MXCuBE Developer's Meeting

Whereby, March 4, 2024

Meeting Minutes

DRAFT

Participants

Rasmus Fogh (Global Phasing)

Marcus Oscarsson, Antonia Beteva (ESRF)

Andrey Gruzinov (DESY)

Elmir Yagudin, Fabien Coronis, Mikel Eguiraun (MAX IV)

Martin Savko (SOLEIL)

Alessandro Olivo (Elettra)

Annie Heroux (ex Elettra)

Michael Hellmig (HZB)

Boyi Liao (NSRRC)

Dan

March code camp

The dates for the code camp are being set at March 14 and March 22, both for a half-day, e.g. 10h-14h CET. The topic is Documentation. An additional half-day or meeting may be set up between those two dates. EY proposes to begin with an introduction to the documentation tools, Markdown, etc. (**ACTION: EY**), after which we should split into small teams, each to document a specific area. The results should be presented as pull requests.

May code camp

The May meeting is pencilled in for May 28-30, but the dates are not quite final yet. The May code camp will be done for the last day at the end of the May meeting at MaxLab. It is noted that that the May meeting will have ISPyB on the *first* day. EY would like to know the topic in order to prepare the agenda etc., but there is no agreement on that yet. The

proposals given most discussion time were to continue with documentation, and to start on Yaml configuration. We shall start an issue on Github to discuss the choice (**ACTION: MO**).

Working groups

Reports on working group topics:

Cybersecurity

All participants should be contacting their local IT departments. EY reported feedback from MaxLab:

Regular updates of libraries and code images; Multifactor authentication; Limit privileges (do not run programs as root); Configure system to deny everything, and then whitelist allowed actions; Use separate networks for different beamlines; Use in-house repository mirror for installation.

At MaxLab all access is via VPN, and access is open only during a session. This means that any access requires a VPN setup on your computer. The VPN allows entry to a specific host with limited access, which runs a browser. It is not possible to ssh from one beamline to another, but this can be done from the in-office wifi network. Machine control commands are done through a separate network, which can only be accessed through a specific Tango device.

At ESRF (MO) the setup is moving in the same direction as at MaxLab. A security audit has been done but the results are still being processed. ESRF will try to avoid requiring VPN for access, exposing MXCuBE but not the computer it runs on, using whitelists. ESRF will be using Keycloak two-factor authentication.

At SOLEIL (MS) a security audit is in progress. SOLEIL is about to deploy two-factor authentication. SOLEIL uses Globus rather than VPN, but it is hoped to retain direct (i.e. non-VPN) access.

YAML configuration

JO apologises for not having progressed on investigating a way to move smoothly from XML to YML configuration. It is agreed that this topic is one of the more urgent pending changes, and might be a good candidate for a code camp.

Centring

MS (SOLEIL) is working on the Murko centring program and still testing different algorithms and edge cases. A number of published algorithms (e.g. PCA-based) turn out

to be surprisingly unreliable. A result is expected within weeks, and will be checked in and shared when available.

MXCuBE queue reorganisation

MO apologises for not having delivered on documenting the existing system.

Abstract LIMS

RF informed of the current status (see https://github.com/rhfogh/mxlims_data_model). It was agreed (nodded through) that MXLIMS would be an appropriate name for this project. RF asked whether anyone was (planning to) use SciCat as the underpinnings of a LIMS system. Max IV and SOLEIL are using SciCAt, and DESY is moving towards it, but no one is planning to use it as an ISPyB replacement. BESSY (AG) plans to keep using ISPyB, as SciCat is not ready for taking over.

Unattended data collection (UDC)

MaxLab reports wanting to move ahead on unattended data collection, but are at the moment using a very old MXCuBE version.

Any Other Business

MO has disabled the code coverage check on github, since it systematically crashed when dealing with pull requests from other forks. All still active checks should now work, and settings will be changed to require all checks passing before a pull request can be merged. It is noted that everybody is now running pre-commit for pre-commit testing. There are some problems. AB notes that it is necessary for everybody to have the same version of black and other linters. It is agreed to pin the version of black and pylint in the requirements, Dan reports problems because he is using Python 3.10, but the pre-commit pipelines require Python 3.8 installed locally

EY raises the question whether to merge automatically Dependabot version upgrade PRs. MO responds that it is preferred to collect them and merge by hand after checking, e.g. monthly. This allows testing on beamlines and catching version incompatibilities. Fabien wonders if security upgrades (but not others) could be merged automatically, or if some facilities could be tasked with testing sets of libraries.

The need for changelogs is discussed. It is agreed that , if introduced, changelogs should be high-level and synthetic, a digest, and so there should not be any pressure to add an entry for every commit or PR. The decision whether to introduce changelogs is postponed, because the particular development structure of MXCuBE does not have the usual division

between developers and downstream users. It is suggested that we should try, for an experimental period.

AB is working on upgrading the XRF spectrum queue entry. Since she is producing a breaking change, she is asking who needs to be consulted. MaxLab is using the queue entry and recommends checking with Mikel Eguiraun.

RF announces that the Web interface for GPhL workflows is now ready for testing, and a release matching this interface will be announced shortly. He thanks Jean-Baptiste FLorial for his work in programming the web interface.