

# 2025-05-13 MXCuBE AutomationWG

## Agenda:

1. Definition of the input parameters in MXLIMS (implementaion, data format, etc...)
2. Fitting MXLIMS in the QueueModel Object
3. Redefinition of the QueueModel Object to integrate MXLIMS input parameters

## Notes:

### Point 1:

- The QueueModelObject in MXCuBE includes:
  - Crystal parameters
  - Beamline parameters
  - Acquisition parameters
- In the crystal parameters,
  - Definition of the "Volume of interest" will come from the software doing the alignment optically (Lucid, Murko, etc) or using a X-ray centering (coarse grid):
    - The "Volume of interest" is not defined as a scalar but as 3D volume is space to be converted to motor position
    - The "Volume of interest" is not be restricted to the crystal itself.
    - The "Volume of interest" include a margin provided but this margin will be calculated inside the alignment software. The margin could be un number of beam size in the 3 direction
    - The orientation of the "Volume of interest" in the beam (omega position) showing the largest or the smallest projection perpendicular to the X-ray beam comes from the alignment software and passed to the beamline parameters
    - The number of meshes to be done inside the "Volume of interest" is configurable by the beamline
  - In case this volume is too big and the mesh would take too long, it will be possible to reduce it accordingly (case of microbeam and large crystals).
  - The "Volume of interest" would be used to calculate the 2D region for the mesh scans ("Line scan will become obsolete in the near future" - MXCuBE Automation WG minutes 2025-03-14)
  - A default volume is needed (beamline configuration) for the option of doing X-ray centering at the current position

- Definition of the crystal sensitivity to X-ray to adjust the exposure time during the X-ray centering

Point 2/3:

- MXLIMS has been based from the QueueModelObject. All parameters that are used in this MXCuBE model should be transferable in MXLIMS

### **Actions:**

- Martin and Rasmus to implement the "Volume of Interest" definition and implementation in MXLIMS
- Rasmus with discussion with all MXCuBE developers to investigate the feasibility of using MXLIMS for inputs (and later outputs) of the automating X-ray centering. This discussion will be wellcome in the Automation/UDC and Queue discussion