Global Phasing Limited

MXCuBE status report

Global Phasing

MXCuBE/ISPyB Meeting, Diamond, 19 November 2025

Global Phasing Ltd 2025

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Unchanged 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 data acquisition Workflow is integrated with MXCuBE
  - In production at EMBL Hamburg P14
  - In various stages of '*watch this space*' at ESRF MASSIF-1 and ID30B, SOLEIL PX2, ALBA XALOC, and MAX IV BioMAX.

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Unchanged MXCuBE status

- 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 pop-up 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

- No progress on Workflow integration outside P14. *Unchanged*
- Participated in Automation WG on modeling and setting up X-ray centring
  - added MXLIMS model of X-ray volume scan (for centring or crystal finding).
- Various improvements to MXLIMS model
- Testing MXLIMS-synchrotron integration for sample submission
  - Thanks to Zac Panepucci (MAX IV), Dennis Stegmann and May Sharpe (SLS), Ed Daniel (IceBear), and Guilherme de Freitas (Diamond)
- GPhL Workflow
  - Submitted StratCal paper for publication
  - Continuous use, testing and improvement of the GPhL Workflow, in collaboration with EMBL-HH P14 (Gleb Bourenkov) and the Ashwin Chari (Goettingen) group

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Plans for the next six months

- Collaborate with anyone interested in making GPhL Workflows available to normal users at MXCuBE beamlines *Unchanged*
- Improvement and promotion of MXLIMS standard and API
  - Complete X-ray centring modelling, and further extend model as needed
  - Collaborate on testing Sample shipment with MXLIMS
  - Collaborate on testing API-driven integration with synchrotrons
  - Further development of MXLIMS collaboration, *seeking input and collaborators*
- In the longer term: Complete mark 2 set of improved acquisition strategies for the GPhL Workflow. *Unchanged*

END