MXCuBE Developers' meeting

August 23, 2022

Participants :

Marcus Oscarsson, Antonia Beteva(ESRF)

Gérard Bricogne (Global Phasing)

Michael Hellmig (HZB)

Gruzinov Andrey (DESSY)

Bo Yi (NSRCC)

Jacob Oldfield (ANSTOM)

Merghdad Yazdi (MAXIV

Letícia G. Capovilla, Nicolas Moliterno (LNLS)

Apologies: Martin Savko (SOLEIL), Rasmus Fogh (Global Phasing), Roeland de Boer (ALBA)

Agenda

Prior to the meeting Ramus communicated the following points for discussion:

- Plans for making and adopting a qt version of the master/develop branch at beamlines. E.g. Qt4 or Qt5? Timings?

- Collaborating to make an interactive version of the GPhL workflow to run under the web interface. I am working on learning JavaScript, but some planning and collaboration would be needed.

The topics are of general interest It was however decided to postpone these for a future meeting as Rasmus could not attend due to connection/location issues.

Site Status

Global Phasing - GB: As Gleb had difficulties to get a VISA, Aswhin from EMBL-HH presented, in Gelbs' place, the results of the work done on P14 at the Gordon Conference. The presentation was very well received.

Rasmus has continued the work to integrate the GPHL workflows across the different sites and mxcube versions. The workflows are now deployed on EMBL-HH (P14), ESRF (MASSIF-1), Soleil. Alba have recently expressed that they are ready to integrate the workflows as well.

There are currently discussions ongoing to find a solution for developing the bespoke dialog(s) for mxcube-web required by the GPHL workflows.

ANSTOM - JO: The construction of the MX3 beamline has started but almost all testing has to be performed on simulated hardware. The integration of mxcube-web has started on the MX1 beamline where they so far had very limited time on the beamline with hardware. There is, despite the limited access to the beamline a running version of mxcube-web although with very basic functionality.

MAX-IV - **MY:** Received a new MD3UP for which he wrote a new hardware object based on **AB**'s new *AbstractDiffractometerObject.*

DESSY - AG: Starting to learn about mxcube and are looking into installation and connection with ISPyB.

BESSY - MH: Currently at the end of a three months shutdown for exchanging the power supply system powering the accelerator and parts of experimental stations. The unavailability of hardware due to the power cut has slowed down the work on the adaptation of mxcube-web significantly.

ESRF - MO and AB: Have installed the new test/beta version of mxcube-web on MASSIF1 and ID29. The code running on these beamlines are using the latest mxcubecore and also includes the latest SSX features. The aim is to continue the tests on a standard mx beamline during the autumn and release mxcube-web 4 once satisfactory results are achieved.

Topics for next code camps

The preliminary date for the code camp was set to 22nd and 23rd of September with the exact times still to be decided and communicated as soon as possible. It was concluded that the topic of the code camp would be *Continuous integration, testing and virtualization (Docker,Podman, Kubernetes)* and that this could serve as a good way for newcomers to get into the code base.

Next meeting

The next meeting will be the code camp the 22nd and 23rd of September