MXCuBE web meeting 5 Feb. 2020

Participants:

Marcus Oscarsson, Antonia Beteva (ESRF)
Rasmus Fogh, Peter Keller, Gerard Bricogne (GPhL)
Martin Savko, (Soleil)
Lais do Carno (LNLS)
Roberto Borghese(Elettra)
Michael Hellmig, (HZB).
Bo Yi, (NSRRC Taiwan)
Jordi Andreu (ALBA), late arrival.

Apologies:

Ivars Karpics,(EMBL-HH).

Status reports

GphL Have mainly worked with strategy determination programs, but have also participated in discussions and refactoring of HardwareObjects and the AbstractActuator class. RF expects to do some detailed refactoring work across the code base as soon as the top abstract classes for Actuators are ready.

ESRF Have been very busy – they now have beam in the ring (but not the hutches). AB and MO have been working on MXCuBE refactoring (AbstractActuator) for the past week. MO was previously on BSXCuBE, with Jean-Baptiste. ESRF have now integrated a B-ZOOM. This included requesting and getting additional functionality from Arinax. There was for instance no facility for getting/calculating x,y positions (for beam positioning). The B-Zoom now comes with a full Lima plug-in, so the camera can be integrated in the same way as other image sources. The Lima plug-in is open-source and will be available on github, the drivers on the B-ZOOM are obviously proprietary. There is still some fiddly fixing going on on the Arinax side, and with network cards. It is hoped to get further improvements from Arinax, e.g. a choice of frame-rate modes, and the capability to fully exploit the 13-bit capability of the camera (as opposed to the current 8-bit images).The B-Zoom is quite resource-hungry – it is reported that it completely fills the capacity of a 4-CPU computer. As one of the CPUs seems to be fully dedicated to the license server, there may be room for improvement.

HZB No time for MXCuBE work, with work on new instruments (SampleChanger, new BeamDefiner (SmarAct). The next step is a new Pilatus 3, 6M detector for beamline 41, which will allow the MAR detector on the fixed energy end station to be retired, leaving HZB with only pixel detectors. Once that is done there should be more time for MXCuBE.

NSRRC These are still early days; and work is progressing on writing the code for connecting the hardware to MXCuBE, MD3, SPEC, . Commissioning is next month. NSRRC is using the Web version of MXCuBE (as are ESRF, MAXLAB, Elettra, and LNLS).

Elettra MXCuBE v3 and its installation are maturing. The first demonstration of remote access (from India) was run in December and was a great success. There are some outstanding questions on how to set up AautoPROC for running on a cluster – which, as it turns out, are awaiting answer from GphL.

SOLEIL Martin Savko has found and fixed a bug that caused delayed program crashes after collection abort. The mechanism is still obscure, but force-clearing the ready_event proved to solve the problem. There has been a problem with the sample-detection of the diffractometer, caused by a loose cable and slip ring (after 8 years of operation); the diffractometer will be sent to Arinax for repairs. The automatic optical centring is being implemented also on PX1. It is clarified that the autocentrign program should be fairly easy to port to other sites – it is a single Python file. The default (and fastest) operation requires pre-acquired background images, but there is an alternative mode where background images are acquired each time with the sample moved out of the way.

LNLS There is local approval for an MXCuBE meeting in Brazil, and the proposal now awaits Steering Committee approval. The proposed dates are 16-18 November 2020, to match up with their annual user meeting the previous week. Lais is starting work on the Machine_info refactoring, and a Pull Request is expected soon. The docker running MXCuBE3 is now on github, and will soon be PR'ed to the master branch. MXCuBE3 has been installed for another beamline, a SAXS beamline, for familiarisation purposes. MO is interested in feedback from the LNLS SAXS people, and LdC promises to send the local config files.

ALBA has been debugging their installation, working on a year-old frozen branch, and installing a B-Zoom. Jordi requests that other developers (re)engage with the open github issues.

Code camp and Refactoring

MO summed up that the code camp had been very productive (if a bit intense) and should definitely be repeated. The possibility of participating remotely should also be kept, even though the practical working of this was somewhat deficient on the first attempt.

The refactoring of AbstractActuators and related areas is well in hand. MO has already incorporated and tested the changes made so far, and is happy with the new clean code. AB volunteers to take care of the next abstract class, AbstractNPosition, which is gratefully accepted. RF will refactor all relevant HardwareObjects to use the new abstract classes once this is ready. Once this is done, the remaining parts of the ongoing refactoring would

be the Beam object, Collect, Machine_info, and SampleVIew (was Microscope), but none of these are expected to be as disruptive or all-encompassing as the Actuator refactoring.

Any other business

None

Further Meetings

There is agreement that the next Code Camp, for documentation and testing, should definitely go ahead. Unfortunately ESRF management is reluctant to allow the necessary time resources any time soon. It is proposed to hold the code camp in connection with the next MXCuBE meeting, but MS notes, to general agreement, that a dedicated meeting is likely to be much more effective. MS volunteers to organise the meeting at SOLEIL. The issue should be investigated further.

The next web meeting should be held a month from date, and MO will send out a Doodle poll