

MXCuBE Developer's Meeting

Whereby, March 14, 2025

Meeting Minutes

Participants

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

Fabien Coronis, Dominika Trojanowska (MAX IV)

Martin Savko, Dan Costin (SOLEIL)

Rasmus Fogh. (Global Phasing)

Lais do Carmo (ESS)

Michael Helling (BESSY)

Pedro Benetton, Pawel Mochio, zrid29, Ezequiel Panepucci, Alessandro Bocciarelli

HDF5 files

It was agreed that this was an important problem. Taking the matter further would require a meeting of all relevant parties, which should include also people involved in processing and probably also Dectris. It was suggested that Global Phasing, who have the widest contact surface and who raised the problem in the first place, should organise such a meeting.

Code camp

Topics were invited for the code camp attached to the May MXCuBE/ISPyB meeting. AG suggested a code cleanup, and all agreed. It was agreed that people should start cleaning up their specific code as homework before the meeting, with common code and more complex decisions to be handled at the code camp. The meeting agreed to RF's suggestion that the configuration files that are checked in as part of the mxcubecore repository also needed revisiting. They are useful as examples and for information on e.g. local goniostats, but they are out of date and not in actual use in this form.

There was some discussion about the introduction of Ruff, with some participants being a little surprised at the speed with which more and new rules were being enforced. It was pointed out that the use of Google doc strings were an old agreement, even if the energetic enforcement of same was

relatively new. Everybody backed up behind the continued use of ruff, and no changes to current procedures were agreed.

Python versions

The lowest supported version is now 3.10. It was proposed to make a PR for adding support to Python 3.12, but AB pointed out that PyTango is still limited to max version 3.11

XML- YAML conversion

The yaml configuration version is ready and checked, with functions needed for ease of change-over still left in. MO promised to rebase the branch so it could be merged.

Reports from working groups

The automation working group is orking on X-ray centring, and renewed the call for adding information on current procedures to the relevant github discussion before the WG meeting on 14/3.

Other working groups are not yet fully active, and some might benefit from being merged. Martin Savko provisionally accepted to eb the chair of the ‘Centring and Sample’ working group.

Any Other Business

Ezequiel Panepucci (Zac) introduced himself as a new member of MAX IV, having moved from the SLS.

There were problems with starting up the mxcube whereby meeting, with the room owner (which is who?) having to let people in, so the meeting had to be held on Zoom. RF promised that GphL would look into ownership and permissions.

Gleb Bourenkov reported being unable to mail to the mxcube mailing list, so his input had to be given through AG. The mailing list has recently become closed because of increasing spam, so Gleb’s problem was likely from trying to mail from the wrong email address.

All participants were urged to go through issues and PRs and clean up anything now out of date.