

2025-01-20 MXCuBE AutomationWG

To inform: [Didier Nurizzo](#) [Marcus Oskarsson](#) [Daniele De Sanctis](#) [Estelle Mossou](#) [Matthew Bowler](#) [Romain Talon](#) [Max Harunobu Nanao](#) [Montserrat Soler Lopez](#) [Antonia Beteva](#) [Yan Walesch](#) [Wout De Nolf](#) [Johannes Kamps](#)

Minutes of Meeting

Approval of Minutes:

- [Minutes](#) of the previous meeting have been approved.

Agenda:

The aim of this meeting is to discuss how x-ray centering is performed at the different sites in order to find a suitable consensus before its implementation in the core of MXCuBE. A detailed description is needed in order to define the level of abstraction that could be then transferred in the code. We divided the discussion as follow:

1. **Modalities of X-ray Centering:**
 - **Types of scans:** Linear vs. helical.
 - **Number of scans:** 1D vs. 2D.
 - **Processing of the scans.**
2. **Required Inputs and Expected Outputs:**
 - **Inputs:** Needed for X-ray centering based on the chosen modalities.
 - **Outputs:** To include the optimal position, the region of greatest interest, resolution limits, etc.

Notes:

1. During the meeting on December 16th, it was decided that "all sites are invited to deposit the information they would like to have as input and output for X-ray centering in the GitHub discussion."
2. Rasmus provided useful [information](#) in our GitHub [discussion](#).
3. A tour de table was conducted to gather inputs and outputs used by different sites to run and process X-ray centering:
 - **ESRF:**
 - Optical centering (automesh) defines a rectangle where the 2D mesh will be performed.
 - After a 90° rotation, a line scan is collected with a default length.
 - Parameters for data collection are default values provided by the beamline and/or embedded in the AbstractDiffractometer.
 - **Soleil:**
 - Optical centering using MURKO allows up to five helical scans at different angles.
 - Future updates may replace helical scans with line scan data collection using the MD3 diffractometer.
 - **MAX IV:**
 - A 2D mesh scan is followed by a line scan after a 90° rotation.
 - **ANSTO:**
 - Optical centering using OpenCV defines two rectangles at 90° apart.
 - Two mesh scans are performed based on these rectangles.
 - **SIRIUS:**
 - No X-ray centering implemented yet.
 - Optical centering aligns the crystal center with the beam.

Discussion Points:

1. **Definition of X-ray Centering:**
 - As a job, procedure or method. For now, all definitions remain interchangeable and further might be needed in the future to clarify this definition
2. **Incorporating Optical Centering:**
 - It was decided to keep optical centering as an independent method rather than integrating it into X-ray centering.
3. **Inputs for X-ray Centering:**
 - The **volume** for scans, with options to simplify it to a 2D polygon or a single point.
 - The **motor positions** of the diffractometer defining the volume. An example of the calculation that has been developed by Martin for Soleil would be welcome.
 - Most parameters will be beamline default values, with user-overrideable options for resolution, beam size, and exposure time /transmission, etc...
4. **Action Items:**
 - Gather all input information used on different beamlines for X-ray centering.
 - Upload this information under the [Automation/UDC and Queue discussion](#) in GitHub.
 - Contributions are particularly encouraged from SSRF, BESSY, and Hamburg before the next meeting.