)
  - Features development (some examples):
    - Better handling of sample changer states
    - Refactoring some HWOs
    - Trying to catch Detector alarms
    - Backporting of @mxcube.route("/mxcube/api/v0.1/detector/display_image/") to call Braggy from MX3 page and discourage usage of Albula through VNC tunnels

Grid-2: Data Collection

Path: MMA_AuCC100Kb_1_#####.cbf

Start °	Osc. °	t (s)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
12.95	0.05	0.300	7	100.00	1.088	12.3987	0.00	0.00

View Results in Braggy

  - Fixes applied (some examples):
    - Restore the emission of Tango signals after a “read attribute” error
    - Prevent negative clicks counting
    - Code clean-up to prepare migration to MXCuBE 4

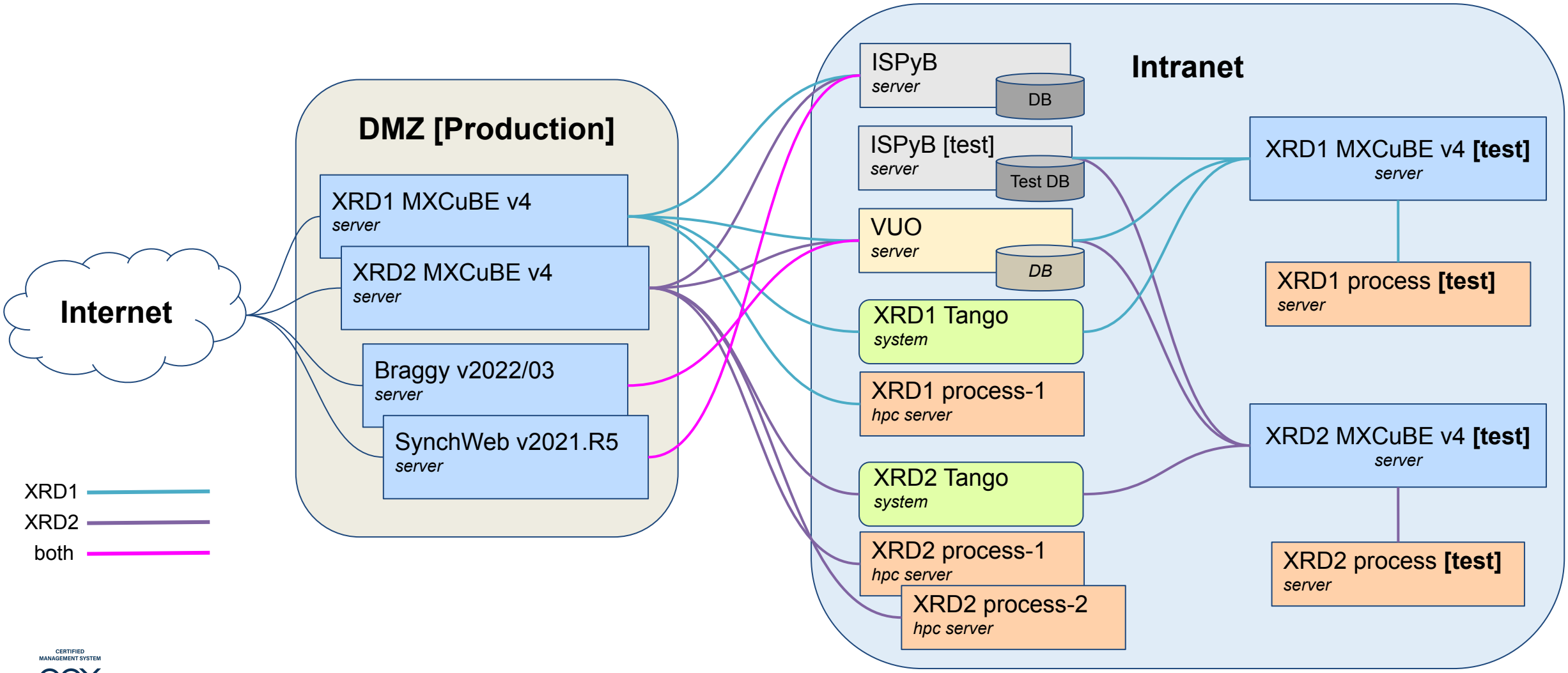
Plans for the next six months (1)

- Deployment of MXCuBE version **4** in the *production server* for **XRD1**

- Upgrade of MXCuBE deployed in **XRD2** from version **3** to version **4**:
  - Porting/refactoring of the current HWO implementations
  - Deployment in the *test server*
  - Real life friendly tests in a new *production server before dark period …?*

- Finalization of the reorganization of the MXCuBE ecosystem (see next slide)

Plans for the next six months (2)



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