

MXCuBE Developer's Meeting

Whereby, June 28, 2024

Meeting Minutes

Participants

Marcus Oscarsson, Antonia Beteva, Jean-Baptiste Florial, Daniele de Sanctis, Axel Bocciarelli, Didier Nurizzo (ESRF)

Andrey Gruzinov (DESY)

Elmir Yagudin, Fabien Coronis (MAX IV)

Alessandro Olivo, Nicola Demitri (Elettra)

Annie Heroux (ex Elettra)

Michael Helmig (BESSY)

Boyi Liao (NSRRC)

Martin Savko (SOLEIL)

Rasmus Fogh (Global Phasing)

Jose Gabadinho (ALBA)

Kangwen, 'Guest'

Apologies

As I missed part of the meeting, these notes will be incomplete. RH.

Discussions

Location of configuration files

It was suggested to reduce the number of (duplicated) configuration files currently found in mxcubecore and mxcubeweb. Separate configuration files are needed for mockup and for test. MO suggests that the configuration files are too low down in the directory hierarchy and should be moved to the top level (but still kept in the same repositories). It is noted

that the production configuration files are generally kept separate at beamlines and not checked in, so that the beamline-specific configuration files in the MXCuBE repositories are out of date and unmaintained.

It is agreed to change the relevant configuration directory name from `mockup` to `demo`.

RF points out that it is possible to specify several configuration directories in an ordered lookup list, which would allow you to use e.g. the demo directory and only override files that you specifically would need to change.

XML-Yaml conversion

It is agreed to do this in two phases, where the change from XML to Yaml is done first and the introduction of Pydantic happens in a second phase. Each change should be done with minimal changes to the code in the initial step.

The desired rules for linting Yaml files were discussed, both MO and RF voted to **not** use mandatory quotation marks around strings. RF and FabCor agreed to provide a set of rules between them. Issues should be put on Github, AND be documented.

EY notes that the yaml configuration would be needed for microMAX, for August, so the matter is somewhat urgent.

Cybersecurity

Cybersecurity is clearly an important topic, but it is not quite clear what this group should do about it, or who the right interlocutors are. It was mooted that the main objective should be to ensure that the MXCuBE web version and the remote access protocols are indeed safe, also in order to avoid demands from IT departments for unacceptably tight access controls. Both interactive access to experiments and post-experiment access to data need to be covered, and Dectris project for in-cloud data storage might be relevant for the latter. ND promises to organise a questionnaire for Synchrotron IT groups, with questions focused on MXCuBE-related problems.

Code camp and code development

The Code camp was acknowledged to be a success. The main code development priority for the moment is to finish the work on configuration and XML->Yaml transition begun at the code camp. The next topics of interest should include documentation, centring, and automation / unattended data collection. MXCuBE only goes as far as populating and executing the acquisition queue; for unattended data collection the big problems are

automatic centring, and, especially, organising what should go on the queue. RF opines that making detailed automation controls part of MXCuBE may not be necessary – Global Phasing workflows trigger all that is needed once they are being acquired on the queue, alternative workflows could do the same, and this could be done using existing queue objects as building blocks. There is, however, a need for applying intelligence in selecting what operations should be carried out, and under what conditions, which could be done as an outer, controlling layer rather than by replacing existing blocks. MS suggests that it would be useful to see this as an opportunity for clearing up the code around the queue, with an emphasis on using message passing.

It was agreed that these topics should have assigned leads, to be selected among those motivated, but no leads were actually assigned at the meeting.

ISpyB

JG raised the question of who were *not* using ISPyB. ALBA is planning to bypass ISPyB and go directly to ICAT for their new Xaira beamline. MH notes that Berlin is not using ISPyB, but has just added a dummy ISPyB object to keep MXCuBE happy.

MO, passing messages from ESRF, reports that ESRF is currently using both ISPyB and ICAT for data upload. Changeover to ICAT will happen ASAP, after the next shutdown. AdM has made a start on an ICAT/ISPyB abstract LIMS layer, using Pydantic, which is still WIP and getting into testing.

RF asked to what extent the ICAT / ISPyB / Abstract LIMS development was purely internal to the ESRF, as opposed to involving also other synchrotrons.

Half-yearly meeting

The next half-yearly meeting will be on 20 November, at Elettra.