

MXCuBE Developer's Meeting

Whereby, September 11, 2025

Meeting Minutes

Participants

Marcus Oscarsson, Antonia Beteva, Yan Walesch, Daniele de Sanctis (ERSF)

Fabien Coronis, Dominika Trojanowska Matheus Luis, Elmir Yagudin (MAX IV)

Rasmus Fogh. (Global Phasing)

Lais do Carmo (ESS)

Michael Helling (BESSY)

Daniel Eriksson (ANSTO)

Cyber security

MO reports that the cyber security audit at the ESRF has started. It will be possible to share selected results in a closed circle of MXCuBE members. A new programmer, 'Matthis Loussert', a university 'work experience' student has started on a one-year job and will try to produce cyber security guidelines.

MJPEG streamer

The ESRF are introducing a new MJPEG streamer hardware object. They are proposing to switch over completely to this HWO in the future, and remove previous video streamers from mxcubecore. This will require talking to the people using MXCuBEQt. ANSTO suggests that this change-over should work.

Configuration repository

A discussion on how to handle configuration data in a repository raised a number of different opinions. There are several use cases:

- One set is needed to run integration tests; these have to be test-specific, and are best kept together with the repository they are testing (mxcubeweb).

- Another use case is for configuration to run MXCuBE in mock mode, separate from synchrotrons; this should probably be public, and it would be preferable that the configuration of the mxcube core mock hardware objects were kept in a single location rather than being duplicated.
- Another use case is for configuration examples and templates, which it would be good to have for e.g. the abstract classes. This need could be catered for in different ways later: Pydantic configuration of configuration parameters would serve for documentation, and example data could be given in the doc string of the class in question
- Yet another would be for sharing actual configuration data, as examples and to promote idea sharing; these would probably have to be kept in a private repository.

It was agreed that for the moment there could be a public repository for configuration data, separate from the configuration data used for testing, and that the need for a private repository could be addressed later, if required. The question will likely need to be addressed again later.

Abstract Diffractometer

AB reported that work on the AbstractDiffractometer was now progressing, and a PR could be expected soon. This would go together with some refactoring moving actions between hardware objects. There would be one breaking change, renaming the phi motor to omega.

Pydantic configuration files

The question was raised where and how Pydantic definitions for configuration should be stored. One proposal was to store them in the class they are configuring. This would be complicated by the fact that you might want to have separate configuration in superclasses (including abstract classes) and their subclasses. One proposal was to have the subclass Pydantic be a subclass of the superclass Pydantic.

As a separate issue it was requested to upgrade from Pydantic 1. to Pydantic 2. This was accepted, as there was no longer any dependencies that required Pydantic 1.

Change log and releases

A proposal by Matheus Luis to start maintaining a detailed change log triggered a long discussion. The underlying reason was that it was hard to know what a change might affect, and generally the underlying structure of the (quite complex) MXCuBE. ML was in favour of having entries in the change log also for small fixes. Others felt that this would be too much like duplicating the git commit messages, and that it would be too onerous for programmers. Another opinion was that the change log should be limited to breaking changes, and/or that better documentation might achieve some of the same results. It was proposed that PRs with breaking changes might be enough, possibly if backed up by a git label like 'Breaking'.

A proposal to limit the change log to ‘releases and milestones’ led to a discussion of how releases should be defined and used. Releases would (apart from being specially marked) be specially tested and validated, and be the code versions you used in installation. Currently MXCuBE is not actually doing releases, in spite of the point having been discussed before in connection with repository procedures. MO noted that dealing with releases would be *additional* work on top of what was already being done, and worried about breaking a good working culture. ESRF currently pulls and merges to the develop branch every two weeks, whereas MAX IV does it every two months. It was argued that in the absence of a strategy for using releases, these releases did not make much sense. Working with releases in the normal way would require having multiple parallel branches, another thing that is currently not done.

In the end the consensus seemed to be to log only breaking changes, possibly with a link to the relevant PR, but it was not clear if this was an action point or who should action it.

Next MXCuBE / ISPyB meeting

The meeting will be on 17-19 November 2025, at Diamond, with the ISPyB meeting beginning at lunchtime on the 17th, The 18th for scientific talks, and the 19th for the MXCuBE meeting. . As this has not yet been officially announced, RF promises to send out an interim announcement ASAP (DONE).

Any Other Business

HDF5 files

RF raised the question of beamlines being able to handle HDF5 files correctly,. With the newest detectors it is becoming prohibitively difficult to convert data to .cbf format, and hdf5 files were mostly not working correctly in two cases 1) when doing short non-consecutive wedges in a single scan, as used in e.g. GPhL characterisation, 2) with any form of interleaving. For 1) there is a known fix (courtesy of Martin Savko), which would need to be integrated at beamlines. For 2) the problem is that e.g. wavelengths are not correctly stored within HDF5; there is no agreement on what would be the appropriate way of dealing with this (virtual data sets were mentioned) or who should be doing the work.