

# MXCuBE Developer's Meeting

Whereby, September 21, 2023

## Meeting Minutes

### Participants

Rasmus Fogh (Global Phasing)

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

Jacob Oldfield, (ANSTO)

Andrey Gruzinov (DESY)

Jose Gabadinho (ALBA)

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

Martin Savko (SOLEIL)

Alessandro Olivo (Elettra)

Nicolas Moliterro(LNLS)

### Working groups

It has been agreed to start a number of working groups to look at upcoming needs. The list of topics was reiterated to be YAML configuration, Cybersecurity, centring, queue organisation, and Abstract LIMS, and unattended data collection.

### YAML configuration

The issue of moving to YAML configuration files has been re-raised. RF noted that it had languished a bit since it was first decided, and that he (RF) had failed in his promise to provide a system that allowed a mixture of YAML and XML configuration, so as to simplify the transition. It is now actual again as people are seeing a need to use alternatives to XML for some complex configuration attributes. JO raised the possibility of using Pydantic. It was agreed to stay with the decision of moving over to YAML, but that an intermediate system to allow a gradual transition was necessary. It was agreed that we would need a YAML working group at some point. Meanwhile JO promised to look into ways to facilitate the transition, and report back. **ACTION: JO.**

## Cybersecurity

For cybersecurity the first task (still not undertaken) would be for developers to contact the local IT infrastructure departments and report on the result. The scope would include both installation, access controls, and hosting. It was noted that many things were completely outside the control of MXCuBE developers, and that the connection to IT departments was often thin. EY noted that at MAX IV the entire problem was solved by allowing access only through VPN, which also included having zero internet access during builds; all software was made available in local mirrors. It was agreed that people should start some general fact-finding, and that the next developers meeting should set up a questionnaire that would be sent to all sites to gather more specific information. MO volunteers to coordinate the questionnaire. **ACTION:** MO, All.

## Centring

It is noted that the Murko program for optical centring and crystal shape determination (MS, SOLEIL) is moving closer to production ready. So far the code is mostly in SOLEIL repositories. Once you have a 3D model of the crystal it becomes possible to register 3D points to centre on. JO volunteered that ANSTO would be able to test the program out at a non-SOLEIL beamline, since they are getting beam but will not have users in February. MS and JO will share background images for the purpose. **ACTION:** MS, JO

## MXCuBE queue reorganisation

One point to address is how to handle interleaving (MO), another the question of how the queue is structured and documented, duplications between Qt and Web implementations, and the signals etc. that put objects on the queue (RF). MO would like to move to a structure where the queue is organised as a series of Pydantic data objects. These structures would have a lot in common with the Abstract LIMS, and it would be desirable to use the same schemas if possible.

## Abstract LIMS

RF informed about the independent project to develop an interoperability data model that would meet the needs for an Abstract LIMS. Details can be found on the (since opened) web site [https://github.com/rhfogh/mxlims\\_data\\_model](https://github.com/rhfogh/mxlims_data_model). MXCuBE has an independent interest and independent goals in this area, and it was agreed that the MXCuBE developers should be kept informed and get the LIMS WG minutes (now available on the github site mentioned above). We should arrange a discussion limited to the MXCuBE developers directly involved at the next MXCuBE/ISPyB meeting.

JO underlined that the main focus of the project had to be *interoperability*. MO noted that the ESRF is fully engaged in building a new LIMS based on using ICAT as an underlying technology, but in the first instance using existing (ISPyB-based) data structures. The

results will be presented once ready; the approach for now is to make something, and then look at converging with the Abstract LIMS.

## Unattended data collection (UDC)

This is something that each site needs to do, where there is still not much experience sharing or standardisation, and a lot of hacky code. The topic overlaps with cybersecurity, and suffers from some of the same problems with close coupling to site IT departments. The need for an Abstract LIMS is in part driven by the requirements of setting up unattended data collection. The general opinion (including at MASSIF-1 that already runs fully unattended data collection) is that UDC should happen *with/within* MXCuBE. A session on UDC should be added to the May MXCuBE/ISPyB meeting

## Code Camps

It is agreed that the first code camp should happen remotely, with a March date. The best organisation would be two or even three successive half-days. **ACTION:** MO. A second code camp should be arranged in connection with the May MXCuBE/ISPyB meeting. It is agreed that the ISPyB meeting should be timetabled *before* the MXCuBE meeting this time, so as to allow for a code camp after the meeting, and that the meeting should avoid using Fridays.