

Current developments and future perspectives of beamline control environment MXCuBE Qt

Ivars Karpics
EMBL Hamburg

Content

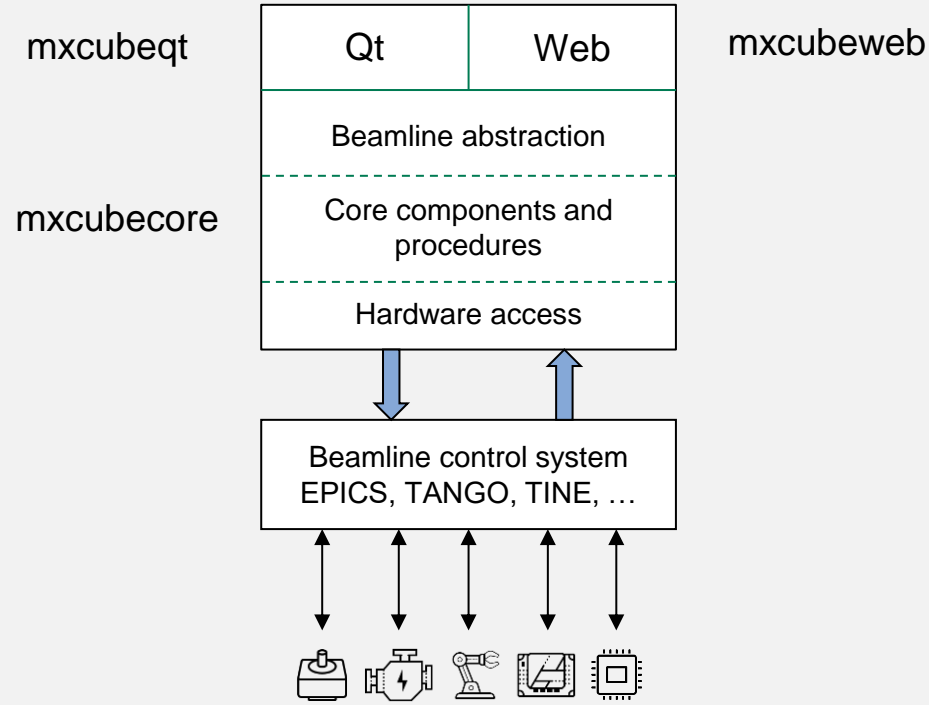
- MXCuBE collaboration
- European Molecular Biology Laboratory and MX beamlines
- MXCuBE Qt frontend
- Future perspectives

MXCuBE collaboration

- Initially developed by ESRF
- Currently supported by 8 members
- More than 20 beamlines currently uses MXCuBE
- Several prospective members
- Steering, scientific and developers committees
- Monthly developers meetings
- Two full committee meetings per year

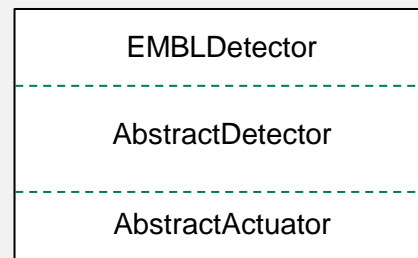
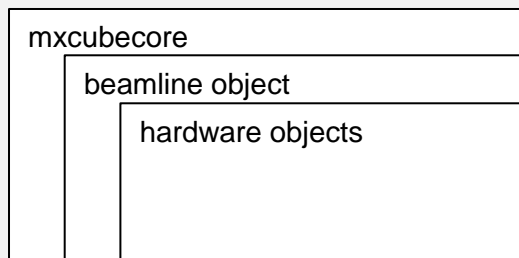


MXCuBE structure



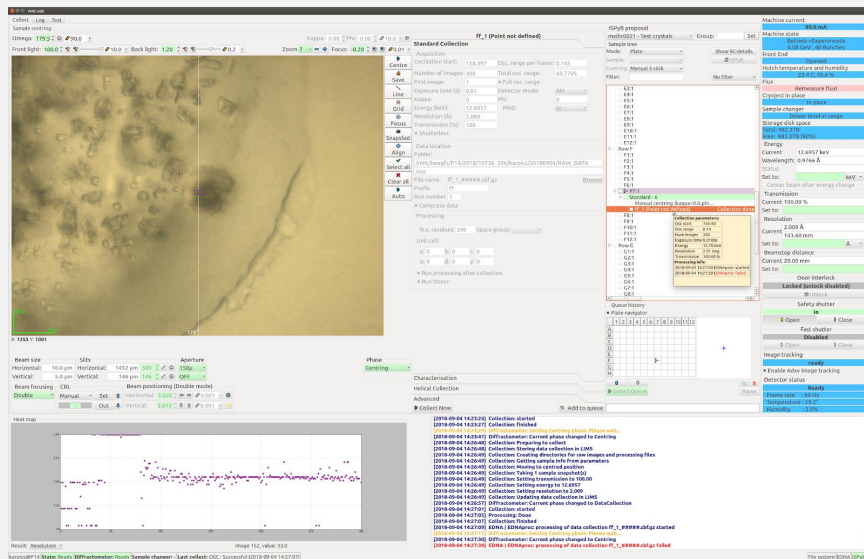
MXCuBE core

- Individual configurable python classes defines beamline equipment and procedures.
- Beamline object defines basic set of python objects and provides an unified api to the gui.
- Default values and limits of data collection parameters defined via “beamline” configuration.
- Abstract classes forces to implement methods required by api.
- Extensive set of mockup classes.
- Functional tests and continues integration.

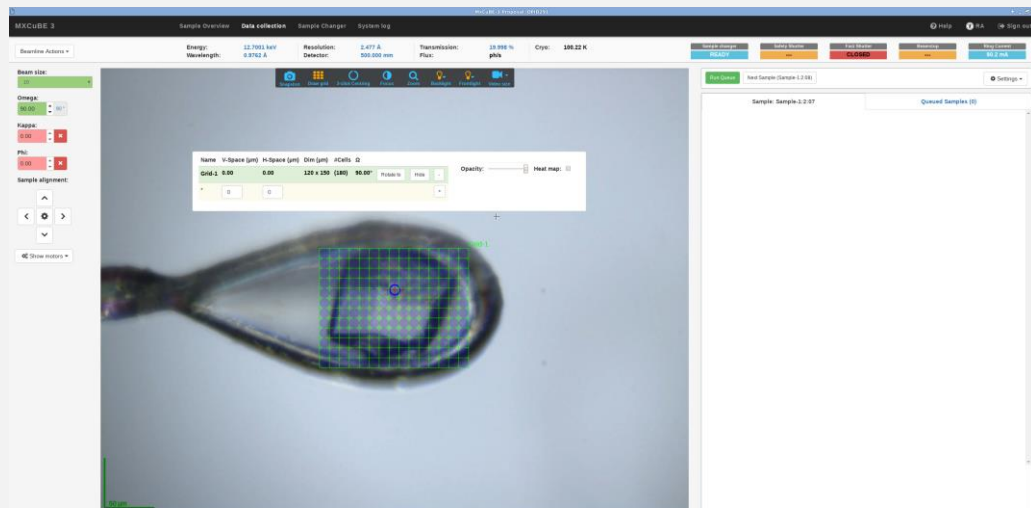


MXCuBE frontend

Qt

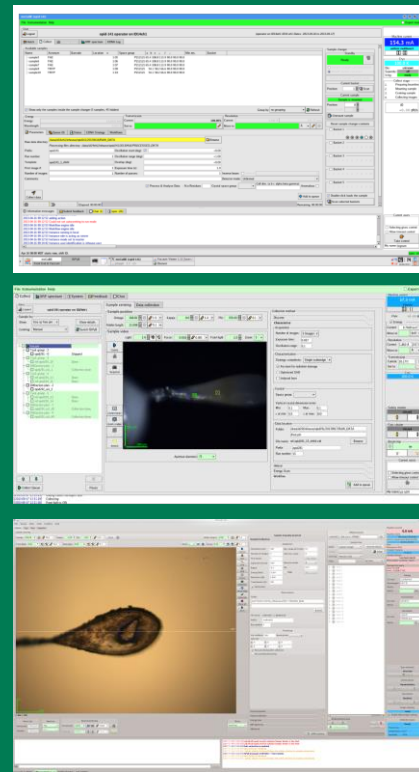


Web

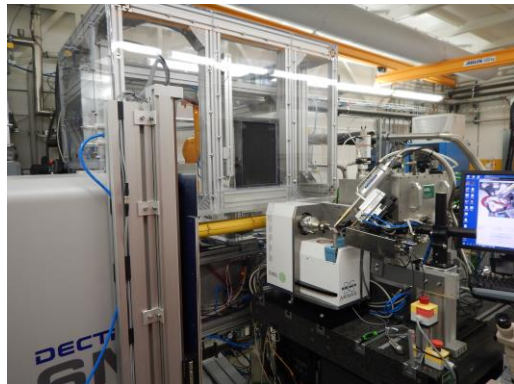


MXCuBE Qt

- 2005 - Python Qt3 based on the BlissFramework (internal ESRF development)
- 2012 - introducing gevent
- 2012 - MXCuBE 2: abstract and mockup classes, sample live view
- 2014 - Porting to Qt4/5, PySide
- 2015 - Qt4 version deployed at EMBL-HH
- 2016 - No Qt3 support.
- 2018 - repository clean up and python3 support
- 2019 - api, unit tests and continuous integration
- 2020 - project refactoring
- 2021 - mxcubecore, mxcubeqt and mxcubeweb

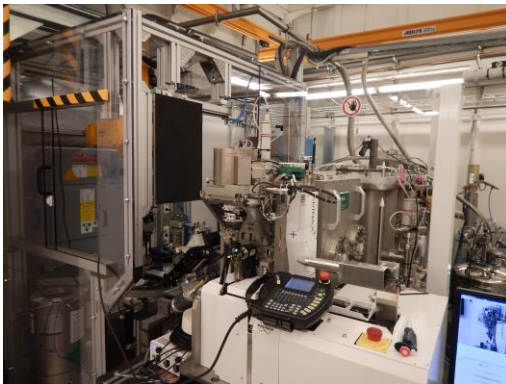


MX beamlines at EMBL Hamburg



P13

- Variable beam size and high flux
- Tunable energy between 4.5 and 17.5 KeV
- MD2 diffractometer (Arinax)
- Pilatus6MF (Dectris)
- Marvin sample changer (EMBL Hamburg)



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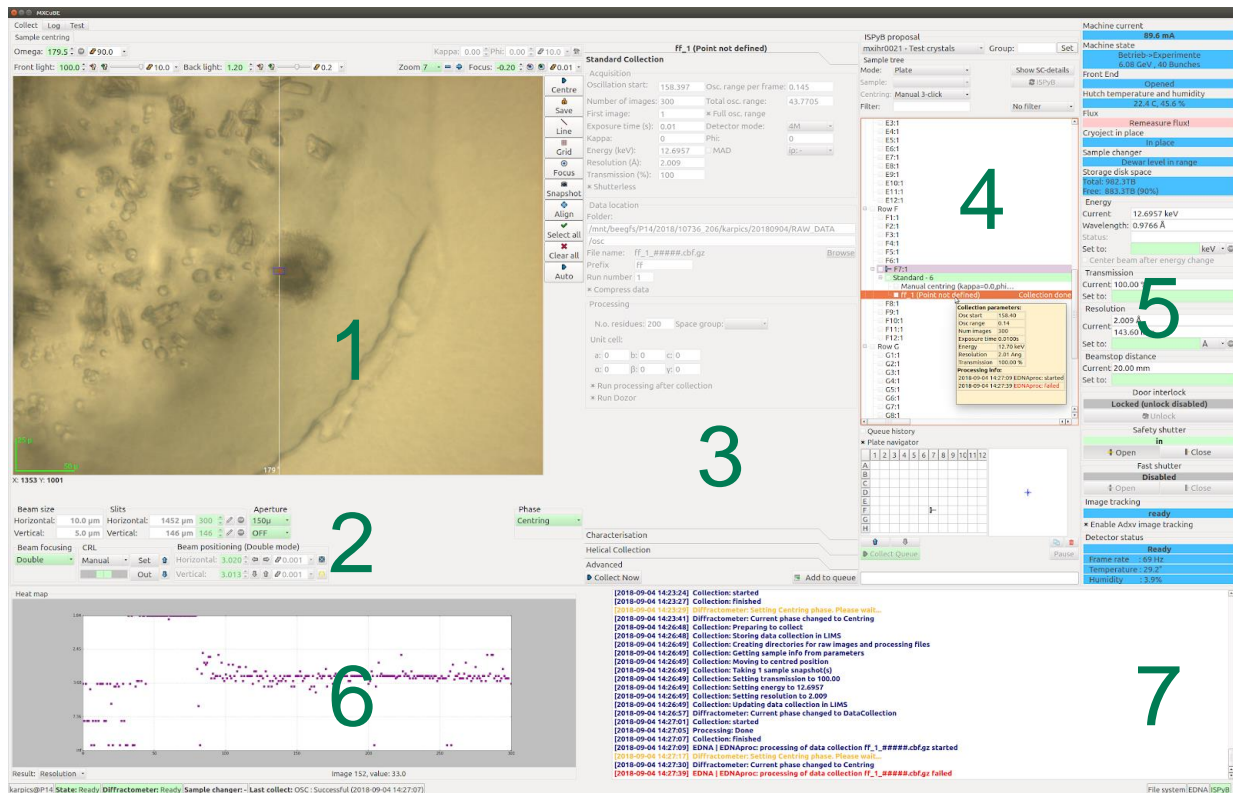
- Micro-beam conditions with 5 x 5 micron beam
- Tunable energy and CRLs (ESRF/CINEL)
- MD3 diffractometer (Arinax)
- Eiger16M (Dectris)
- Marvin sample changer (EMBL Hamburg) and plate scanning



PE2 TREXX

- Time resolved pump/probe experiments
- Beam shaping unit (Arinax)
- Compound reflective lenses CRLs
- Eiger4M (Dectris)

MXCuBE at EMBL Hamburg

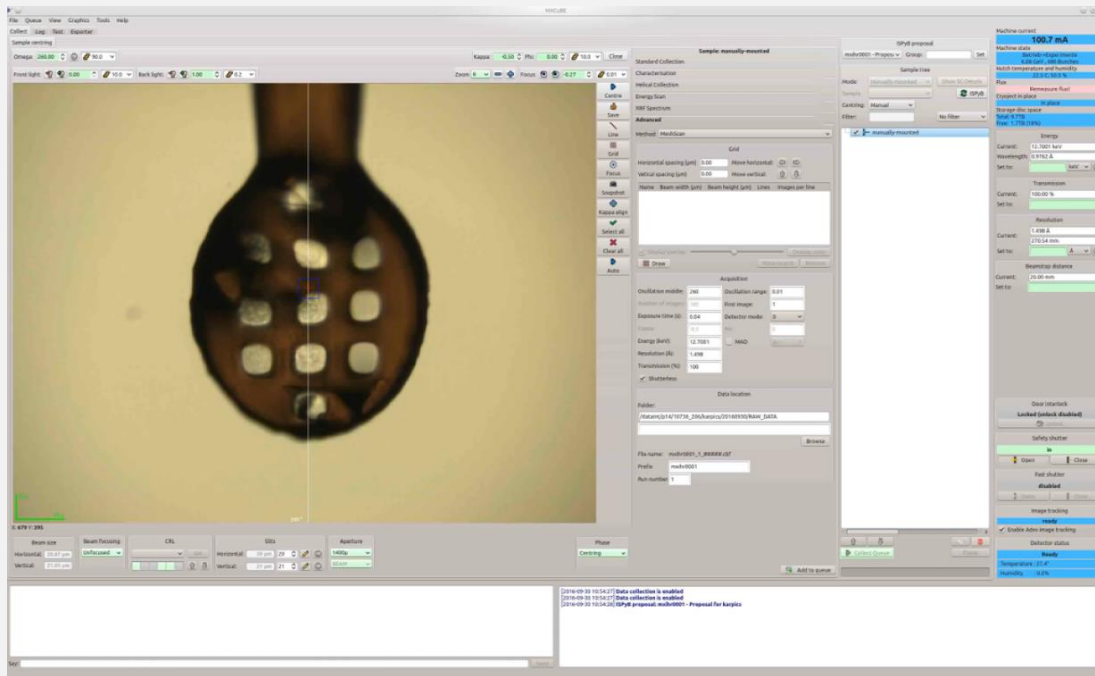


1. Sample view and control
2. Beam characteristics
3. Task menu
4. Queue
5. Beamline control
6. Online processing results
7. Logging

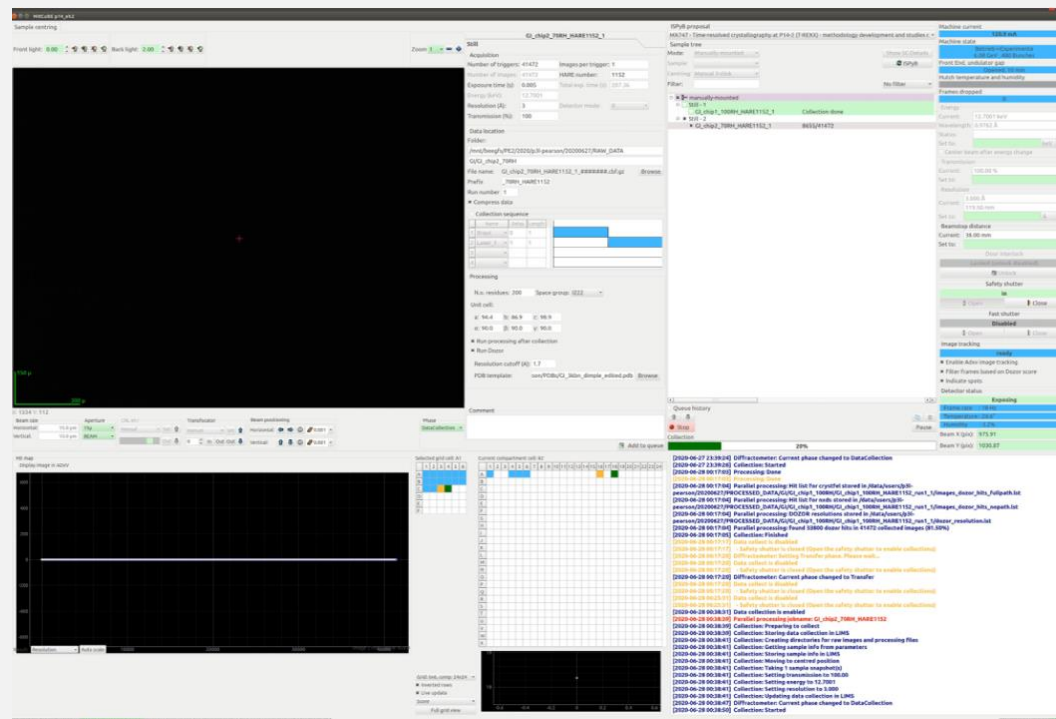
Beam characteristics



Mesh and collect

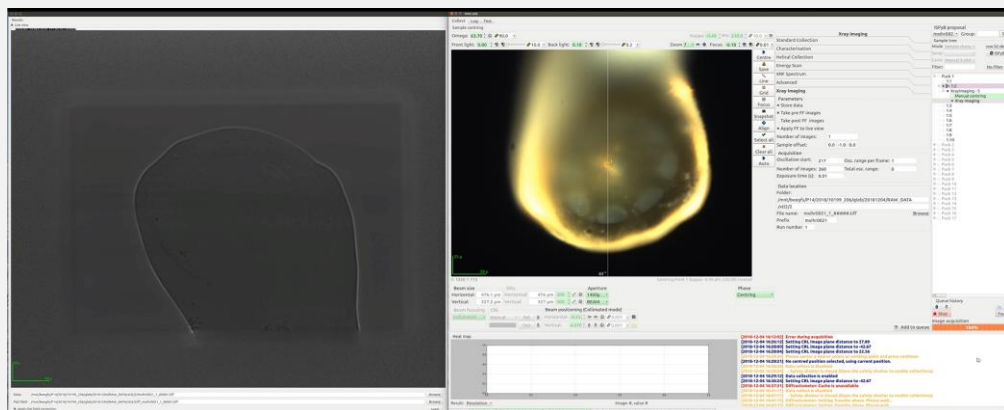
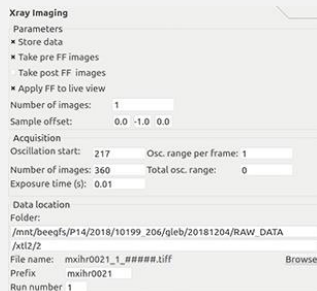
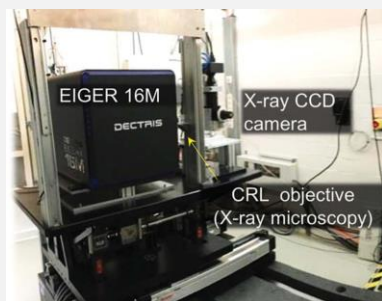


Serial crystallography



von Stetten, D. et al. (2019). Acta Cryst. A75, e26

Phase contrast xray imaging



Polikarpov, M. et al. (2019). Acta Cryst. D75, 947–958

Future perspectives

- DataPublisher
- Extended and configurable queue and tasks
- State persistence and message broker (apache airflow, kafka, redis)
- Not just MX

Thank you for your attention