MXCuBE meeting

Hamburg 20250520

Developers' meeting

Present:

YAML configuration

Agreed that people will at least try out yaml configuration on a real beamline before next half-yearly meeting, with a view to have integration by May meeting (for those who are not far behind, anyway). For the process you should move over xml to yaml configs, and at the same time make pydantic models to represent the config. ESRF will begin looking at pydantic models. The process should be followed at monthly meetings. The agreed file extension is '.yaml'.

Out-of-date config files should be removed from repos, but there is demand for a place to see current configs, for inspiration and imitation. Pydantic will help once it is there, but till then there is still a need. It was temporarily agreed to look at using a private repo to put it in, to keep configuraton data out of the public eye. ESRF will check if we can get a private Github repo or ESRF Gitlab, PK if we can use the GPhL github account if needed. ACTIONS: PK, ESRF. Unmodifiable configuration files (MK3??) to be kept visible somewhere.

MO has been looking at getting mock mode simulation for Arinax FlexSC and Lima detector and would like to use this to build a better mock beamline.

Collaboration

Agreed to have a slot in developers' meetings where you talk about interesting ongoing/started work, to avoid different groups doing the same thing alone in parallel. Send in bullet points beforehand, talk as needed / requested. Should avoid time consuming status report phenomenon

Automation

The point was discussed both in connection with the talks of Didier Nurizzo and Martin Savko, the developers' meting proper, and the automation section of the code camp. The results are presented together.

MXLIMS should be used for specifying queue input – given that the MXLIMS model was based on the queue model objects in the first place. The current activity and the biggest need is to define the model for X-ray centring.

The X-ray centring model should define the allowed input parameters and leave it to per-beamline configuration to set defaults and define the procedures to use rather than trying to model all possible strategies. Gleb Bourenkov notes that you need beamline-specific subclasses as well as configuration parameters.

It is agreed that:

- Line scans are (becoming?) obsolete, and the new approach is to use multiple mesh scans
- X-ray centring input should be a volume of interest. In some use cases (re-centring) this could be just a 3D point with default volume, in most current situations a cylinder or box, eventually a precisely defined volume such as a point cloud.
- The X-ray centring process also needs to include processing.
- There is no need to specify X-ray centring as an explicit series of mesh scans. Rather the basic unit should be a block of n mesh scans rotated relative to each other to cover a volume.
- There should be an AbstractCentring hardware object to unify input and output, and allow calling the locally preferred centring routine in a uniform manner.

Martin Savko presented the status of his Murko optical centring program at the meeting. The program has the potential to provide many detailed results, but some (particularly determining precise crystal volumes) still require research. The closest achievable result would be to use Murko to determine a crystal coordinate system and to re-centre by superimposing the overall volume. Whatever functionality is supported, it would be ideal to have a Murko hardware object for easy integration. Gleb Bourenkov noted that for detailed reconstruction the process had similar requirements to tomography. Martin Savko envisaged a 'Sample environment' model that would hold detailed information on coordinate systems, volumes and shapes, points of interest etc. The meeting liked the idea, but accepted that a simpler centring model might be required as a first step pending the availability of routines to determine the sample environment in detail.

In the specific context of MXLIMS the meeting was not particularly interested in specifying jobs (experiments, processing) explicitly as nested subjobs. For X-ray centring the chosen approach mostly make this inappropriate anyway. For the more general case it is clear that a queue

specification needs mainly to specify the time order of the steps, but this could be done by tree traversal as well as by a linear list. One way or the other it will be necessary to group the various sub-experiments (characterisation, centring, which sweeps to merge and process, multi-crystal experiments, …) to allow searching and processing. As a first step RF will try to get an overview of the systems of identifiers currently used in various places for this purpose, and see if this would be an easy replacement for a nested subjob structure – ACTION RF.

Code camp

There was some dissatisfaction with the short time effectively available for the code camp, between the synchrotron visit, the morning talks, and the need for people to leave early on the last day. The next meeting will not have a code camp, but there was agreement on doing better next time, be it through having a dedicated code camp slot, or through changing the format.

Steering committee report

Next meeting 17-19/11 at DLS. Long meeting with science day, not code camp.

Topic: automation and large scale (computing?).

The progress of adopting mxcubecore is commended. The LS-CAT accession is postponed a little, as Solaris is looking at documents in order to join as well, so that both can be added to agreement at the same time.

The automation WG work is also commended and asked to continue, and other WG are asked to follow in the footsteps of the automation WG.

Quotations for a cybersecurity audit were inconsistent. The goal remains to finish by end year and get some certifications.

MW recommended putting more into PR work, and putting this topic on the standard six-monthly meeting agenda. The proposal was well received. It was considered to have a Linked-In profile for MXCuBE. Who would do it, though, and ensure enough traffic? Gleb will check with the EMBL PR team. Mabe this should be done with/through institution PR, since those already have followers.