

MXCuBE web meeting 15 Oct. 2019

DRAFT

Participants:

- Jordi Andreu, (ALBA)
- Marcus Oscarsson, (ESRF)
- Rasmus Fogh, Peter Keller (GPhL)
- Martin Savko, (Soleil) – connection permitting.
- Lais do Carno (LNLS)
- Roberto Borghese, Milan Prica (Elettra)

Apologies:

Michael Hellmig (HZB), Ivars Karpics,(EMBL-HH), Mikel Equiraun (MAXIV)

Status reports

Elettra Engaged in upgrading MXCuBE prior to installation. There are users now, and it is a very busy time. Work is ongoing on enabling remote operation; for now there are some features missing (e.g. shared streaming), thought it has been tested once. There is a team from India coming in mid-November for a high-powered (ministerial level) demo. Elettra is using MXCuBE3, with the Synchweb front end to ISPyB, and have integrated Diamond autoprocessing.

LNLS Continuing as of last meeting. Preparing presentation for Berlin. There are some Python 3 dependency issues.

ESRF MXCuBE 3 is up to date with latest hardware objects. There were quite a few changes. An update is coming. ESRF is switching from an OAR-based to SLURM-based queueing system.

ALBA Still in the process of migrating from Tango 7 to Tango 9, and from old OpenSUSE 11 (?) to Debian 9. The processing job submission library has been changed. The new library is ALBA-specific and based on SLURM, with YAML configuration. ALBA can make it available to others for inspiration. ALBA can run GPhL autoprocessing through the EDNA plugin mechanism – though this is not in MXCuBE yet.

ALBA (with GphL) found a bug in the cbf header file for Pilatus – ESRF can kindly provide a patch. At the moment the production environment cannot in any way be modified. At next opportunity will upgrade the ALBA hardware objects to use the beamline object (?) and work with Python 3; the results should be in use after the Christmas shutdown.

GphL Have mainly worked with strategy determination programs and less with MXCuBE directly, but hope to put some work into MXCuBE now. The ISPyB face-to-face meeting produced some good agreements on refactoring, but raised a difference in priorities and approach that caused a significant disagreement on how to proceed with refactoring of the

Sample tables. Considering that Diamond and ESRF ISPyB installations actually have very little code in common this is a serious problem that has been referred to the ISPyB Steering Committee. It is noted that the MXCuBE collaboration seems to be in a much healthier state. GphL has been collaborating with Martin Savko on calibration using the SOLEIL optical centring.

SOLEIL Martin Savko was only able to speak to the meeting for brief periods He managed to report that SOLEIL was working on X-ray centring and mesh screening, expanding the characterisation procedure to include X-ray centring.

Refactoring

- The location for the detector distance was briefly discussed. It was agreed to leave it as `detector.distance`, since this was at least no worse than the alternatives (under Resolution or directly under the Beamline).
- It was discussed how to organise `AbstractProcedures`. The desire was for each beamline to be able to add its own procedures, and the use of beamline-specific `Beamline` subclasses was (still) not popular. RF raised the question of how one could call procedures (e.g. centring) from central, beamline-independent code if there was no central agreement on naming or input parameters. He also noted that as currently coded, `AbstractProcedures` were not compatible with the `ConfiguredObject` mechanism they used, which by deliberate design choice does not allow using the configuration files to add attributes or objects that are not already defined in the code. RF volunteered to make a fast, lightweight modification to `ConfiguredObject` that would allow `AbstractProcedures` to work with the `ConfiguredObject` superclass, pending further discussion on how this could be reorganised.
- For the `AbstractActuator / AbstractMotor` PR RF asked whether a `set_limits` command should be included. The meeting was in favour [LATER NOTE: the `set_limits` function was not added in the latest draft – because of problems with adding a `set_limits` function when some subclasses might have unmodifiable limits]

Further it was discussed how to set waiting and timeout in `set_value` (etc.) commands. It was agreed to have no 'wait' attribute, to have `timeout=None` mean 'wait forever', and `timeout=0` mean 'do not wait'. RF promised to replace the `AbstractActuator` with an updated version.

- It was discussed how to continue the refactoring and clean-up. MO raised the question whether it was worth the work and trouble to continue changing function names from camelCase to snake_case; JA suggested that this should continue and the meeting agreed.

It was generally agreed to get as much clean-up as possible done before Berlin. Many things need doing: `AbstractDiffractometer` (suggested that AB will consider), removing obsolete classes and functions, snake_case. PK suggested, and the meeting agreed, that removing obsolete code first would make subsequent refactoring easier. RF promised to make a clean-up PR within the week.

Roadmap

The status of the roadmap was discussed, in preparation to presenting the development status to the steering committee and populace at the Berlin meeting. It was agreed to move AbstractCollect from Milestone 2 to Milestone 3, and to concentrate on finishing Milestone 2 completely soon after the Berlin meeting. There was no agreement on which target dates to put on the Milestones. LdoC raised the question to what extent the Milestone 1 tasks were considered finished. It was agreed that they were all 'in principle' finished, but for testing especially it was considered that a certain amount of practical work still remained.

Any other business

None

Next Meeting

At Berlin meeting