

# MXCuBE Developer's Meeting

Whereby, February 6, 2025

## Meeting Minutes

### Participants

Marcus Oscarsson, Antonia Beteva, Yan Walesch, Jean-Baptiste Florial, Didier Nurizzo(ERSF)  
Andrey Gruzinov (DESY)

Elmir Yagudin, Fabien Coronis, Dominika Trojanowska Ana Gonzalez (MAX IV)

Nicola Demitri (Elettra)

Dan Costin (SOLEIL)

Rasmus Fogh, Gerard Bricogne, Peter Keller (Global Phasing)

Nicolas Moliterro (LNLS)

Lais do Carmo (ESS)

Michael Hellimg (BESSY)

Pedro Benetton

### HDF5 files

GB gave an introduction to the problem. HDF5 files as normally used do not support either interleaved data collection or multi-trigger acquisition. There is a built-in assumption that images are a single linear sequence, acquired in order, and with image numbers proportional to the omega position, which is not the case in these instances. The problem does not appear with mini-cbf files, but with high-data-rate detectors coming up more sites (like e.g. Massif-1) can be expected to switch over to HDF5-only. As an example GB referred to a test dataset acquired on ID30B which had ended up with incorrect omega values. This is a problem that will hit the use of multi-trigger acquisition (used e.g. things for multi-wedge characterisation sequences, among others by GPhL), and interleaved data collection (used mostly for phasing experiments, but that is still an important technique in a number of applications).

There is some interest in this field, Graeme Winter has reopened a discussion in HDRMX formats, and Dectris is also involved though some of the key people have been quite busy lately. A consensus initiative from MXCuBE would be very useful to carry things forward.

It was agreed that this was an important and timely topic, but too big to take up at this meeting, and people were encouraged to contribute all relevant information to the discussion at <https://github.com/mxcube/mxcubecore/discussions/1130>

## Code review

The situation around merging and code reviews was discussed. The process currently does work, but relies excessively on a few people to do the merging. One problem is that not all relevant people can merge (e.g. contractors). Current rules say that before merging there should be two reviews, at least one from a different institution, but that the originator can merge himself after two weeks of inaction. It was reiterated that code review was good and necessary, even for site-specific code to ensure consistency and promote best practices, and that we should keep up with the principle that merging required review from a different site. People were encouraged to do more merging, both of their own PRs (once reviewed) and other people's.

## Python 3.8

Python 3.8 is EndOfLife, and Python 3.9 will be so this year, so all agree that support for these versions should be dropped when practical. The critical point is which sites are using these old python versions *\*while following the develop version\** (e.g. EMBL-Hamburg is using a very old MXCuBE so its Python version is not relevant). Pre-commit testing currently tests Python 3.8 (as it should) but that could be changed. Elettra (ND) are using Python 3.9 with the October MXCuBE version, but believes that this could be changed. It is agreed to remove support for Pythons 3.8 and 3.9 (unless someone objects), and to support Pythons 3.10-3.12, while raising an issue to investigate what it would take to support Python 3.13.

## XML- YAML conversion

EY has tested the yaml configuration branch earlier, and ESRF (AB) has rebased on the YAML branch before Christmas and tested the result. AB reported that she was happy with the architecture of the new branch, in particular also with the automatic generation of new yaml configuration files from the older xml files. It should be noted that this is a breaking change; it is necessary to initialise all role attributes in the code, and to avoid deprecated functions, also in abstract classes. There were also some specific points on properties that were really objects (like beam definers) that needed cleaning up, and the hardware object name would need explicit definition as a parameter in some places. The `get_object_by_role` function was found to be very useful and AB wanted it to be preserved, for ease of transition and the greater flexibility it offered. RF opined that this function left a hole where the goals of having well-defined attributes and documentation for what was supported could not be met. After some discussion on the point, it was agreed that

- We should now merge the `xml_to_yaml` branch into `develop`
- We should keep `get_object_by_role` for now, for ease of transition
- We should be tightening up the code in connection with the more widespread introduction of Pydantic definitions, with a view to eventually retire `get_object_by_role`.

- We should *not* make a separate branch for the yaml-configured code but stay in develop, but should up the major version at some point in the transition since this is a breaking change.
- We should standardise file names to use ‘.yaml’ as the file suffix.

## Reports from working groups

The automation working group is actively working, and is asking people to put information about their X-ray centring set-up on <https://github.com/mxcube/mxcubecore/discussions/1105>

Other working groups are not yet fully active, and some might benefit from being merged. It was proposed to volunteer Martin Savko (not present) for the ‘Centring and Sample’ working group.

## Any Other Business

Ideas:

- Make and distribute dockers for ICAT/ISPyB LIMS to use as mock instances for testing.
- Start using an automated testing tool for testing the UI (YW).