

MXCuBE Developers meeting, 7/6/2018

Present (virtually): Jordi Andreu, Antonia Beteva, Gerard Bricogne, Lais do Carmo, Gabriel Fedel, Rasmus Fogh. Michael Hellmig, Ivars Karpics, Peter Keller, Andrey Nascimento, Marcus Oscarsson, James Piton, Milan Prica, Martin Savko, Ana Zeri, Roberto.
Apologies: Mikel Eguiraun, Pavel Palau

1. Minutes of last meeting, and matters arising

The minutes were not discussed, and are deemed to be approved, pending objections.

2. Status reports

Ivars Karpics: Just installed a new computer that can analyse 500 frames per second for number of spots and Dozor score, before data are written to disk. Written an API test prototype ACTION ALL: Please test it. Added a [Collect Now] button to the UI. ACTION Rasmus: test and merge.

Ana Zeri: The Qt4 version is installed but suffers from mysterious crashes, which were not alleviated by changing from CentOS to Debian. MO suggests to check if this could be caused by video buffer overflow.

Energies are concentrated on moving to MXCuBE 3 for the Sirius synchrotron. MO and AZ agree to organise a remote test of the MXCuBE3 installation at the ESRF.

Roberto: Installed new sample changer, which caused some problems with the core sample changer code. Upgrading to a newer step on the branch solved this problem but cause multiple others. Roberto raised a problem with MXCuBE3 mediator code that imports specific classes (e.g. TangoShuttle) and how to handle the case of using a TangoShuttle subclass locally. MO agreed to discuss the problem after the meeting.

Marcus Oscarsson, Antonia Beteva: Remote operation of MXCuBE3 by users (at the moment AstraZeneca) is active and running. Main activity at the moment to install MXCuBE3 on all beamlines and prepare the upcoming MXCuBE3 release.

Michael Hellmig: Currently in a short shutdown, and busily upgrading the active version to master.

Martin Savko: Finished bringing code and configuration files on Proxima2 up to master branch, and will push the result before the end of the week. The exercise reduced the amount of Site-specific HardwareObject code by 75%. Will start working on UI API once this is finished. ACTION Rasmus: Test integration of GPhL code to new branch when available.

Jordi Andreu: About to commission new version, which is almost Qt4 master, including sample changer, postprocessing, ISPyB, collection. Release before summer to friendly users. Will improve on data collection code over summer. Four week shutdown starts 23 July. Using MD2 motors with

direct motor control without a server, and looking to new Icepack firmware. AB comments that e.g. helical scans can be run from the MXCuBE level, but JA answers that it has been decided to do this at the hardware level. GB comments that if you bypass the Arrinax driver routines for the diffractometer it is necessary to do careful backlash compensation yourself.

3. ESS interest in MXCuBE collaboration

The interest from ESS is welcomed, and MO and MK have already responded (on github) with offers of a remote demo session and a visit to MAX IV. ESS participation in the next (Elettra) MXCuBE meeting is possible, the only limit being the number of participants. Since ESS is only at the stage of preliminary interest as yet, it is agreed to mention the possibility of participation and leave the initiative to ESS.

4. MXCuBE refactoring

The feeling of the meeting is that the UI API is generally both desirable and feasible. There are a number of outstanding questions, and the time and resources needed, as well as those available for the task, is still not fully clear. The current draft is seen in general in a positive light, but is still likely to change, maybe significantly, as implementation nears.

IK showed the code of his test SampleChanger brick. Conversion did not seem a big challenge, the implementation had been easy and taken about an afternoon. The possibility to write a user interface using only signals, without knowing about or calling HardwareObjects was a clear advantage. Others (MO, RF) were also positive.

Signalling is one technical problem that needs to be overcome. The Web interface requires http-compatible signals, whereas the Qt interface can run with Qt signal of PyDispatcher on both sides.

Attempts to pin down the likely resource requirements by comparing to the effort of bringing local implementations up to the master branch were inconclusive. Some exercises (IKs test brick, individual motors) have proved quite simple, but the upgrade to master had proved unpredictable and very non-linear (MS). Some hardware objects proved particularly difficult, and integrating all the individual changes is also unpredictable.

GB proposed, and the meeting agreed, to hold another meeting in two weeks' time, to get a better picture of the situation before the holidays kick in. The goal is to have the situation sufficiently clear by the time of the Elettra meeting to enable the various committees to take sensible, binding, decisions. The following people volunteered for various tasks over the next two weeks:

- MO, AB cannot put test code into the upcoming MXCuBE release version, but might for the following one. Meanwhile they volunteer to write draft interfaces for LIMS and data processing.
- MS volunteers to produce a detailed draft for the diffractometer.
- IK will look at different signalling mechanisms, including PyDispatcher.
- RF will produce a draft interface for the workflow component.

Next Meeting

The next meeting is planned for June 21 1400-1530 (UK time), on appear.in/mxcube.