

MXCuBE Developers meeting, 27/2/20189

Present (virtually): Jordi Andreu, Antonia Beteva, Roberto Borghese, Gerard Bricogne, Mikel Eguraun, Rasmus Fogh. Michael Hellmig, Peter Keller, Marcus Oscarsson, Daniele de Sacntis.
Apologies: Ivars Karpics
Trying but failing to connect: Martin Savko,

1. Minutes of last meeting, and matters arising

The minutes were approved.

2. Agenda

The agenda was approved

3. Status reports

Roberto: Done some bug fixing, and set up characterisation data processing. Mostly stuck as far as MXCuBE development is concerned.

Marcus Oscarsson, Antonia Beteva: All work is on (web)version 3.0, now the shutdown has started, and code is Python-3 compatible. Working on a BIOSAX BCS, and a web-based image viewer (Braggy). AB is making tests on the AbstractDiffractometer HO.

Michael Hellmig: Concentrating on set-up of new fixed energy beamline. Currently using 'really old' MXCuBE version.

Jordi Andreu: Working on version 2.3.0, and has refactored ALBA-specific code to be Python-3 compliant. Will merge into version 3.0 next week. Asks when master version will be ready to start using, and is referred to the Roadmap (late fall 2019).

Mikel Eguraun: Not much happening on MXCuBE lately. Characterisation close to finished. Installing a new fluorescence detector.

Global phasing: Done tests at ALBA and SOLEIL. Done some development in branch 2.3.0, which will be ported to master starting next week.

4. Report to the steering committee

The draft report to the steering committee and the report (by RF) on the UI-API development were accepted as written, except for some discussion on the handling of the UI-API in the draft report. MO and DdeS proposed that the UI-API should be in the roadmap, as a question mark, whereas RF preferred discussing it as a possible future decision without timetabling it for now. GB recommended reporting how the current refactoring has cleared the way for future UI-API work

(which the Steering Committee was keen on). MO notes that Ivars (not present) seems positive to continuing with the UI-API. It is agreed to have discussions about UI-API plans at the Lund meeting, and to limit the current report to reporting this. MO to finalise reports and send them to the Steering Committee.

4. Scheduling of release 3.0.0a

MO proposed making a release 3.0.0 α to incorporate the changes summed up in the first milestone of the road map, more precisely after the Lund meeting. The general idea was positively received, but there was discussion of the details. What did the word 'release' imply, when the code was not in a state to be used in anger? Would the following release, according to semantic versioning, then have to be 4.0.0? What was supposed to be ready by release time, and to remain reliably unchanging after it (or was it unnecessary to spell this out)? Would 'milestone' be a better name? It was agreed to settle on a precise course of action after discussion at the Lund meeting.

5. Lund MXCuBE meeting

ME reported that there were 61 registrations, and that the meeting program was complete for MXCuBE and getting close for ISPyB. The program for the MXCuBE developers meeting was still open; a hands-on test of MXCuBE3 would not take nearly the whole time. Proposed topics were 'Procedures and etiquette for pull requests' (MO), as well as 'Discussion of the roadmap', 'Plans for another face-to-face meeting', and 'Future plans for the UI-API' (arising out of the discussion here). People are requested to email ME, who will put the topics together in an agenda.

6. X-ray centring

RF asked around about X-ray centring capabilities. The specific GPhL need is for fast top-up centring partway through a multisweep data collection, based on an initial calculated centring position. This should be possible to do fast, with only a very small centring grid.

It was reported that the actual scanning was done using firmware embedded in the microdiff. Ivars was not present to account for the Hamburg procedures. At ESRF the X-ray centring is done with a Passerelle workflow, and the scanning grid can 'relatively simply' be set and passed to the X-ray centring routines. At Massif-1 the standard procedure is for rough optical centring of the loop, followed by X-rays for fine centring, which should have similar tolerances to GPhL's problem. Olof Svensson should be contacted for details.

Next Meeting

The date for the next meeting (tentatively: April) would depend on whether and when a longer face-to-face meeting was arranged. The decision is postponed to discussion at the Lund meeting.