

MXCuBE web meeting 11 July 2019

DRAFT

Participants:

- Jordi Andreu, (ALBA)
- Ivars Karpics, (EMBL-HH)
- Marcus Oscarsson, Antonia Beteva (ESRF)
- Rasmus Fogh, Gerard Bricogne (GPhL)
- Martin Savko, (Soleil)
- Milan Prica, Roberto Borghese (Elettra)

Minutes of previous meetings

Minutes of the Hamburg meeting were approved – with no positive or negative comments.

Status reports

SOLEIL MS has been working on drawing overlays for mesh scans. There is a bug in the HardwareObject that assumes the drawing must start at the top left hand corner as origin. This fix is likely relevant also for MXCuBE3.

A major problem has materialised with the SOLEIL MD2 diffractometer, that homes to $\kappa=180$ (instead of $\kappa=0$) and freezes every few hundred mountings. The goniostat has been sent to Arinax for servicing, and the beamline has reverted to single-axis operation. This revealed some interface problems, as the interface failed when motor objects or positions were None or missing. MS has fixed these temporarily by passing motor positions as 0.0 if the motor is absent. These fixes are likely present also for other beamlines and their code, and should be checked for.

Elettra has been in a long shutdown, and RB and MP took the opportunity to integrate with ISpyB. After experiencing great difficulties with the ISPyB GUI it was found that SynchWeb was very simple to install and configure. A cron job is used to transfer information between the local access database and ISPyB, which then is used to log into MXCuBE. ISPyB is now replacing the csv files previously used to import sample information. There have been some problems with synchronisation and directory naming, but ISPyB should be in production use in a few months.

GPhL: Since Hamburg meeting GPhL has finished its yearly Consortium meeting, and RF has worked on the MXCuBE refactoring. A recent ISPyB meeting confirmed that there would be a face-to-face meeting for refactoring on 12-13 September. Preparations are in train for a remote test at ALBA on July 18-19.

ALBA: Intense work on integrating the new Arinax two-focus camera. The camera is run via a (pseudo-Lima) Arinax server, which supposedly should be changed (by Arinax) to a full Limas plugin later. The double gripper sample changer is reported to be working without problems.

ESRF: Software preparations for December restart are now in progress. The installation uses the refactored HardwareObject layer, and Python 3. The Exporter package has been upgraded to use Python 3 string handling, and a PR is expected shortly. Some changes to motor hardware objects are in the pipeline as well. Much work with Jean Baptiste on the new (MXCuBE based) BioSaxsCube, and a new framework for general beamline applications, which will reuse some of the work done for the Braggy viewer. MXCuBE will not be moved to the new framework, and will remain based on the HardwareObject layer.

EMBL-HH have tested maximum image throughput, acquiring 1 million images at maximum speed. The test worked up to 500 000 images where frame dropping started. IK has tried out a new (published) neural-network-based centring approach, DeepCentring. The idea is interesting, but seems overkill for loop centring, and was found not to work too well for crystal centring, probably because the test objects were too different from the crystals being centred.

Refactoring and scheduling

There is general satisfaction with the conclusions of the Hamburg. Current PRs are seen as going in the right direction, but more time for examination is needed before a firm decision on exactly how to proceed. Both the BeamlineObject and the AbstractActuator PR will require very widespread code changes when fully rolled out (as will adopting YAML configuration more widely). ESRF needs to install and prove the current state of the code before being able to take on board additional major changes, and SOLEIL will not have time for major interaction before September. This makes some degree of parallel development unavoidable. RF requests a timetable, promising to devote significant time to implementing his PRs once there is agreement on what to do. It is agreed to continue discussion on github, and to expect major comments to be in by 20/7, so that implementation work could start soon after that.

The milestones in the current plan clearly need to have their timing adapted – they are probably too optimistic – but no one has a precise proposal. It is agreed to reconsider the milestone timings in a web meeting at the beginning of September, that can also serve to concentrate minds and do some planning ahead of the Berlin MXCuBE meeting.

There were some detailed points:

- The BeamlineObject PR by Rasmus is considered the most complete, and the competing PR is closed. Antonia will help test the BeamlineObject once it is implemented and needs testing at a beamline.
- The AbstractActuator PR is not ready for adoption and should have been marked as WIP. The two most obvious question marks are whether the basic structure are OK, and a closer look at the ExporterMotor implementation example, to check that it makes sense from an

actual hardware point of view. There is not felt to be a need for caching current motor positions in the HardwareObject, as opposed to getting them through channels when needed. Antonia and Rasmus will take the lead on implementation.

- As people review the AbstractActuator PR, they are requested to consider also the possibility and requirements for future replacing HardwareObjectNode (XML configuration) with ConfiguredObject (Yaml configuration), reducing or removing the functionality in the current HardwareObject.

Any other business

MS reports that the newest ISPyB version has a call findSessionByProposalAndBeamline that takes tens of seconds (over two minutes having been observed). This has not been observed anywhere else, probably because 1) people have not yet adopted this version, or 2) because they are in shutdown (ESRF) Marcus promises to check out the problem.

Next Meeting

The next meeting should be in early September. A doodle poll has been set up at <https://doodle.com/poll/9sqa99e3iyxatxyt>, covering 6/9, 9/9, and 10/9