

MXCuBE Developers meeting, 21/6/2018 DRAFT

Present (virtually): Antonia Beteva, Marcus Oscarsson, Jordi Andreu, Michael Hellmig, Ivars Karpics, Milan Prica, Roberto, Martin Savko, Rasmus Fogh, Gerard Bricogne

Apologies: Mikel Eguiraun, Pavel Palau

1. Minutes of last meeting

Minutes passed without comment; no matters arising

2. Status reports

MO (ESRF) reports having done a remote access test in MXCuBE 3 with Swedish and UK big pharma company(ies). The test was successful, the company is learning the new UI behaviour, and liked the experience.

MS (Soleil) reports having finished bringing the local installation up to the master branch level, greatly reducing the need for Soleil-specific code. Only a few bricks still left to change. There had still not been time to do the diffractometer UI specification. The aim is that each beamline should have a single .yaml file that would work for both production and mock setup.

IK (EMBL-HH) reports a hard time with two power cuts. Also a new 4K screen that will require some configuration changes (fonts), to make use of additional screen space.

MP, Roberto (Elettra) reports a very successful remote test of MXCuBE3 test with ESRF. Three-click centring now works. There are some problems with configurability of data file names. AB recommends that all file name management should be done in the Session HO, which is accessed from many places in the code, and MO comments that it might be better to have NON-user-modifiable file paths.

MH (BESSY) is still upgrading of the master branch, having finished the hardware objects and working on the mxcube repository.

ALBA is in the process of moving up to master, and expects a PR with changes to follow on completion in July. They are currently working on configuring EDNA, ISPyB, and expect the first friendly users over summer, with start of operations in September.

AB (ESRF) has changed the handling of XREFS scans, moving code from brick to HO, and separating fitting from graphics, with results written to file. IK asked how information was transmitted to the UI (with signal?), but the results display is no longer in the brick.

3. UI interface specification

MO has pushed (the start of) a LIMS+Login specification, taken from MXCuBE3. He will define data structures later, but IK has already merged his WorkInProgress. Processing is not there yet but is expected for the coming weeks – there should be few functions defined here.

IK accepted the PR, has added LIMS to testing, and is working on new and better signalling. IK and MO concur on the need for a separate transport layer to transfer information between the HO and UI layers, to supplement the specification.

A general discussion on interfaces and signal handling followed. MXCuBE has HTTP, remote procedure calls could be added. The transport layer could have emits that triggered the appropriate method. Some clever use of decorators might fit the bill. The interface functions should be implemented as wrappers – which for Qt could be *very* thin wrappers dealing with exception handling etc. IK considered if the HO mediator objects from NMXCuBE3 could serve as a model, but MO replied that they had been conceived as a temporary shim layer to preserve an unchanged HO layer while modifying the UI functionality, and so might not be appropriate. JA points out that MXCuBE3 is client-server, whereas Qt is a single process, and asks if there are HO0HO signals as well as (or the same as) the HO-UI signals. Qt uses dispatching, and MXCuBE3 sockets; some kind of interface layer would be needed to translate signals to the appropriate mechanism. The whole point should be discussed further in an issue.

RF asked whether the refactoring was considered desirable, feasible, and what the resource needs would be. There is general agreement that the reorganisation ought to happen. The pure specification phase is mostly finished. There seems to be agreement that the next step should be somebody coming up with an implementation, and trying; others would then move over to it later, much like the current master branch has been handled. There was no appetite for a more precise overall plan, and resource requirements were seen as a matter for each individual site. MO hoped to be able to present a possible implementation at Elettra in September. The actual work would likely take within 2-3 months (presumably full-time), doing one category at a time, but as for the testing, ...With summer on us, something might be ready around the turn of the year, but it depends on the priority it gets. One way or the other this will presumably be settled at the Elettra meeting.

4. Any Other Business

- IK: What is the status of the MXCuBE paper? A: GB admits that it is currently held up on his desk, but promises to do something.
- IK: What is the status of serial crystallography? Has ESRF a document on how to deal with it, how to visualize the results, ... MO says 'it is being looked at. IK and MO discuss a possible separate meeting on the matter. Serial crystallography will be discussed at the Elettra meeting, and MO hopes to have done some refactoring by then.
- MO mentions the acquisition issue raised by RF, with the first image in a wedge having a different scaling. The consensus is that this is a beamline-specific issue that should be dealt with locally, rather than at the MXCuBE level.

Next meeting

It is agreed to hold a meeting in the first part of August, ACTION: RF to start Doodle poll.