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Global Phasing Limited

Status Report for Global Phasing Ltd.

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Global Phasing Ltd, Cambridge, UK

MXCuBE-ISPyB Meeting, 29-30 November 2023, ALBA

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Summary of Main Activities

- Active participation in developers' meetings for MXCuBE and MXCuBE3 frequently including the writing up and broadcasting of Minutes (Rasmus Fogh). **We are up to date with the development branch.**
- Participation in the MXCuBE Code Camp (9-11 October) at MAX IV (Rasmus Fogh).
- Continued development and deployment of the GPhL Workflow and its associated autoPROC-essing at MXCuBE synchrotron beamlines (Rasmus Fogh, Peter Keller, Claus Flensburg, Clemens Vonrhein), especially
  - on P14 at EMBL-HH (Gleb Bourenkov) with MPI Göttingen projects (A. Chari)
  - on MASSIF-1 at ESRF/EMBL-GR (Olof Svensson, Matthew Bowler)
  - on PROXIMA-2A at SOLEIL (Martin Savko, Bill Shepard)
- Progress towards a UI for the Workflow to run with MXCuBE3 (Rasmus with Jean-Baptiste Florial at ESRF).

The Global Phasing Workflow on EMBL-HH P14 after ~~2~~ 3 years of routine operation

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Overview

- Uses a separate side-branch of MXCuBE2 (Qt)
- Over ~~1500~~ 3000 high-quality datasets collected
- Asymmetric unit contents ranging from 21 kDa to 2.5 MDa
- Various ligand soaks and enzymatic reaction intermediates
- Resolutions ranging from 3.2 Å to ... ~~0.59~~ 0.55 Å !!
- Work reported at the GRC 2022 and the LEAPS Conference 2023

Some projects require pushing various frontiers:

- ✓ Overcoming pseudosymmetry/pseudocentring problems
- ✓ Handling of huge files (e.g. MTZ with 440M unmerged reflections), pushed as an update to the CCP4 MTZ library.
- ✓ Reliable high-quality data processing (WF/autoPROC improvements)
- Speeding up scaling (almost finished ...)
- Efficient and accurate model building, esp. AltConf networks
- ✓ Automated, standardised model refinement protocols (aB_autorefine)

Courtesy of Ashwin Chari (MPI Göttingen)

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Workflow connection to other beamlines - 1

ESRF MASSIF-1 (with Olof Svensson and Matt Bowler)

Uses the Web branch, without needing a Web UI since it is “wrapped” by the ESRF MXPress Workflow

Previously reported:

- Translation calibration using tungsten pins and image analysis software to automate the collection of a large grid of mini-kappa recentring translations for analysis by TransCal
- Use of Recen to predict recentring translations after crystal reorientation on the basis of TransCal results
- Stable operation of the workflow driven by the ESRF MXPress workflow in fully unattended mode
- Data have been collected for two industrial clients, with a high level of user satisfaction.

Still a few fixes required in the grouping of items in a DataCollectionGroup object.

SOLEIL PROXIMA-2A (with Martin Savko and Bill Shepard)

- Successful “rendez-vous” at the development branch of MXCuBE2 (Qt5) on both sides.
- The connection tested over two working sessions was put to the test by a request from a local industrial group to use the WF to collect data on a P1 crystal system.
- Two separate data collections were done, resulting in fully satisfactory data.
- Latest beamtime test on 19 November, next one scheduled for 3 December.

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Workflow connection to other beamlines - 2

MAX IV (with Jie Nan)

- Contact established during the MXCuBE Code Camp
- Interest in using the WF for MASSIF-1-style unattended data collection.
- Translation calibration using tungsten pins and the GPhL TC Workflow to assist the collection of a large grid of mini-kappa recentring translations for analysis by TransCal. Analysis gave the best results ever (7 microns rms) – more in Rasmus's talk
- Further work awaits the availability of the Web-based UI and possible coordination with MASSIF-1

ESRF: towards deployment under MXCuBE3

- Work by Jean-Baptiste Florial and Rasmus Fogh towards providing a UI suitable for operating the Workflow with the Web version of MXCuBE
- Will open the way for connecting the WF to all ESRF MX beamlines, e.g. ID30B and ID23-1