# 2025-03-14 MXCuBE AutomationWG

# Agenda:

Following the inputs we received, the tentative agenda for the Automation WG meeting (tomorrow 1:00 pm) for defining the steps of the X-ray centering:

1. Area definition of the mesh from Lucid, Murko or other approach ?

2. number of mesh scan (1, 2, 3 or more?): All sites are moving away from line scans and want to put in place mesh scan instead?

3. Processing and outputs: How do we launch? Which outputs do we need? How do we retrieve the outputs?

4. How can we integrate all of these in the MXLIMS framework

## Notes:

Several answers from different sites (MaxIV, Soleil, ANSTO, EMB-Hamburg) gave the information on how the X-ray centering is done on their beamline. Starting from this, the discussion came on the points of the agenda:

#### Point 1:

- Instead of defining a 2d area a definition of a 3D volume would cover all cases. Martin will provide a definition of this volume
- The volume definition will come from different software that are already in use. This discussion will be driven by the sample environment WG Martin is chairing
- The volume could be reduce to a 2D area if the sites does not need the definition of a 3D volume
- The volume definition will have to be incorporated in the definition of MXLIMS by Rasmus

#### Point 2:

- Line scan will become obsolete in the near future. It should not be implemented and only keep the option of 2D-mesh
- The mesh parameters for the data collection will be defined by the beamline in different config files as a method (coarse grid versus fine grid, small grid versus large grid, etc,,,)
- The method will include the standard DC parameters (resolution, transmission, exposure, etc...), the beam size, fast axis and slow axis of the 2D-mesh

• The number and type of the mesh scan to be done for the X-ray centering will be defined as a list with angle and methods. This option also covers the option of multi sweeps with a need of recentering between sweeps (kappa re-orientation)

#### Point 3:

- The processing of the 2D mesh images starts as soon as the mesh starts
- in a first instance it should output only the list of diffraction spots
- If the beamline has the Dozor, dozorM, XDS, Dials or any other programme to characterize the diffraction images, the processing will be launched also (this option should be configurable)
- The outputs:
  - presence or absence of any crystals in order to decide to have the option of stopping the X-ray centering if there is no diffraction
  - best positions. This must be a list depending of the software in use if it is able to differentiate between multiple patterns like dozorM does
  - resolution to be able to adjust the detector distance during the next step
  - size of the crystal to adjust the transmission/exposure and reduce radiation damage

## Point 4:

- The MXLIMS framework is able to cope with most of these definition above
- Some adjustment to be made depending on the future implementation
- Martin to provide 3D model definition and Rasmus to define the implementation in MXLIMS