

MXCuBE meeting, SOLEIL, May 25, 2023

Minutes

Developers meeting

Meeting format

It is agreed that the next MXCuBE/ISPyB meeting(s) should be held over three days, not two, to put more time in the schedule. Proper information should be in real talks, with status talks shaved down. One proposal is to have status reports written up and sent out ahead of the meeting.

Status of pull requests

Martin Savko (Soleil) and Rasmus Fogh (GPhL) have some fairly big PRs coming up, that should be merged in before a release. ALBA will wait till after the release, as there is too much in hand to get ready beforehand.

Marcus Oscarsson (ESRF) notes that PRs in general are good to do also if still WIP, to communicate work in progress and solicit comments. RF notes that whenever possible PRs should be rebased on the current development tip, or alternatively marked as WIP, or, failing that, discussed.

It is agreed that from now on the minor version should be bumped for each PR to give a clear and distinct identity to all stages.

For the Qt branch MS, RF, and Andrey Gruzinov (DESY) agree to share the handling of PRs, as being the developers most involved with that branch; MO also promises to give them a look.

AG notes that as a matter of policy the master branch should **always** be in a functional state, which will require (RF notes) that it is checked out, installed and tested after changes.

Code camp

There are three topics for the code camp: The MXCuBE4 web version release (and how to code it), mxcube-core, and better documentation / code integration. All agree on holding the code camp, at some time after the summer. The meeting should be hybrid. The meeting should be at MAX IV; MAX IV has informal approval to hold the meeting – and the MAX IV people have difficulties being allowed to travel. The meeting should have two and a half days. The possibility of having parallel sessions was raised, but not agreed on.

Someone should put together materials (use-ready guide, simulator, etc.) so that people could install them on their laptop and do homework and preparation, particularly for the mxcube web work. Mikel Eguraun (MAX IV) will do a Doodle poll for dates

Any other business

MS notes that incorporation of the GPhL workflow serves as a mobilising factor for moving to the mxcube core/develop branch.

Peter Keller (Global Phasing) notes that with sample shape data becoming available, the connection between transmission, dose, and sample shape would deserve a closer look.

Steering Committee meeting

Collaboration agreement

The collaboration agreement is now going out to institute directors to sign. The new agreement revises the Steering Committee membership to account for new members, and it is REALLY IMPORTANT that this be signed in a timely fashion. The agreement is up for renewal in 2024 (Daniele de Sanctis, ESRF), and last time it took a year to get all signatures.

Meeting format

The next MXCuBE/ISPyB meeting should be over three days and two nights. Status talks should be strictly limited to 10min each, and slides and videos should be uploaded to the venue beforehand. The next meeting will be at ALBA sometime in December 2023.

It is noted that ISPyB participants cover fewer time zones than MXCuBE, and that this should be taken into account for scheduling. Also, sharing a scientific session between MXCuBE and ISPyB could be useful. GB seconds this proposal, and notes that setting some purely scientific targets to feed to the developers would be productive.

CATS/Bluelce/MXCuBE

BoYi had mentioned an interest in Bluelce, in part based on the impression that combining CATS and MXCuBE was problematical. SOLEIL is running CATS with MXCuBE and is offering to help on this point. It is noted that Beijing lacks a computer engineer at the moment.

To Developers

It is a strategic goal that *all* centrers should upgrade to mxcube core, and the Steering Committee wishes a report on this every six months. Developers should concentrate on sharing code, and the various sample recentering methods developed up to now should be put into the shared repositories.

The Steering Committee thanks the developers for their hard work.

Manpower problems

There are known resource/manpower problems, and the different sites are encouraged to inform each other about available positions so that other sites can steer promising candidates in the right direction.

Giufre suggests that participating sites could contribute money to hire external developers (as was done in the Tango collaboration); this could be put into the agreement at renewal. In the original agreement the 'participation fee' was man-hours matching 10-20% FTE for a site. DdS notes that this is a recurring point, but that it has been given up. It is too hard to find someone qualified to help, and too few beamlines in each case who can share the fruits. Matt Bowler thinks a membership fee could be problematic also with respect to what to do with unspent money. Gerard Bricogne (GPhL) also notes that external contracting requires quite precise specifications for what works needs doing.