MXCuBE ALBA Scientific and Developer's Meeting

November 29, 2023

Meeting Minutes

Participants

Peter Keller, Rasmus Fogh, Gerard Bricogne (Global Phasing)

Marcus Oscarsson, Antonia Beteva, Daniele de Sanctis, Axel Bocciarelli, Mael Gaonach (ESRF)

Jean-Bapriste Florial (EMBL-Gr)

Olga Merculova, Andrey Gruzinov (DESY)

Jose Gabadinho, Roeland Boer, Judith Juanhuix (ALBA)

Ana Gonzalez, Oskar Aurelius(MAX IV)

Bill Shepherd, Tatiana Isabet, Martin Savko, Dan Costin (SOLEIL)

Alessandro Olivo (Elettra)

Michael Hellmig (HZB)

Gleb Bourenkov (EMBL-HH)

Nicolas (LNLS)

Kate Smith, Ezequiel Panepucci (SLS)

Scientific meeting - Roundtable session

With mxcubecore getting stable and deployed on the various sites the aim was to identify the next set of areas to focus the development on and discuss what needs to be done to carry out that work. There are additionally few sites that have features that are of general interest and which can be standardised and transferred.

RF, MS and DdS opened the session by presenting a few slides. Thereafter followed discussions around some of the main topics; cybersecurity, abstract LIMS, centring, queue tasks and abstract diffractometer. Each topic was briefly covered and it was decided that working groups should be created for continued in-depth discussion on some of them. It was decided that the creation of the working groups should be handled during the next developers meeting (**ACTION MO**)

Cybersecurity

Recent events and the general situation in the context where MXCuBE is deployed requires more efforts to be made regarding cybersecurity. ESRF have recently carried out a security audit and will shortly be asked to implement stricter deployment routines. MO notes that work around two factor authentication is currently being carried out and will be made available shortly. A.Gonzalez mentions that the MAX-IV IT department applies very specific internal regulations on how software is deployed. As each site has a similar situation, with internal routines, it's decided that each site should briefly investigate what applies on their site and report back to the developers committee. A summary will be put together by the developers' committee and a common suggestion for a best-practice deployment could hopefully be made.

Abstract LIMS

So far all sites in the collaboration have been using ISPyB making the need for an abstraction layer in MXCuBE unnecessary. Today, however, it's no longer the case, with ESRF replacing ISPyB with ICAT, other sites already supporting SCI-CAT as metadata catalogue (SOLEIL, MAXIV) and some sites staying with ISPyB creates a need for a LIMS abstraction layer. Even more importantly, some sites, such as ANSTO, are not using an ISPyB derivative at all.

MO suggests that a thin abstraction layer should be created for MXCuBE, comprising the definition of the data exchanged between the LIMS and the methods needed to retrieve user and session information as well as upload of collection metadata. PK and RF suggest that there should be an effort made to create a more general LIMS abstraction layer that not only includes functionality needed by MXCuBE. MO clearly sees the need for a more general abstraction layer and that the MXCuBE LIMS abstraction layer would not prevent the creation of a more general solution. MO further notes that it is important with a solution that can be implemented in MXCuBE relatively soon.

Centring

MS presented how his software Murko could be used for re-centring and to create the concept of a reference frame attached to the sample. The idea was received with general enthusiasm. RF made a note in his presentation that the use of kappa in some cases greatly improves data collection quality and that a kappa calibration and correction routine is needed. RF refers to the work previously done by G.Bourenkov and that it would be of great value if this could be made widely available.

Queue tasks

RF and DdS both brought up that there are features that currently are site specific but potentially transferable and that could be implemented natively in MXCuBE.

Many of these could be implemented as queue tasks. MS notes that for instance the current implementation of interleaved data collection is quite complicated and sort of squeezed in the standard data collection and could benefit from being reworked. MO, DdS suggest that the X-Ray centring could be made available as a native method. RF suggests that implementation of more complex sweep patterns with multi-trigger detector execution would be a caondidate for such (a) tasks(s). A wider discussion regarding the granularity of a task follows, i.e what's a task and what's considered a workflow.

DdS and A.Gonzalez state that there is general interest in unattended data collections. G.Bourenkov notes that the majority of the efforts in unattended data collection lies in error handling and falls outside of the scope of MXCuBE. There is a general agreement that a request to Didier Nurizzo and Matthew Bowler from MASSIF-1 should be made to discuss what can be ported.

AbstractDiffractometer

JG and (Who else) mentions that it is difficult to use the GenericDiffractometer hardware object as their diffractometer is quite different from the standard Micro diffractometers. AB notes that the work on the AbstractDiffractometer is more or less done and could be used instead but needs a final review. It's decided that AB will re-open the PR for review **(ACTION AB)**.

Developers meeting

The discussions from the previous session continue during the developers session. MO asks if there are any other general topics of interest for instance blocking points to bring up. Nothing was reported at the moment.

The developers committee has been discussing the organisation of code camps on a regular basis, Especially after that the last code camp was held with great success. The idea is generally well received and the discussion is then focused around how the codecamps can be organised. MO and MH suggests that one of the biannual MXCuBE

meetings also should include a codecamp, and that the agenda of that meeting should be kept lighter so that the total number of meeting days in the end remain the same. MS makes the point that it's easier to get away from the everyday beamline work for shorter amounts of time and that it's an activity that requires a different mind set than a standard MXCuBE meeting. MS argues that the code camp would thus be better held apart from the MXCuBE meetings. A show of hands indicate that the prefered alternative is to host the codecamp together once a year together with one of the biannual MXCuBE meetings.

It's suggested that the developers committee would recommend that the steering committee should consider adding a codecamp to the next MXCuBE meeting.

Any Other Business

None

Appendix - Status of mxcubecore integration

Site	Python version	Virtual env	Current HWR or mxcubecore	UI	Manpower (of one full time)	mxcubecore status	Update to mxcubecore, roughly timeline
ALBA	XALOC:2.7 soon 3.9 XAIRA:3.10	conda	XALOC:HWR 2.2 XAIRA:mxcubecore	XALOC:Qt5 XAIRA:WEB	20-50%	XALOC:Testing XAIRA:BL commissioning	Summer 2024
ANSTO	3.9 soon 3.11	conda+docker	mxcubecore develop branch	WEB	25-50%	Testing Develop	Jan-Feb 2024
BESSY	2.7	conda	HWR 2.2	Qt4	50%	Testing Develop	Summer 2024
DESY	3.7	venv	mxcubecore develop branch	Qt5	50-80%	Testing	
ELETTRA	2.7 and 3.10	conda	HWR 2.1 and mxcubecore develop	WEB	10%	Testing	First half of 2023
EMBL-HH	2.7 and 3.10	conda	HWR master (2021 March) and mxcubecore develop	Qt4	0%	Testing	
ESRF	3.9.18	conda	mxcubecore develop and HWR master	WEB (4.5.0 for mxcubecore and 3.2 for HWR)	70% + 50% (EMBL Gr)	In production (develop + internal)	All beamlines during first half of 2024
LNLS	3.7	docker (podman) + conda	HWR 2.2 and mxcubecore develop	WEB	10%	Testing	First half of 2023
NSRRC	3.9.12	conda	mxcubecore develop and HWR master	WEB	10% ; 40% (2024)	Initial develop	First half of 2024
MAX-IV	2.7 and 3.10	docker (biomax), conda (micromax, and later	2.2 (biomax) mxcubecore develop	WEB		latest version in prod in micromax, testing	Q1 for biomax. Micromax already

							in biomax	done
			biomax too)	(micromax)				
SARI	3.7		Conda (Mamba)	mxcubecore develop branch	WEB	20%	Testing	
Soleil PX2	2.7			HWR 2.2	Qt4 moving to Qt5		Testing	
Soleil PX1	2.7		Conda	HWR 2,2 moving to MXCUBE CORE	QT4 moving to web	100% for 1,5 years	Testing	
ARINAX	3.7		venv	mxcubecore arinax branch derived from develop	WEB	90%	Testing	