

# MXCuBE developers' meeting

## 6 October 2021

### Participants:

- Marcus Oscarsson, Antonia Beteva (ESRF)
- Rasmus Fogh (Global Phasing)
- Ivars Karpics, (EMBL Hamburg)
- Michael Hellmig (HZB)
- Martin Savko (SOLEIL)
- Lais do Carmo (LNLS)

Minutes: Rasmus

### Site status

None volunteered

### PR guidelines and repository workflow

The guidelines proposed by Jordi Andreu are still viewed very positively, but no one had had time to try out the test installation, and JA was not present at the meeting. The point was postponed to a future meeting.

### Outstanding issues and PRs

- #640 [Wavelength dependence for AbstractResolution functions](#)

Accepted for progression to PR and merging.

It was noted that this issue had remained uncommented for over a month, which is an argument in favour of accepting it. A proposal to introduce a minimum wait for API-changing PRs before they could be accepted was rejected as too bureaucratic. Instead we shall keep to the rule that API-changing PRs must be passed by the developers' meeting, and we would count on the meeting not rushing through proposals before all interested parties had had a chance to give input.

It was agreed to introduce a new repository label, 'API change', to highlight API-changing proposals.

- #630 [mxcubecore module, python path and import](#)

It was agreed that runtime changes to the Python path could and should be avoided. Also site-specific code should be added to the common repository under e.g. HardwareObjects/ESRF/, so that they could be imported using the standard Python path.

If necessary we can always change over to a more complex system later.

It was noted that configuration files already have a functioning system for setting up lookup paths, in both Qt and web versions.

ACTION: RF to check for remaining path modifications and propose necessary fixes.

- #641 [Merge ExporterZoom HO and MicrodiffZoom HO](#)

The meeting agreed to proceed with the proposed changes. ACTION: AB

- #635 [\\_collect in AbstractCollect](#)

The outstanding question remaining in the discussion of this (by MO) was whether the specific issue raised by Bernard Lavault had been resolved – which it had. RF raised an additional question about further reorganisation / consolidation of AbstractCollect. The situation is that the master AbstractCollect has been reverted from a more refactored state (which did not work), and the current version is in production use at P14. There is still a fair amount of refactoring outstanding, but this is a major task and is connected to finalising abstract procedures. Meanwhile there are no immediate changes to be made.

- PR #633 (connected to issue #628). [Add sample\\_environment to the beamline properties.](#)

The idea of the PR is to add an object SampleEnvironment to the beamline, to serve simply as a container for objects like sample temperature, pressure, humidity. Since the SampleEnvironment object is in itself empty, there is no need for an AbstractSampleEnvironment, only for SampleEnvironment. MO noted (correctly) that it would be simpler to add these objects directly to the beamline, but meeting preferred to accept the PR in order to get a less cluttered and more logical organisation.

ACTION: MO to make merge.

## Release for mxcubecore

Point postponed to a future meeting after minimal discussion.

## Any Other Business

### Automatic Centring

RF raised a question about availability and calling interface for X-ray and other automatic centring at different beamlines.

There are three sites that support automatic centring: EMBL-HH and ESRF (X-ray centring) and SOLEIL (optical centring). Of these EMBL-HH uses the XrayCentringQueueEntry and the normal queue mechanism, ESRF uses calls to an external workflow, and SOLEIL also uses an external mechanism. Only at P14 is automatic centring integrated in the queuing system. It was agreed that in the longer term automatic centring should be accessible via QueueEntries and the queuing system, but it would clearly require a certain amount of work to make this happen even at the sites that have automatic centring available.

### Upcoming ISPyB/MXCuBE meeting

The next ISPyB/MXCuBE meeting will be organised by Elettra for October 26 and 27.

It was discussed whether to organise a 'status of MXCuBE' talk, but agreed to wait till a future meeting after the first mxcubecore release. Three people announced the intention of giving a talk:

- ☺ Martin Savko on automatic centring
- ☺ Rasmus Fogh on implementation of experimental strategies and workflows.
- ☺ Marcus Oscarsson on Braggy (which is now production ready) and possibly also the status of MXCuBE3

### Contacts to Australia and Ophid/BlueSky

The Australian synchrotron has shown interest in MXCuBE and possible connections with their own Ophid and BlueSky software. Ophid is a hardware abstraction layer, which is spreading rapidly in the EPICS world. It has a role similar to our HardwareObjects / mxcubecore. From later emails it is noted that the Australians are studying the MXCuBE documentation, and would like a (virtual) meeting as soon as this has progressed.

### Next Meeting

The next developers' meeting was not discussed, as we shall meet at the ISPyB/MXCuBE meeting.