

MXCuBE developers' meeting

25 Feb. 2021

Participants:

- Marcus Oscarsson, Antonia Beteva (ESRF)
- Mikel Eguiran, Meghdad (MAX IV)
- Jan Meyer (DESY)
- Michael Hellmig (HZB)
- Ivars Karpics (EMBL Hamburg)
- Jordi Andreu (ALBA).
- Bo-Yi Liao (NSRRC)
- Lais do Carmo (LNLS)
- Martin Savko (Soleil)
- Rasmus Fogh (Global Phasing)

Minutes: Rasmus

Last meeting

Minutes approved

Additions to agenda

no additions

Site status

Lais do Carmo (LNLS)

Pull request with configuration for Sirius has been finished and submitted. LNLS is currently restarting a new MX beamline, which should be taking users in the second week of March. The new beamline will be using a sample changer under MXCuBE3; robot simulation tests have been done this week, real tests are for next week. There is a bug in motor widgets that do not refresh properly; the bug is not seen in the master branch proper.

Ivars Karpics (EMBL Hamburg)

The P14 shutdown will end in two weeks, working on a frozen Qt version. The (close-to) master branch has been tested. PySide 6 and Qt6 are to be released soon, and EMBL-HH

plan to support them. Meanwhile much time is being spent on the T-REX serial crystallography beamline, using EDNA.

Jordi Andreu (ALBA)

In a few days the implementation of mesh scans in the frozen Qt branch used at ALBA will be completed. The next task, to be started in a month or so, is to start migrating to the master branch.

Martin Savko, (SOLEIL)

MS is working on moving to the master branch for PX2, currently in shutdown. In parallel he is addressing user reports and complaints, mostly slowdowns rather than actual bugs. Updating of motor widgets is happening sequentially and slowly, which is an irritating effect. Remote operation can take up to three times longer in practice due to slower refresh; the cause is often inefficient firewalls, and (academic) institutions close by may work much slower than users in New Zealand.

MS is integrating snapshots and videos from optical centring and storing them together with the acquisition data, which should be very useful for debugging. Longer term he is considering to store also images from other in-hutch cameras. ME notes that at MAX-IV the hutch camera is on continuous acquisition, and any instance of sample changer clash will trigger an email including a video of the last 60 seconds.

Together with Global Phasing MS has rooted out a bug in centring, where the use of the F2 shortcut (end centring) also triggered the centre-to-point routine, partially undoing the previous centring. This caused a significant number of missing images for high-powered (CRO) users working on thin-plate crystals.

MS is looking at reducing the total number of signals emitted. More long-term he is thinking of revisiting the idea of treating MXCuBE as a finite state machine (Comment from IK, 'should be for interface part only').

Rasmus Fogh (Global Phasing)

Global phasing is at the stage of installing the data acquisition workflow as a β version for beamlines to use independently. Testing with EMBL-HH P14 has given much useful feedback to improve the user interface (thanks Gleb Bourenkov and IK), and further testing is expected by mid-March. Meanwhile Roeland Boer and JA are also installing the workflow for imminent testing (thanks!).

The next tasks contemplated would be a similar effort at SOLEIL, improvement of release system, recoding in Cython (etc.), but we hope soon to be able to start porting to MXCuBE version 3. AB is interested in this, and notes that there have been in-house requests for this to happen, with particular reference to the calibration workflows.

RF asks whether beamlines in general are supporting the specification of acquisition with repeat count and overlap. This is the case, the capability is in core MXCuBE, and is in use

for characterisation images. The interleaved acquisition capability, on the other hand, is not used outside of raster scans.

Jan Meyer (DESY)

Upgrading of MXCuBE is paused, but will be taken up again as soon as Vicente Rey is again able to travel.

The implementation of the new Eiger2 16M detector is finished, and will be used for the next user run in two weeks time. Implementation ultimately required a hand-coded Tango server, as the DESY controls group did not accept LIMA, and the existing Tango servers at DESY were not capable of handling the Eiger2. The Tango server (unusually) accesses the Dectris REST API, and JM is happy with the way it is working. The API code is on SourceForge.

It is noted that the Eiger2 produces a more standards-complying version of HDF5, which is good but has the unfortunate side effect that older HDF5 access code may not work for Eiger2. It is further noted that only EMBL-HH and parts of ESRF use the streaming interface for Eiger, whereas the more common approach is to use FileWriter.

Michael Hellmig (HZB)

BESSY is in user operation, with one beamline for remote operation and the other one (still) in a mixture of mail-in and in-person operation. There is no progress on MXCuBE development, energies being taken up by user support.

Bo-Yi Liao, (NSRRC)

February has been mostly holiday season. The first component for the new MX beamline, a mirror, has just arrived.

Antonia Beteva (ESRF)

A pull request to bring ESRF-specific HardwareObjects up to the current master has been completed. Locally ESRF has not upgraded to snake case, but the PR has been engineered to fit. A new Eiger2 16M has been installed on one beamline. A recent meeting with beamline scientist gave rise to a long wish-list. The demands of supporting remote operations have reduced over time, as remote operation is gradually settling in.

Marcus Oscarsson (meeting chair)

Notes that the status rounds take a long time at every meeting, and proposes to consider reducing the frequency to one every other meeting.

Pull Requests

#596 Abstract Actuator

There is still disagreement on the PR, whether AbstractEnergy should store a separate wavelength value (AB) or store only energy and convert to and from wavelength as needed (RF). The question was postponed to be settled after the meeting.

mxcube repository snake_case

Before accepting the PR, it was discussed whether and for which parts of the code base module and package names should be changed to lower case / snake_case to conform to PEP-8. The consensus was that we should aim for PEP-8 compliance across the board, apart from accepting underscores fairly freely (snake_case) where this seemed helpful. The PR was accordingly accepted as the first step on the way. In clarification it was confirmed that file names should be snake case but class names should be CamelCase (this distinguishing modules from classes of the same name) and that also abbreviations should be in lower case when part of module or package names.

Implementation order

It was established that the order should be

1. Merge the above Pull Requests.
2. Clone the old HardwareRepository to a new location, and rename it mxcubecore
3. Fix all import statements
4. Make setup.py and make the new repository structure work. This should be version 0.1
5. Continue with conversion to snake_case.

RF and MO will endeavour to finish this before the next developers' meeting.

AbstractProcedure

Reference is made to the discussion during the last developers' meeting, as summarised in the minutes, including the proposal to use another name than 'AbstractProcedure'.

There is some discussion about what scope is desired for this object. On one hand it could be integrated with the queue system, which would make it match the Task / QueueEntry. On the other hand there is also interest in having procedures as combined sequences of steps at a lower level and usable also outside of the queue context.

JA notes that this is the first time that the developers as a group are designing something new from scratch. He proposes that we should make a joint draft specification / enhancement proposal to clarify what we want to do and how to do it. There are various pitfalls here, a single-person draft might unduly bias the subsequent discussion, whereas

collecting ideas and requirements from all might give a heterogenous and unwieldy result. It is agreed that IK will do a first, code-level proposal, but that this should be seen as a discussion starter.

MXCuBE meeting

The next MXCuBE/ISPyB meeting will be arranged jointly by EMBL-HH and DESY. It will be fully virtual, with one afternoon for MXCuBE and one for ISPyB, and will be approximately in the period 17-21 May. Anybody who has major problems with these dates are requested to communicate this as soon as possible.

Next Meeting

The next developers' meeting will be in week 12, 2021.