

MXCuBE web meeting 8 Sep. 2020

DRAFT

Participants:

- Marcus Oscarsson, Antonia Beteva (ESRF)
- Rasmus Fogh (GPhL)
- Martin Savko, (SOLEIL)
- Roberto Borghese (Elettra)
- Jan Meyer, ((DESY).
- Ivars Karpics (EMBL Hamburg)
- Jordi Andreu (ALBA).

Apologies:

Lais do Carmo (LNLS)

Status reports

DESY It has now become possible to hire Vicente to work on MXCuBE for DESY. He has worked on bringing the DESY installation up to the level of the master branch, and in two more weeks should have got close enough that JM can take over. DESY is running the Qt MXCuBE version.

GPhL has done a lot of work on refactoring over the past year and will continue, but is looking forward to things settling. Current plans concentrate on getting acquisition strategy code to the point where it can be used in anger by third parties, working most closely with EMBL Hamburg and ALBA where the work is furthest along. The MXCuBE web version will be next on the agenda.

EMBL Hamburg. Lately most work has been on ISPyB (but including a connection to MXCuBE). In addition, IK has made a first working installation of the master branch for P13, which is at the point of at least starting collection. A PR incorporating fixes and enhancements arising from this is expected for this week. It is noticed that the new PyISPyB will not be able to support the old ISPyB GUI.

ALBA has been working on a major upgrade of the entire ALBA installation, including lower levels, OS of control computer and installation of B-Zoom. This work will be ready for release at the end of next week. The new version will allow upgrading to Python 3. ALBA uses Conda for installation management. The next job will be incorporating Sardana scans into the MXCuBE layer.

Coming up is the start of the Xaira serial crystallography beamline, and help or starting points in setting up MXCuBE for this would be appreciated.

New hardware is also coming up, which will need software support. Of particular interest is a new goniostat, produced in-house as no commercial company could meet the required specs. The goniostat is a mini-kappa, sitting entirely inside a helium chamber (with the

sample changer outside), with a very small sphere of confusion, meant for use with small crystals.

ELETTRA is looking at starting to use automatic centring and asking for advice. One suggestion is to use Lucid 3, which is in use at ESRF and maintained by OS. There are some new fixes from ESRF that will be merged in RSN, and apparently a very effective debug mode that saves all images. MO also mentions a native raster scan capability in MXCuBE 3.

SOLEIL In answer to the question from ELETTRA, MS suggests trying out his optical auto-centring software, and both RB and MO show interest. The code is available on github, as a small part of a huge repository. It has been greatly cleaned up, but MS plans to clean it still further, separate it out as a separate module, and give it a name. The calling interface is not identical to that of Lucid 3, but MS is planning on making it so. The program still does not use training (next step). It is now very robust and can function also from single images and no longer needs to loop over multiple omega values. The program is pure Python, with SKimages (?) as the main external dependency.

Martin Savko has been setting up configuration for installation, using Ubuntu 20.04, and is debugging a version that is close to current master.

ESRF Version 3 has been updated to the latest HardwareRepository and has been running on three beamlines, including ID30B, for a couple of weeks. The next beamlines to be added will be MASSIF 1 and 3. Throughput is comparable to pre-shutdown, with one example of a bag running 150 samples in a single time block (of 18 hours ?). Some teething problems were caught. Operation is fully remote, which may be relaxed in exceptional cases by next year. There is a need for some remote-working enhancements, e.g. showing images directly in MXCuBE.

There is some parallel work on a user interface for an X-ray microscopy beamline using an (MXCuBE-inspired) Qt version.

Jean-Baptiste is working on a BIO-SAXS program 'inspired by' MXCuBE 3.

B-zoom integration is finished. Arinax has provided a full Tango-Lima server to the B-zoom, which is being run under Windows on the beamline control computer.

Pull Requests

#532 Camel-case-to-snake-case. It is confirmed that this PR should be merged in during the next code camp.

#584 Limit handling in Abstract classes (Vicente). AB confirms that AbstractNState objects will have **no** limits checking – limits (if any) will be only for the purpose of showing on display. RF proposes to put implementation of limits checking inside AbstractActuator (as per Vicente's PR), but to distinguish AbstractNState and AbstractActuator behaviour by overriding functions rather than by a `check_limits` attribute. It is agreed to check in a bug fix that will make PR #576 work (ACTION: RF to send proposal to MO, who then solves the matter), and to raise an issue to handle discussion of further refactoring.

Any other business

- RF asks whether .yml configuration is still seen as desirable (long-term) since even the beamline uses xml configuration in the branches he sees. It is settled that
 1. move from xml to yml configuration will be slow and gradual
 2. Beamline should use .yml configuration, and indeed does so already in the newest branches.
 3. It is agreed that it would be good to refactor away getHardwareObject, getObjects and other functions that rely on the HO name (i.e. file name) as opposed to the role. RF puts this on his TODO list (ACTION RF)
- MO proposes to (eventually) make HardwareRepository into a proper Python module with its own install script. This would require moving the directory down one level in the directory tree, and removing the sys.path manipulations currently used for import handling. RF enthusiastically backs the proposal.
- AB now needs to have AbstractProcedure and has been writing some relevant code. She will raise an issue on the topic shortly.

Next Meetings

- The next meeting will be a code camp, not just a meeting. MO will set up a Doodle poll for Mid-October, and organise the meeting.
- Depending on how work goes with open issues a meeting between interested developers may be organised around the last week of September.