

MXCuBE site report

Global Phasing

MXCuBE Meeting, Lund, May 2024

Brief beamlines summary

- autoPROC processing software
 - Installed and run post-acquisition at all MXCuBE beamlines
- GΦL acquisition workflow
 - Generation and execution of multi-sweep acquisition strategies
 - Accessible to favoured users at EMBL-P14, MASSIF-1 and SOLEIL
 - Installation and validation in progress at ESRF-ID30B, ALBA-XALOC and BioMAX

- mxcubeqt version with mxcubeqcore, up to date with develop branch
 - mxcubeqweb version with mxcubeqcore, up to date with develop branch
 - Branch for EMBL-P14 maintained separately
 - MASSIF-1 installation of GΦL workflow is interleaved with MXPress workflow and supports fully automatic operation
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Developments since last meeting

- GΦL workflow now uses a generic, JSON-Schema-driven mechanism for user interface queries.
 - The new system now works with the web version as well as the Qt version
 - Thanks to Jean-Baptiste Florial for porting to the web version, and Marcus Oscarsson for extensive help
 - Numerous workflow improvements
 - Better support for ambiguous space group information
 - Support for reference MTZ files
 - Workflow refactored for better maintainability
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Particular contributions

GΦL has done the initial work for converting from using XML-based configuration to YAML-based configuration - which should lead to significant code simplification. This is the basis for the MXCuBE code camp at the end of the meeting.

Plans for the next six months

- Support installation and deployment of GΦL workflow at the ESRF, MAX IV, ALBA, and SOLEIL
- Continue workflow collaboration at EMBL-P14
- Contribute to MXCuBE refactoring