MXCuBE site report

P11, DESY (Hamburg, Germany)

Brief beamlines summary

The High-throughput Macromolecular Crystallography Beamline P11

Crystallography Experiments

- In user operation since 2013
- Broad energy range: 5.5 28 keV
- High-speed sample changer with capacity (23 unipucks = 368 samples)
- High precision single axis goniometer:
 0.0001° at 120°/s
- Eiger2 X 16M
- XRF for experimental phasing (SAD/MAD) and element analysis



MXCuBE status

- Latest mxcubeqt (develop branch),
- Latest mxcubecore 1.104.0 (develop branch)
- Python 3.8.9, PyQt 5.15.10
- Cybersecurity: mxcubeqt is running on a separate VM (Kiosk mode), TFA

Developments since last meeting

- Finished moving to the latest development branch (core, qt)
- Live view as an ADXV-based executable (Eiger monitoring interface)
- Automated optical centering can now be done with murko (M. Savko) – PR#932

Plans for the next six months

- EDNA-Characterization + processing
- Code cleanup
- Roll-out to the users
- Interaction with ISPyB
- X-Ray centering + mesh-scans
- Move installation to Debian 12
- Optimize usage of *murko*-centering
- Aligning temporary *murko* setup with local IT infrastructure