MXCuBE Developers meeting, 15/4/2019

Draft

Present (virtually): Jordi Andreu, Antonia Beteva, Roberto Borghese, Lais do Carmo, Rasmus Fogh. Michael Hellmig, Ivars Karpics, Peter Keller, Marcus Oscarsson, Martin Savko,
Apologies: Gerard Bricogne, Mikel Eguiraun,

1. Minutes of last meeting, and matters arising

The minutes of the last two meetings were approved without comments.

2. Agenda

The agenda was read out and approved.

3. Status reports

Rasmus Fogh Global Phasing is busy this spring with test visits at EMBL-Hamburg (early May) and ALBA (end of May). The data collection metrics meeting of the previous week went constructively, and further collaboration and (hopefully) agreement is expected. GPhL is now on the master branch, tested in mock mode.

Jordi Andreu Sample changer problems (syncronisation issues with Tango) have left little time for adding new features, but Jordi has contributed reviews on the current issues and PRs. There are some changes for the running version 2, which have not been PR'ed to the central version. RF comments that he would find such a PR useful.

Michael Hellmig Work has been going on with finalising the use of MXCuBE on several fixed energy beamlines. There should soon be time to start harmonising the latest branches, First HardwareRepository, then the Qt GUI

Ivars Karpics Extensive clean-up of the repositories. Code is fully PYthon2/3 compatible , 'from *' imports have been replaced by individual imports, Travis is run for both Python 2 and Python3. The use of their new computing cluster is now stable.

Roberto Borghese Some features have been added, such as phases and custom actions. ISPyB is now being suncronised with local databases using a cron job.

Martin Savko There is not much change, and the interfaces are stable. There is a problem with the characterisation stage taking unconscionably long after running the program for 4-5 hours, but none of the other developers have experience with any similar issues.

Lais do Carmo LNLS is now signing the MXCuBE collaboration agreement, just some final legal details being sorted. Nobody was quite sure about the signing process (Daniele de Sanctis should know) but Gerard Bricogne (guest appearance) said it was done by sending around papers to sign. LNLS is going ahead with moving to MXCuBE3, reusing work from the Qt version, and have connected up to their EPICS code. Starting to use ISPyB will come later.

Marcus Oscarsson There is an unofficial rumour that the Taiwanese synchrotron will sign up to MXCuBE. MO has been working mostly with the BSXCuBE (SAXS) and the Braggy viewer. AB has been updating the AbstractDiffractometer PR. It is reported that ESRF is now Python3 only.

4. Feedback on the Lund meeting

A few scattered comments:

- The hands-on session on version 3 was commended

- It was regretted that the MXCuBE hands-on session clashed with the ISPyB meeting.

- It was hard to keep track of what5 the program was and when talks were due etc. in the run-up to the meeting

5. AbstractDiffractometer

- AB proposed to reduce the number of possible states for the diffractometer from the current 26(!) to maybe half a dozen or so. The meeting was generally favourable.

- The AbstractDiffractometer is ready for use, and it is agreed that it can be merged and tried out now as soon as currently discussed changes are incorporated.

- It was discussed if functions in the AbstractDiffractometer should be marked as raising NotImplementedError, as abc.AbstractMethod, or not at all. General opinion was that abc.AbstractMethod was the right approach, but that it should be used sparingly, and that a default implementation (e.g. get_phaase returnign None) should be preferred where possible.

- The order of moving motors in the code was discussed. Looping over a dictionary of motor positions means that the order of function calls is indeterminate, which can make for tricky bugs if there are other problems as well. One solution proposal was to use an ordered dictionary of motor positions as input, another to configure the order of calling the motor move commands. Gerard Bricogne raised the point that some beamlines may require tight control over the moving trajectory in order e.g. to avoid taking the sample out of the cryostream. The best proposal seems to be 1) that move_motors guarantees to move all motors in the input to the inpout position, 2) that the movement order is done in a deterministic manner at each beamline, 3) that the movement order be configured or set at the beamline level, so that calling code does **not** set or depend on the movement order.

- It was discussed whether (and how many) functions could be moved out of the AbstractDiffractometer. E.g. snapshots, centring maths, and move-to-beam were candidates for a move, as they involved also functionality outside the diffractometer. One proposal was to move all functionality that implicate more than one component to the Beamline object. It was objected that this might led to a single highly unwieldy object with too many functions attached. One proposal was to use the Beamline object for general access to HardwareObjects that did not have an obvious alternative home, but to use another system for procedures. Procedures might be put in an api object, with some kind ODF internal structure.

6. Preparations for face-to-face meeting

The face-to-face meeting is around 13/6. To make it a success considerable homwwork will be needed.

- IK will make a GoogleDocs to track preparations, both administrative and scientific, and put up proposals and tasks for people to sign up to. The link is https://docs.google.com/document/d/1eWDrNS-_PpZN140aoxhDtG7n-iwGdch7I7k_fUPDNEE/edit
request permission to edit.

- One general task is for all to engage with the issues on github, and consisder the linter and test output.

- It is agreed that all parties should make a local ersion of a new Sesasion HardwareObject for merging at the f2f meeting.

- RF promises to make a PR with a first draft Beeamline object.

- Draft PRs or preparatory work for other issues, such as Queue, api, data hilding objects etc. are eagerly solicited.

Next Meeting

It is agreed that there will not be a full developers' meeting before the face-to-face meeting. A quick meeting for finalising preparations might be useful, and will be called at shortish notice if necessary.