

MXCuBE Developer's Meeting

Whereby, September 21, 2023

Meeting Minutes

DRAFT

Participants

Rasmus Fogh (Global Phasing)

Marcus Oscarsson, Antonia Beteva, Daniele de Sanctis, Jean-Bapriste Florial, Axel Bocciarelli (ESRF)

Jacob Oldfield, (ANSTO)

Andrey Gruzinov (DESY)

Jose Gabadinho (ALBA)

Elmir Jagudin, Fabien Coronis (MAX IV)

Martin Savko (SOLEIL)

Alessandro Olivo (Elettra)

Michael Hellmig (HZB)

Nicolas (LNLS)

Boyi Liao (NSRRC)

PyQt and licensing

RF raised the point of PyQt licensing.

As Global Phasing workflow code is proprietary, and the workflow and MXCuBE unmistakably form a combined work, groups who develop the PyQt version need a commercial PyQT license. The condition is on groups 'distributing' PyQt code, which would mean pushing code to the mxcubeqt repository (purely internal use does not require a license). The cost is \$550 per seat per year + VAT, and details can be found at <https://www.riverbankcomputing.com/commercial/license-faq>. It may be noted that even though MXCuBE proper does not itself distribute either non-free software or PyQt libraries, the licensing conditions for GPL have been carefully set up by the FSF lawyers to make it impossible to combine proprietary and GPL code in any way, direct, indirect, or sneaky.

Distributing MXCube Qt without the relevant commercial license would therefore put MXCuBE in violation of both the Riverbank Computing license and the GPL license.

A round of the participants gave:

- ESRF does not have a PyQt license but agrees they should have at least one, as the originators of the first PyQt version and regular contributors to editing, pull requests etc. - even though they are no longer actively developing the PyQt version.
- Global Phasing has a current PyQt License.
- The following other groups are using mxcubeqt and to varying degrees pushing code to the repository: SOLEIL (MS), HZB (MH), DESY (AG), ALBA XALOC (Jose).
- The following are working only with the MXCuBE web version and so have no need for a PyQT license: ANS (JO), LNLS (Nicolas), Elettra (AO). MAX IV (EJ). NSRRC (Boyi)
- EMBL-HH (not represented at this meeting) is known to be using a QT-based MXCuBE, but are not currently 'developing', as in contributing to the public mxcubeqt repository.

It is agreed that the matter should be put before the Steering Committee, with the recommendation that the relevant participants should buy a PyQt license.

Status with mxcubeqt integration

- RF (GPhL) reports that the Global Phasing workflow is now integrated with the develop branch tip of both mxcubeqt and mxcubeqt, and should be ready to set up for anyone at a similar stage. The code is prepared for setting up a user interface for the web version also. RF would need help from someone making a prototype first, as it would be too much work for him to do a JavaScript interface on his own. On the latter point there is interest from ESRF ID30B, and J-B F might be able to contribute.
- AG (DESY) has been busy catching up with the develop branches and has been making numerous Pull Requests lately; he thanks for the reviewing. There are still a couple of bug fix PRs to go. AG would be interested in trying out the web version at some point. AG was invited to talk to the Code Camp about getting started, but notes that his main experience is upgrading from an old mxcubeqt branch, which is a particular set of circumstances.
- MH (HZB) has no new developments to report or in progress, as HZB is still recovering from the June cyber attack and has no functioning internal network.

- EJ (MAX IV) has one pre-mxcubecore web version running on an active beamline, and is trying out the latest web version on a new beamline. There are still bugs being found and some HardwareObjects not yet coded for.
- JG (ALBA) is setting up the latest web version on the new XAIRA beamline, while the XALOC beamline is running the mxcubecore version. Functionality (sessions and ISPyB handling) is being transferred from XALOC to XAIRA.
- MS (SOLEIL) has last year's mxcubecore version on the PX2 beamline, and is moving up to the current version. The upgrade has been quite smooth, but is not yet finished; it should be done by the October code camp. The Global Phasing workflow has been running; there had been some bugs, and SOLEIL is working to get it all ready and installed themselves. SOLEIL is setting up a campaign to upgrade the PX1 beamline to the mxcubecore version tip, and also intends to take a look at the web version.
- AO (Elettra) is finalising the latest web version. There are some problems with signals.
- Nicolas (LNLS) is working on the web MXCuBE3 version, and are adding HardwareObject code, most recently a Flux class. They have given version 4 a try.
- JO (ANS) ANS are in the process of commissioning a beamline right now, so not much is happening on the MXCuBE front. They will have beam in a month. They do not really have time to participate in the Code Camp, but could do a presentation on Ophyd. They expect to commit some tests they already have written.
- BoYi is working with the latest version MXCuBEweb.

Any Other Business

JG asked about the relationship between signal handling in Qt and React. In Qt there were cases where signals passed between different interface components, where React seemed to allow only communication back and forth to the core layer. It was confirmed that this was indeed a core principle of React.

MS proposed adding some code to handle on-screen overlays as the sample was reoriented. The meeting supported the idea. On a related topic it was agreed that the code for re-centring as kappa and phi changed should be introduced across the board – it has been present and in use by the (EMBKL-HH) inventors for years, but has not so far been widely adopted

Next meeting

The next meeting will be the Code Camp at MAX IV. MO noted that there was no required reading to be done first, but recommended that everybody installed the web version on their computers, both to test the install procedure and to have it ready before the meeting.