

MXCuBE status report

Global Phasing

MXCuBE/ISPyB Meeting, Trieste, November 2024

Brief beamlines summary

- We have no beamlines of our own
- autoPROC processing software is in use at all MX beamlines, and by end users
- Global Phasing acquisition workflow is integrated with MXCuBE
 - Functioning or being integrated at EMBL Hamburg P14, ESRF Massif-1 and ID30B, SOLEIL PX2, ALBA Xaloc, and MAX IV BioMAX.

- The workflow follows the local implementation
 - GPhL code is beamline-agnostic, as it must work at multiple sites
 - The code is kept up to date with the MXCuBE develop branch
 - Site-specific branches are disfavoured
 - We support both Qt and Web interfaces, using popup UI windows specified with JSON Schema
 - autoPROC runs in stand-alone mode, but results need integration with local LIMS/viewers
 - Multi-sweep experiments and detailed processing quality output go well beyond the standard templates
 - Cybersecurity is NMR ('Not My Responsibility')
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Developments since last meeting

- Progressed workflow integration and testing with Massif-1 to get ready for routine production use
 - Added extra attributes to AcquisitionData needed to support treating data in ISPyB-DRAC LIMS.
 - Multiple visits to MAX IV to set up workflow integration, to be used for unattended operation
 - Tackling problems in using HDF5 files for storing complex and interleaved sweeps.
 - Collaborated on setting up X-ray centring so that it can be called programmatically from mxcube core (GPhL workflow). *In progress.*
 - Written prototype MXLIMS exporter from MXCuBE queue
 - Described in more detail in ISPyB session talk
 - Solved problem of auto-estimating transmission for large crystals with small beams (to be merged)
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Plans for the next six months

- Collaborating on making GPhL workflows available to normal users at interested beamlines
- Completing a first usable version of MXLIMS, use it for import/export of data to GPhL software, and collaborate with others on expanding MXLIMS
- Submit Stratcal paper for publication
- In the longer term: Complete mark 2 set of improved acquisition strategies for the GPhL workflow.

GΦL

Global Phasing Limited

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