MXCuBE web meeting 19 Sep. 2019

Participants:

- Jordi Andreu, (ALBA)
- Ivars Karpics,(EMBL-HH)
- Marcus Oscarsson, (ESRF)
- Rasmus Fogh, Peter Keller, Gerard Bricogne (GPhL)
- Martin Savko, (Soleil)
- Lais do Carno (LNLS)
- Michael Hellmig (HZB)

Apologies:

Roberto Borghese (Elettra)

Status reports

SOLEIL MS is working on bringing his installation up to the current master. It should take three weeks more to get to the point where the ongoing pull requests can be validated in real life. MS has added a dose display in the main MXCuBE GUI, based on running RadDose3D, but without the capacity to calculate contributions form heavy metals. RF proposes to compare notes with the dose calculations in the GphL user interface code.

ESRF: Has upgraded to the master version on ID30B, which runs as before (though there is no beam to test with at the moment). There are a few issues still to test. Working on integrating a plate interface, with Jean Baptiste. The plan is to get the latest version of MXCuBE 3 installed by January, however the shutdown ends in August, so that's when ESRF will take first users. The plan is to have everything running for March when ESRF gets beam to the experimental hutches. In house test usage might start in May depending on how things goes before that.

LNLS is migrating from MXCuBE 2 to 3, rebasing code, and working on their control system The new system is well liked, and all changes are available on github. LNLS is using the HardwareRepository repository and MXDocker, and generally using dockers for their implementation. Review of detector code is in progress and will be put on github. Shutdown was last month and work is fully focused on the new synchrotron, SIRIUS, starting with MX.The second beamline to start will be SAXS, and LNLS is interested in integrating SAXS in MXCuBE, also reusing some equipment. LNLS will be coming to the Berlin meting. MO points out that ESRF has done a lot of work on BioSAXSCube, and proposes that the two sides should discuss synergies and collaboration.

EMBL-HH Do not have much to report. Work has been going on on the second beamline hutch, for serial crystallography, with GUIs for processing results and control of the sample holder chip. In plotting IK has introduced PyQtGraph as a (much faster) replacement for

matplotlib. When asked, IK says that it should be fairly simple to use PyQtGraph also for energy scans.
There has been improvements on the Crysfel pipeline; all data are being added to ISPyB.
A student is working on ACElab (?) integration.
There are data processing facilities missing in MXCuBE, and IK hopes to add something here soon.

ALBA has just restarted after a 6 week shutdown, and is working on integrating the new Arinax on-axis viewer with digital zoom. This should be done before the short shutdown four weeks from date. ALBA is in the middle of a complex upgrade to Debian 9 and Tango 9. The database has been upgraded, and work is in progress on the Tango servers. MXCuBE is run, successfully, in a Conda environment, using Qt4 and Python 2. It is planned to migrate SARDANA also to Python 3. There is no time for refactoring at the moment, but JA will give the code a look. Advance planning is in progress on SSX, also with respect to integration with ISPyB.
MH adds that there will be an SSX session at the Berlin meeting to discuss SSX and its processing.

GPhL: Work is progressing on refining the strategy calculation workflow. Further MXCuBE refactoring is currently awaiting the processing of the (large) BeamlineObject PR.

Refactoring

The main topic is the BeamlineObject PR – which most people think ‘looks sort of OK’, with a ‘sound concept’... MS proposes to wait the three weeks it would take for SOLEIL to be ready to test the PR at the beamline, and in general to hold up the merging till it has been tested at 3 beamlines. After some discussion the meeting however agrees to merge the PR as soon as possible, and to proceed at speed with refactoring, snake_case / CamelCase, cleanup etc. for another month or two, before calling a halt to the high-speed phase and testing all changes together. It is ‘now or never’, and thorough testing is demanding and depends on scarce resources – IK, for instance, has only one day a month for such work. After further discussion it is agreed to **not** make a separate branch for refactoring, but to do the work in the master branch. Specific points:

- Could Beamline hardware objects be implemented as properties after all? It is agreed to check, but shortly after the meeting the main proposer, MO, decides that this is not practical, and to do the merge with module attributes. RF promises to replace the get_beamline calls in the PR with HWR.beamline.
- Is the system of dividing HardwareObjects into categories as a top part of the implementation useful? The general opinion is that it is not, and RF agrees to remove it from the PR.
- It is generally agreed that there is no need for ‘hot-swapping’, i.e. changing hardware objects (and/or their configuration) during an MXCuBE run.

It is agreed that there is no need for joint planning on the next refactoring steps. First the BeamlineObject PR should be cleaned up and merged, and MO will do some refactoring on Python 2→3 and fixing CamelCase in the code. IK and MO agree that there is a need for having an abstract Procedure object, and will try to come up with something. Work on individual abstract HardwareObjects is left to individual initiative, but could well be done

before the Berlin meeting.

Preparations for Berlin meeting

Postponed to a later meeting

Any other business

None

Next Meeting

October 15, at 1400 UK time on whereby.com/mxcube