2025-09-05 MXCuBE AutomationWG

Agenda:

1. Definition of the input parameters for X-ray centering
2. Definition of the output parameters from X-ray centering (if the time allows)

Notes:

Introduction to the new comers on the aims of the Automation WG.

Point 1:

- Crystal parameters:
    - From the meeting in May, one of the action was "Martin and Rasmus to implement the "Volume of Interest" definition and implementation in MXLIMS" (see minutes). For the time being, we decided to restraint the "Volume of interest" as a 3D rectangle.
    - Renaming "crystal parameters" to "sample parameters" to avoid confusion with unit cell etc...
    - Discussion on whether to include additional information such as loop type ((mitegen, etc...) or the composition of the liquid in the loop (heavy atoms, etc...). These are more related to the sample environment than to X-ray centering itself.
    - The sample parameter is the volume to scan, not just the crystal volume which could be extracted from Murko for example
- Beamline parameters:
    - Keep the same as those already defined for any data collection.
    - Discussion on the X-ray dose to be deposited during centering which depends on the transmission factor. This parameter will be part of a configuration file that would be defined by the beamline staff.
    - The X-ray sensitivity of a given crystal should be defined at the level of the sample, not at the level of X-ray centering even though this parameter will be taken into account during the process.
- Acquisition parameters:
    - Keep the same as those already defined for any data collection.
    - Default parameters to be set in a configuration file by the beamline staff, with the option to adjust based on sample-specific information such as crystal size and sensitivity etc ...

General remarks:

- X-ray centering is a process that allows positioning the crystal in the X-ray, A higher level of decision making layer should be integrated in the general workflow to decide how many times centering should be performed or whether to adjust some parameters after a failed attempt e.g. increasing the transmission, in order to reduce the logic inside the process.
- The number of meshes to be used for centering should be decided by the beamline staff. The input is the number of orientations required to perform the N meshes needed for centering.

The next meeting will be dedicated to the output parameters. Participation from colleagues in data processing is welcome.