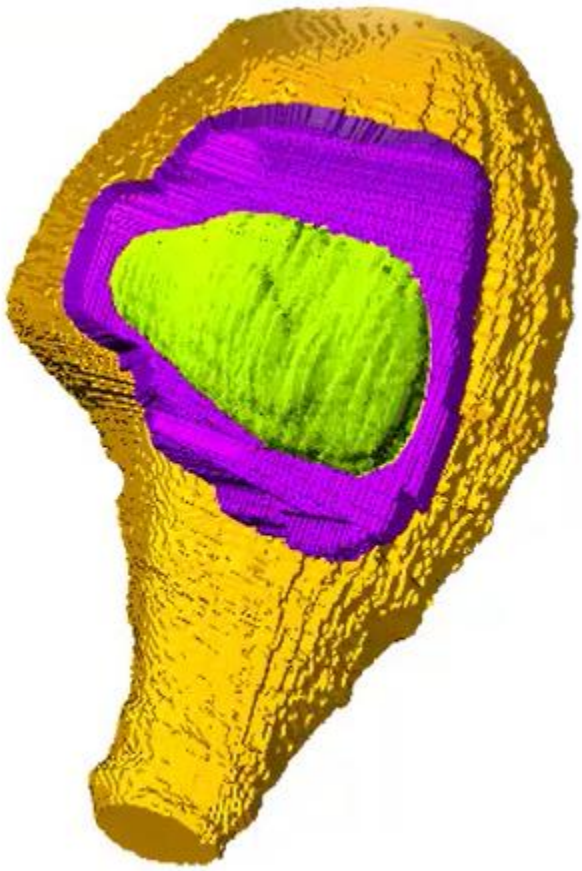
2026-04-07 MXCuBE AutomationWG

Agenda:

1. Further discuss the output of the X-ray centering
2. Up coming tasks

Notes:

- Rasmus and Martin proposed a definition of the diffracting volume based on this type of volume coming from Murko:



Yellow: Volume of the loop, Purple: diffracting volume, Green: best diffracting volume

The implementation in MXLIMS could follow this type of framework:

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  - The VolumeScan is defined with:

        - experimentType (string)
        - rotationAngles (list of floats)
        - searchVolume (PointCloud)
        - boundingBoxSize (list of float) in the OAV coordinates
        - boundingBoxShape (string)
        - resultVolume (PointCloud)
        - subolumes (list of PointCloud
    - PointCloud are:
        - best position (a dictionary of string with float) for motor position that are common for all the points
        - grouping (a list of integer) as 0 is background, 1 is crystal1, 2 is crystal2 ....
        - motorPosition1 (list of float) offset from the the previous best position
        - motorPosition2 (list of float) offset from the the previous best position
        - motorPosition3 (list of float) offset from the the previous best position. The 3 last positions could be all put together as a triplet instead.
        - quality (list of float)
        - etc....
- The PointCloud is converted in motor position for MXCuBE as an output of the X-ray centering
- Matrix of indicators indicators should be kept open for one to be able to add any new indicator to the list:
    - dozor score
    - maximum resolution
    - number of spots
    - I / sigI
- Definition of the matrix of indicator should be per point
- Selecting the BEST part of the crystal is not part of the X-ray centering bit left to decision maker later on.
- The default quality indicator of the matrix could be defined in a YAML file
- Showing the results of the indicator matrix in MXCuBE means that the definition of the quality indicator must be introduce in MXCuBE.
- Abstract diffractometer is now available. The Xray centering can be introduce so.
- Marcus and Antonia will draft a PR to define the volume scan to be the first part of the Xray centering.
- The display of the results in MXCuBE is more part of the discussion the MXCuBE GUI WG.