

MXCuBE Developers web meeting

27th Jan. 2021

Participants:

- Marcus Oskarsson, Antonia Beteva (ESRF)
- Roberto Borghese (Elettra)
- Michael Hellmig (HZB)
- Ivars Karpics (EMBL Hamburg)
- Jordi Andreu (ALBA).
- Bo-Yi Liao (NSRRC)
- Lais Pessine do Carmo (LNLS)
- Martin Savko (Soleil)

Minutes: Marcus

Last meeting

Minutes approved

Additions to agenda

No additions

Site status

Marcus Oskarsson, Antonia Beteva (ESRF)

Just restarted after winter shutdown in full remote user operation.

New FLEX sample changer software from EMBL installed for Linux and Windows.

Worked on PR with Rasmus for the HWR 3.0 python package.

Lais (LNLS)

Currently in startup, have been working on code review and improvements in general PR with LNLS specific code and more general EPICS HardwareObjects that is meant to be shared with the EPICS community.

Marcus Oskarsson (ESRF) oscarssso@esrf.fr

Bo-Yi Liao, (NSRRC)

Constructing the beamline, TPS15-A, and network infrastructure.
Will soon start working on experimental control (EPICS) and MXCuBE3, using a MD3.

Roberto Borghese (Elettra)

Just restarted (In full remote operation), XRD2 beamline.

Working on the raster scans and the latest MXCuBE3 with Python3.
Running synchweb, IK asks how is the database populated. RB is using a modified ISPyBClient hardware object and using the SQL Python library from DLS.

Michael Hellmig (HZB)

In operation local users are still allowed on site. Some issues with the sample changer when doing remote, gripper from irelec does not work as foreseen.

Ivars Karpics (EMBL Hamburg)

Winter shutdown end of February startup (remote). Eiger 2 for P14, Eiger 1 will probably move to P13. Played with AbstractProcedure, Queue and DataPublisher, worked on separation of concerns. Deploying the latest HWR on P13.

Jordi Andreu (ALBA)

Working on helical and raster scans for the Xalloc beamline. Raster scans implemented using Sardana (No MD software used). Working on the Qt part trying to backport the current master version mesh scan feature to their frozen Qt MXCuBE. Basic feature works, hope to have a full solution in a few weeks.

Also hoping to be able to migrate to new HWR (Python3 and Qt5) as well as a new version of Sardana aim is to do this for and during summer shutdown.

Xaira installed optical elements, planning for a beam in the optical hutch for June.

Beamline are operational (remotely)

Martin Savko, (SOLEIL)

Starting implementing HWR master on PROXIMA2, interesting debugging case with misaligned samples, sample moved after final alignment.

Release of version 3

PR #605 (Hwr repository rename)

It was decided during the last meeting that HardwareRepository would change name and RF made a PR #605 introducing mx3core as a placeholder for the new name until a name had been decided.

MO continued the work and created a corresponding module and package name, with a setup.py.

Package/Module name (mxcubecore)

Agreed on the module name, *mxcubecore*, as discussed in the issue, [Python package name ideas #604](#), none opposed.

Setup.py and Bumpversion

Bumpversion to handle versioning and tagging is discussed. JA have previous positive experience with this tool and think it works well. The developers in general think it's useful with a tool that handles tagging and updating all version instances in one go. It's decided that Bumpversion will be used for the moment.

Pending PR's

- **[WIP] Fixes for setup.py in mxcube #607**
 - To be done after *PR #605 (Hwr repository rename)* is merged
- **LNLS site-specific config #608**
 - Can soon be merged, Lais to finish a few last things
- **WIP Hwr repository rename #605**
 - Discussed above RF asked to perform the last name change to mxcubecore. Developers asked to go through the new structure a last time before the PR is to be merged.
- **validate_value in AbstractActuator #596**
 - AB and MO to discuss with RF for a final update.
- **[WIP] PyISPyBClient to be used to read and store data via py-ispyb #58**
 - IK still working/investigating
- **[WIP] AbstractDiffractometer issue #276 #334**
 - To be closed and reopened in a different shape when the discussion on AbstractProcedures have been held.

AbstractProcedure

Ivars presents some work he did with AbstractProcedure, Queue and DataPublisher. IK proposed to use a schema based on JSON Schema to define data objects. These models are then attached to a queue entry that inherits a base queue entry that defines the execution steps.

MO mentions the previous work done with Pydantic also using JSON schema that could also be a good solution.

It's said that the approach is interesting in general and that dynamic import of schemas and entry logic would be a nice addition.

AB and IK makes the remark that the name AbstractProcedure should perhaps be changed to something else

It's decided that the topic should be discussed during the next meeting to specify what we want in more detail.

Next Meeting

The week of 22nd of February