

2024-12-16 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](#)

Notes

- Introduction to the automated ESRF MASSIF-1 data collection steps.
 - Sample loading (it could be lead by a unload step)
 - optical centering
 - optical analysis of the loop over 360° (called "automesh" at ESRF) to find the largest area of the loop to be scanned by X-ray during the first 2d mesh of the X-ray centering
 - X-ray centering:
 - 2d-mesh scan using the area defined during the automesh
 - line scan at 90° on the hottest point of the 2d-mesh. In the near future we will have the option of replacing this line scan with an other 2d-mesh around the hottest point
 - Characterization
 - Data collection

With each of the last 4 steps , the autoprocessing is launched as part of the Workflow. These steps cover the entire process of "data collection automation" if we keep in mind that all the steps can be rearranged in different orders and called several times in case of data collection with helical translation, multi-sweeps, kappa- reorientation, etc... For the time being all these steps are embedded in different types and Workflow engines meaning they are not part of MXCuBE. The aim is to create abstract objects for some or all of these steps that will cover all the actions required for producing an accurate result. It is noted that not all sites use Arinax goniostats (e.g. Smargon), but the MXCuBE AbstractDiffractometer should handle this.

- Some elements needs to be left to the discretion of each sites
 - the option of launching the processing job inside MXCuBE
 - the option of using local developments for automation instead of the steps cited above. The way to populate the inputs could be done via popups in the interface but this is not part of the scope in the automation WG where all the processes are done without human intervention. Populating inputs is left to LIMS.
- Replacement of XMLRPC:
 - the exchange of information (input and output from processing) needs to be done using JSON format
 - a rest API could be one of the option but it needs more thoughts if any other message queuing protocol would be of interest
 - Any choice to be made will have the possibility of populating the MXCuBE queue from outside

The work on data modeling already done in MXLIMS (https://github.com/rhfogh/mxliims_data_model/tree/rhfogh_develop) and others will have to be incorporated in the discussion to define the needs of Inputs and outputs to be given and retrieved from the abstract object that are defined in the automation data collection cited above.

It is agreed that the first step to model, also to start the ball rolling, is X-ray centering with a development of an AbstractXrayCentering. Next meeting in week 3 or 4 (a doodle will be sent in the next days or so). It would focus on the data model to be provided to the X-ray centering step. In order to prepare for this, all sites are invited to deposit the information they would like to have as input and output for the X-ray centering in the GitHub discussion <https://github.com/mxcube/mxcubecore/discussions/categories/automation-udc-and-queue>