

MXCuBE status report

P11 beamline, DESY Hamburg

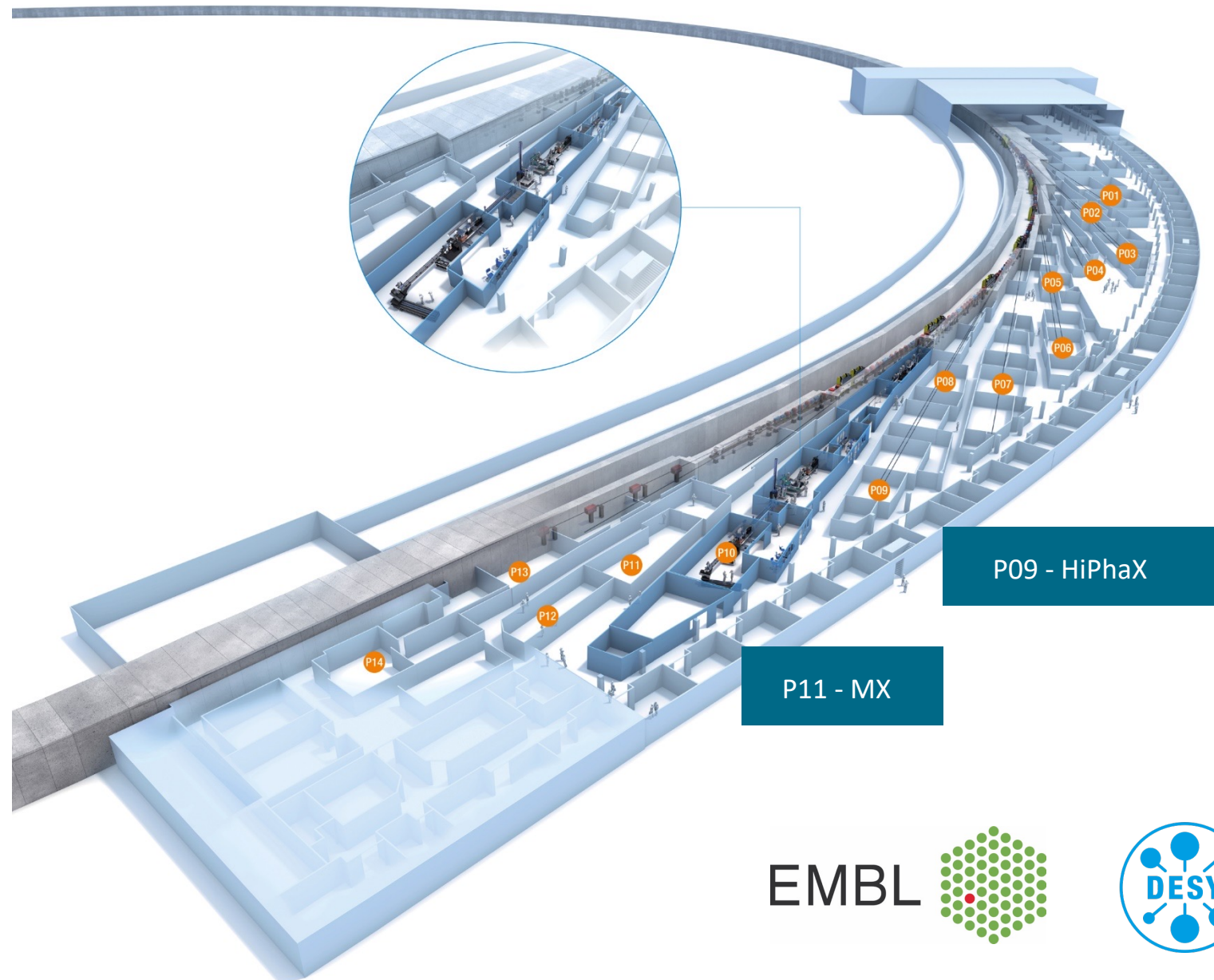
Andrey Gruzinov
MXCuBE/ISPyB - ALBA Synchrotron
29.11.2023

HELMHOLTZ



Structural Biology Village of PETRA Beamlines

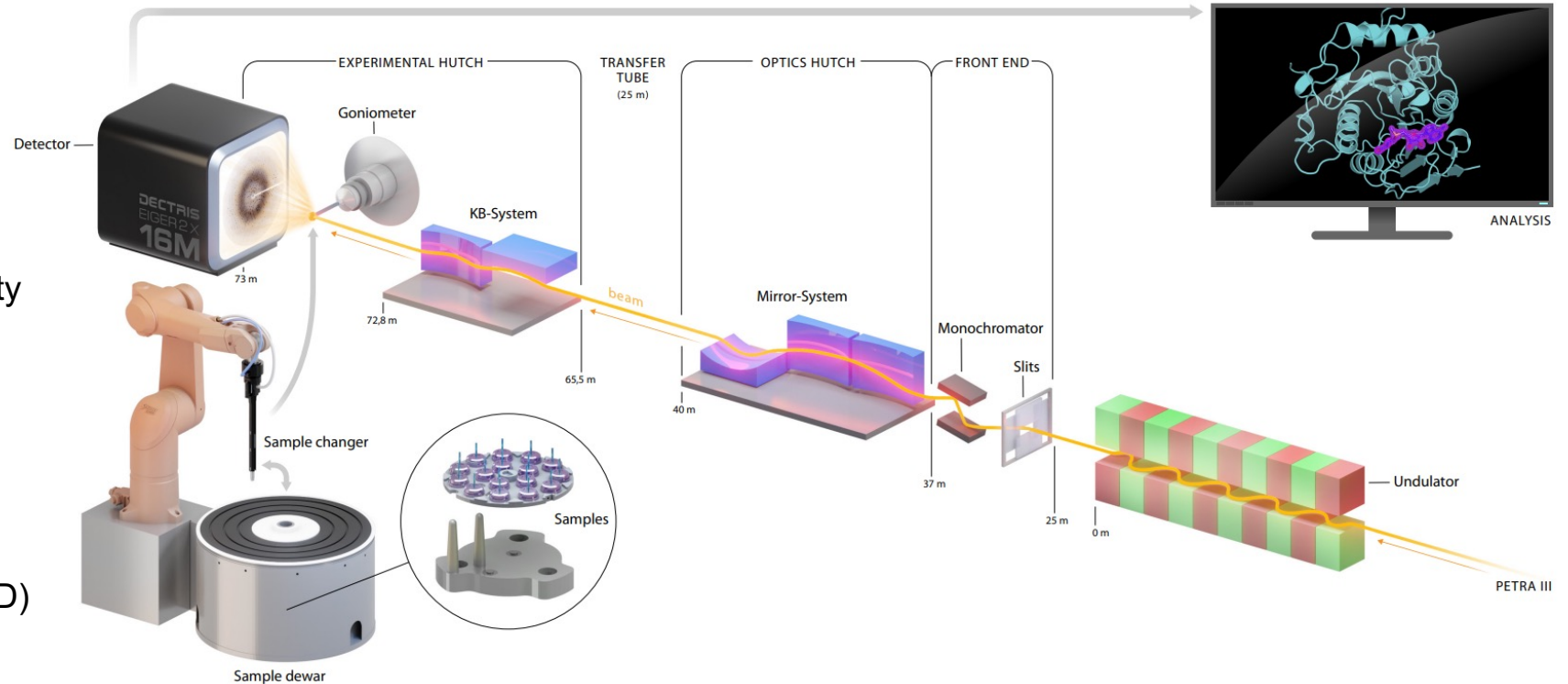
- P12 – bio-SAXS
- P13 - MX
- P14 – MX, imaging, TREXX
- SPC-facility HTX and characterisation



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 $120^\circ/s$
- Eiger2 X 16M
- XRF for experimental phasing (SAD/MAD) and element analysis
- **Currently in-house developed control software (Tango/Tine + Qt front-end) moving to the MXCuBE**



Current status and challenges

December 2023

Deployment Strategy:

- Internal GitHub CI/CD pipeline (as soon as stable version is achieved).
 - Workflow:
 - Check-out latest dev branch (core/qt) -> Debugging.
 - Move to p11_master/stable for user operation.
 - Develop in p11_develop -> Test -> PR to p11_stable.
 - Scheduled Wednesday deployment (shared FS) after complete merging and update.

PR #800 P11 develop (mxcube_core):

- Finishing upgrading and integrating the latest code into the develop branch (Thanks for the comments!)
- Ongoing issues with refactored queue? (acq_parameters.osc_start etc are lost on the way...)
- Sporadic recursion error probably in **TangoMotor.py** <- **AbstractMotor.py**?

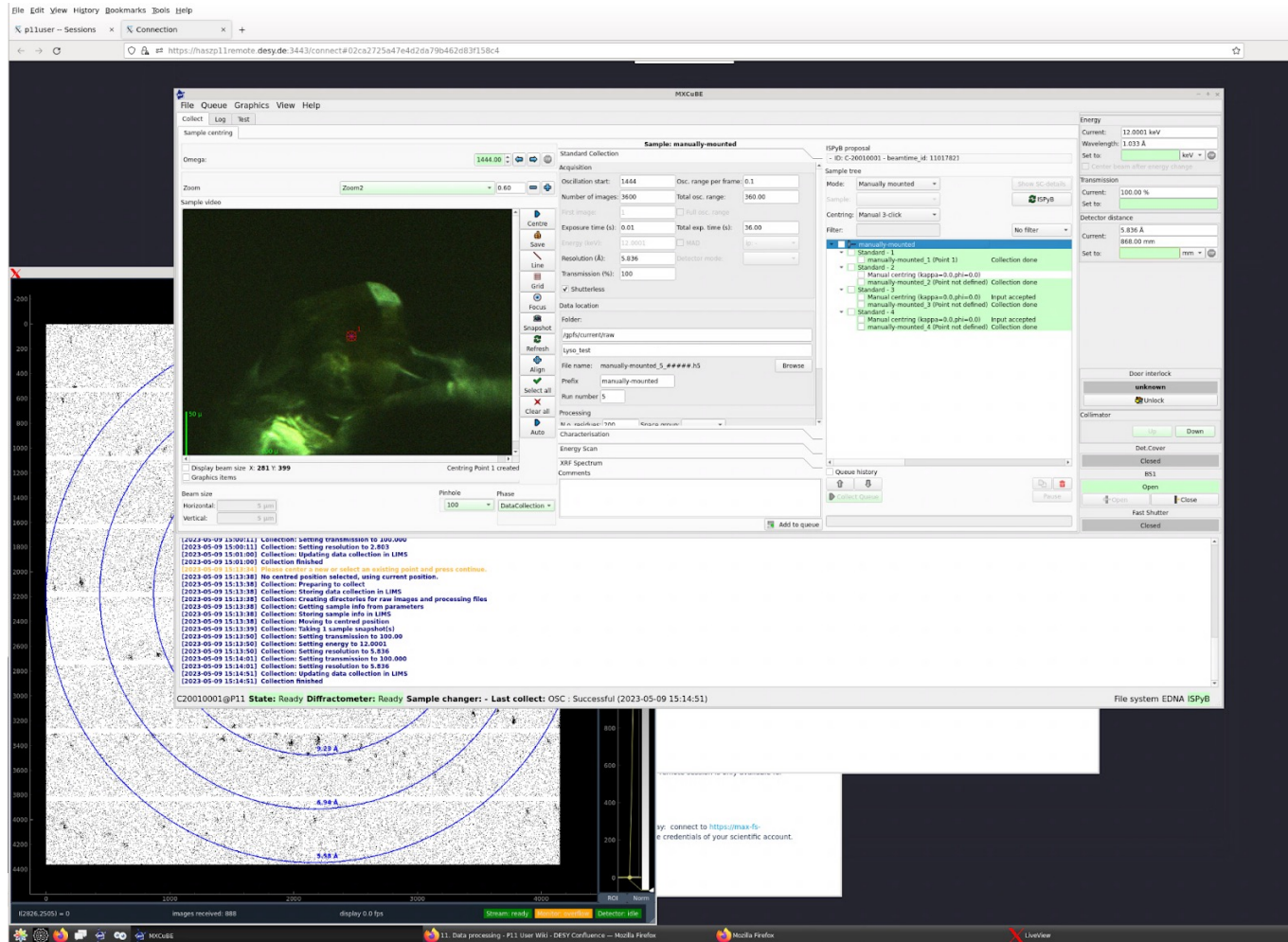
Updates:

- PyQt licence is purchased
- **mxcube_core**: PR #780, #782 , #790
- **mxcubeqt**: PR #452

System info:

- Python 3.7.3 on Linux
- Qt 5.15.2 – PyQt5 5.15.9
- Matplotlib 3.4.3

MXCuBE at P11



- **MXCuBE Upgrade:** Pending upgrade for enhanced functionality.
- **EDNA Characterization:** Implemented basic functionality (G. Bourenkov)
- **AI-Centric Approach:** Exploring AI-based beamline centering (M. Savko)
- **Tech Upgrades:** Considering Python 3.8+ and Qt updates

Acknowledgements



P11 Staff

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P11 Users

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MXCuBE

collaboration

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