

MXCuBE developers' meeting

March 29th 2022

Participants:

- Marcus Oscarsson, Antonia Beteva, Olof Svensson(ESRF)
- Rasmus Fogh (Global Phasing)
- Michael Hellmig (HZB)
- Clemente Borges (DESY)
- Bernard Lavaut, Daniel Homs (Arniac)
- Martin Savko (Soleil)
- Roeland Boer (ALBA)

Minutes: MO

Workgroup status - Diffractometer:

AB explains that there is a PR ([WIP] Abstract diffractometer #663) containing an AbstractDiffractometer class and a concrete example implementation. AB asks for input and comments regarding the PR. BL will once their current code is synchronized with the current master make an attempt to use the AbstractDiffractometer and try it with one of their MD3-Ups. MO explains that ESRF will try the new AbstractDiffractometer on ID29.

MS asks if anyone has seen or is using a diffractometer with a vertically oriented goniometer with the OAV in portrait mode/position. BL explains that this has been discussed but never put in use.

Workgroup X-Ray centring and Queue integration

OS and RF are currently working on combining Global phasing strategies with the ESRF BES workflows. That work have amounted to the creation of a Processing hardware object and a X-Ray Centring hardware object and queue entry.

OS and MO explains that the idea is to create a Processing hardware object that contains most of the basic processing functionality used by MXCuBE. The first implementation will use Celery to distribute the processing but this could later be made interchangeable. OS explained that the X-Ray centring routine will be brought from the workflows and made into a native MXCuBE routine. The first implementation will rely on the ESRF BES workflow but this could later be replaced by the Processing hardware object (for instance). There will also be a X-Ray centring queue entry.

MS asks when there could potentially be something ready to be used. MO explains that the intention is to develop and test the Processing hardware object on ID29 and that there likely will be something by the end of summer. The work on ID29 will almost certainly also result in a reworked collect routine.

Data- model/classes and possible new style task

MO explains that he made a PR (<https://github.com/mxcube/mxcubecore/pull/680>) that was discussed by himself and RF. The aim of the PR was to make it possible to export schemas for hardware objects with type hinted methods, so that the basic generic interfaces could be generated by the UI.

This feature is used by MXCuBE3 to generate basic “maintenance” interfaces as well as to generate interfaces for the beamline actions.

MO explains that an idea that still is being explored is to generalize the idea and create a Task object that is associated with a DataClass (exporting the same schema as previously mentioned). This Task object could then be used in the queue as a beamline action or as a “maintenance” task.

One flow

It was foreseen with a more in depth discussion around the One Flow branching model with the goal to simplify the current process partly based on Git Flow.

RF unfortunately arrived a bit late to the meeting and only had the opportunity to summarize his ideas. The main idea is to keep the current process, but to remove some of the intermediate steps of creating release candidates and instead only having a master (stable) branch and a develop branch.

RF also explained that the one flow process comes with a set of git usage recommendations that mantinas the git history clean.

Next Meeting

Next meeting in April. MO to send out a Doodle.