

2026-10-12 MXCuBE AutomationWG

Agenda:

- Recap of previous decisions
- A round-table check-in to confirm everyone's on board
- Action plan going forward

Notes:

A brief introduction on was previously discussed. Marcus presented an early draft pull request summarizing the principle: [mxcube PR #1680](#). The current code runs several mesh scans at different omega angles to determine a crystal's diffracting volume.

Orientation and bounding box

MXLIMS allows the bounding box and the omega angle to be defined. The optical centering performed before the X-ray centering could present the crystal in different orientations, such as the largest or smallest surface perpendicular to the beam, or any other orientation.

Scanning strategy

- The first scan relies only on optical information, either a user-supplied bounding box or the result of the optical loop centering.
- Subsequent scans give priority to the X-ray results of previous scans, even if the size of the surface to scan is derived from the earlier optical centering. The output of one scan becomes the input of the next.
- Questions were raised about efficiency, and whether it would be simpler to scan the whole volume defined by the optical analysis. One suggestion was to let scanning continue while processing jobs run in parallel. One option is to scan only at 0° and 90° , then add 45° increments with nested meshes, refining until the volume is stable. This raises the issue of radiation damage.
- Two projections already give a rough idea of the volume to scan. The current PR does not support nested meshes. It was concluded instead to offer the option of relaunching the X-ray centering with finer omega steps to refine the volume.

Processing and results

- At the time of the presentation, the PR included neither the image processing launcher nor a way for MXCuBE to retrieve the quality indicators.
- The WG should agree on a standard output for the image processing job used in X-ray centering. A minimal layer, such as a “processing_results processor”, could make results MXCuBE-compliant.
- This connects to how quality indicators are displayed over the crystal image in MXCuBE, which was discussed in the UI/UX working group.

- The result of the Xray centering could be a point cloud with quality indicators. How it is used is deliberately left outside the X-ray centering procedure, to keep it generic.

Next steps

- Test the X-ray centering functionality before moving on to other automation topics.
- Test the PR at ESRF first, then at other sites to check transferability.