Global Phasing

Status report

Rasmus Fogh

MXCuBE Collaboration meeting

Zoom Webinar, June 2020

Contents

- **MXCuBE refactoring**
- Synchrotron collaboration
  - Test EMBL-P14 February 2020
  - Test ALBA-XALOC June 2020
- Developing workflow strategies

Refactoring efforts

- See Antonia's talk for all that happened
- Major part of my work since last meeting
- Abstract classes
  - Standard, consistent function names
  - Maximise shared code
  - Maintainability
- A single location to get hold of hardware objects

Why GΦL thinks it is important

- Our code must work at all synchrotrons
  - A healthy integrated software suite is a necessity
  - "*An ounce of unification is worth a pound of customisation*"
- We come from the outside
  - Clear, consistent code is easier to learn and adapt to
  - We would need to learn all the local styles
  - Duplication, multiple standards, and obsolete code makes the program hard to figure out

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EMBL-P14 test

- One-day test slot, without beam.
- Set-up required some work merging disparate branches
- Translational calibration successful after some debugging (and a too-long pin)
  - 8+28 centring points, ~25µm reproducibility
  - Auto-recentring during acquisition did not work
- Tested diffractometer calibration and data acquisition (without beam)
  - Earlier data storage problems had been solved.

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ALBA: preliminary tests

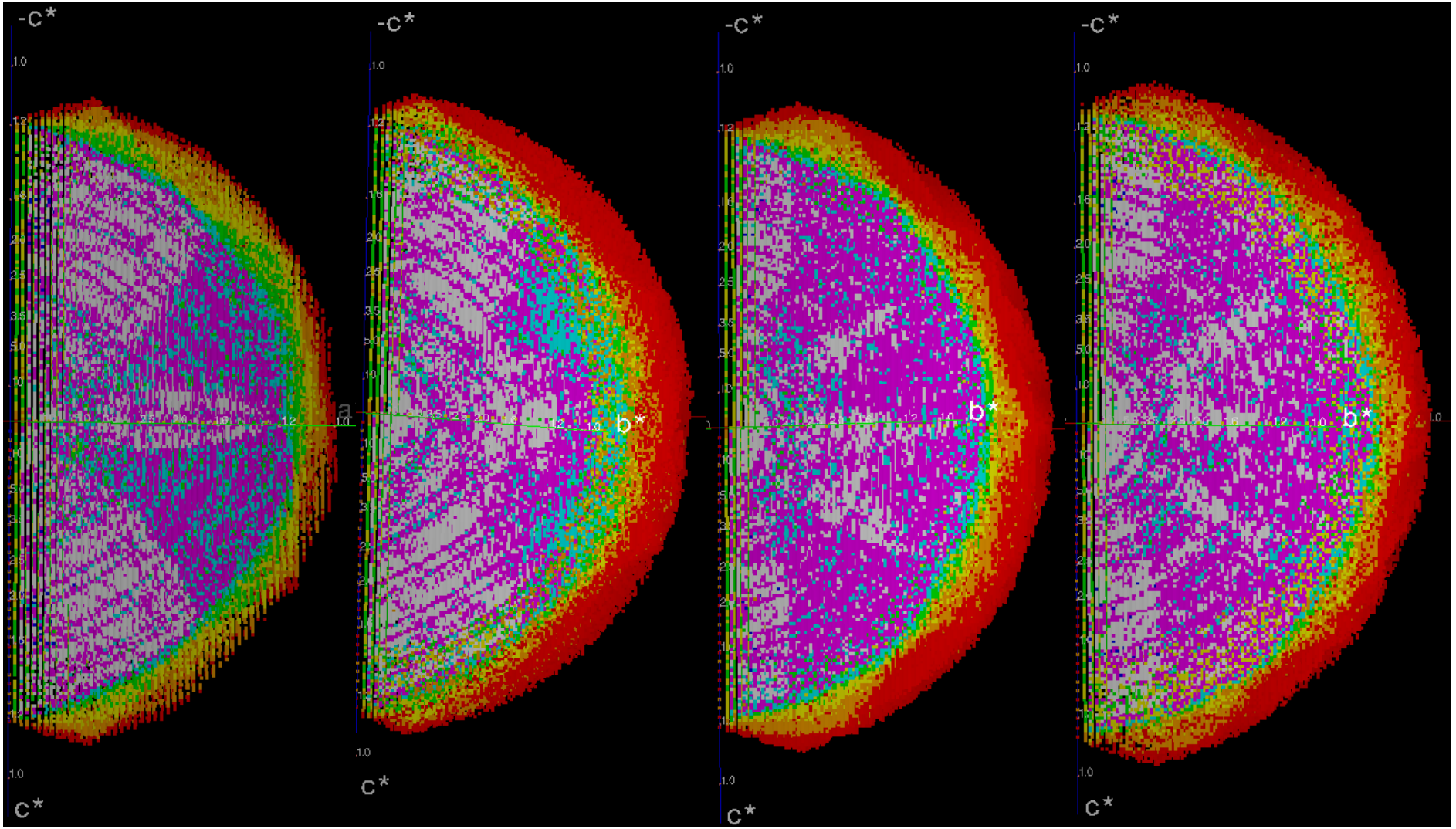
- Setup went quickly and smoothly
  - owing to the availability of production code in a git repository branched off the main repositories
  - and to keeping GΦL workflow development in a compatible branch
- Translational calibration in a one-hour window
  - 8+36 centring points, 10μm reproducibility
  - Auto-recentring during acquisition did not work - interference with ALBA pseudo-motors?
- Successful short diffractometer calibration in two-hour window

ALBA: Data Collection

- June 16, remote, 8-hour shift at ALBA
- Real-life fragment screen crystals
  - Point group 32
  - Anisotropic, 1.9/1.5Å
  - provided by the Marquez group

- Six successful data sets,
  plus work on data processing queue
- Extremely clear density for ligands
  - Cannot show results as they are confidential at the moment
- Next step: integration with ISPyB for
  repatriation of data sets and processing results

Testing new strategies



360˚ *180˚ : 360˚* *180˚ : 360˚ : 180˚* *360˚ : 360˚*

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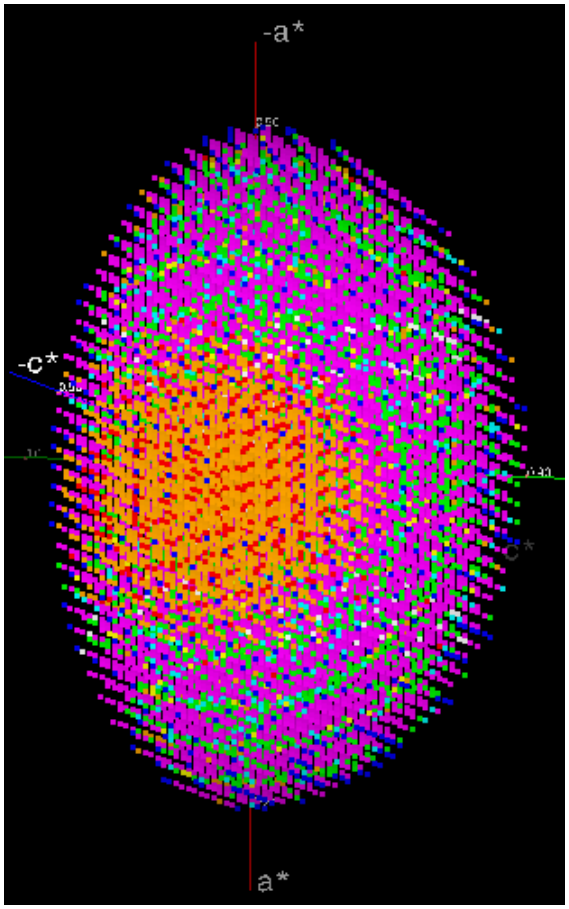
Where we are - strategies

- We have improved our native and experimental phasing strategies
- We have set up fully functional simulation and display facilities for strategies
- Our workflow is functional at ALBA and EMBL-Hamburg

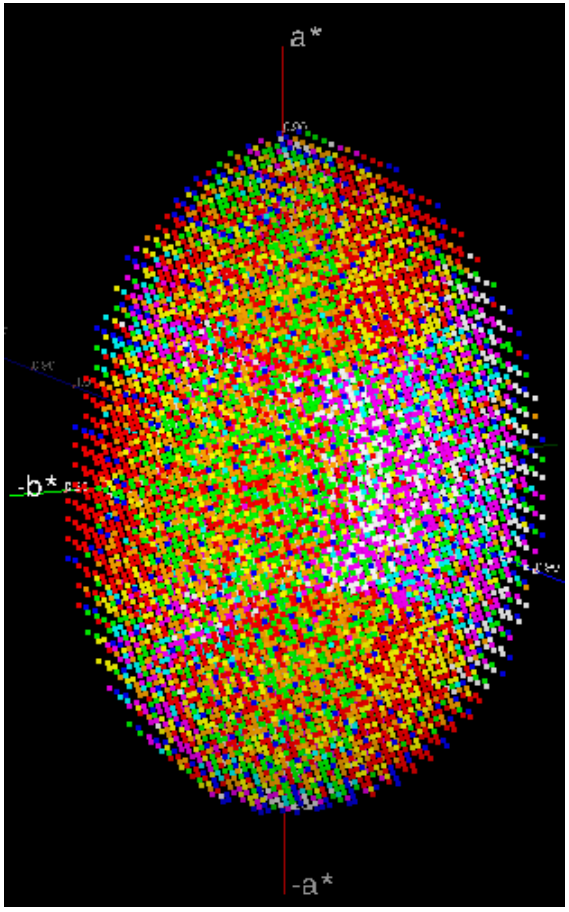
Redundancy from multiple sweeps

P21 – One sweep



Red 2/8 Green 6/8
Orange 4/8 Magenta 8/8

P21 – Three sweeps



Red 16/24 Green 20/24
Orange 18/24 Magenta 22/24

Next steps

- Investigate and clarify interaction between GΦL and beamline recentring operations
- Invoke X-ray centring to fine-tune recentring
- Standardise integration with auto-processing resources at synchrotrons
  - We need on-line as well as off-line processing
- Clarify the meaning and reliability of flux values to calculate dose budgets and radiation damage
- Integrate with Web-based UI

Thanks to

- Roeland Boer and Jordi Andreu at ALBA
- Gleb Bourenkov and Ivars Karpics at EMBL-Hamburg
- Josan Marquez group for providing crystals
- My colleagues at Global Phasing.
- All of you, for the refactoring

END