Global Phasing's MXCuBE-related activities since the ELETTRA meeting

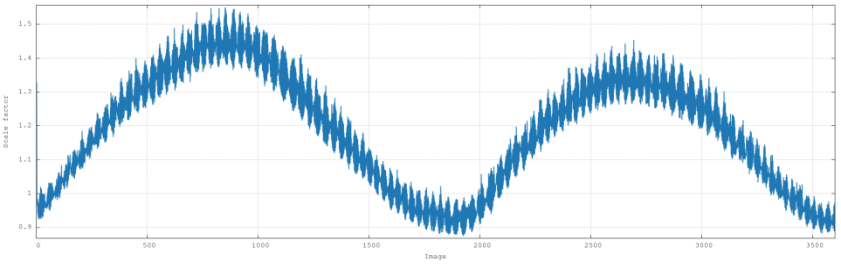
Rasmus Fogh, Peter Keller,
Claus Flensburg, Wlodek Paciorek,
Clemens Vonrhein, Gerard Bricogne

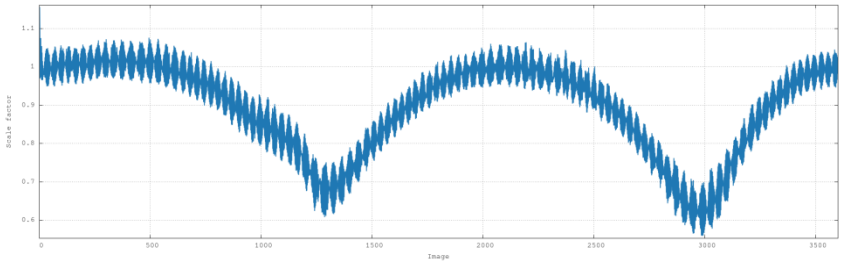
Global Phasing Ltd., Cambridge, UK

Overview

- Oct/November — Remote tests on ESRF ID30B
- 26-27 October — Visit to ALBA
- 22 November — Workflow-driven remote multi-orientation data collection with GSK
- 21-24 January — Visit to SOLEIL Proxima2
- 19-20 February — Visit to ALBA
- Throughout — Participation in all DEV VCs

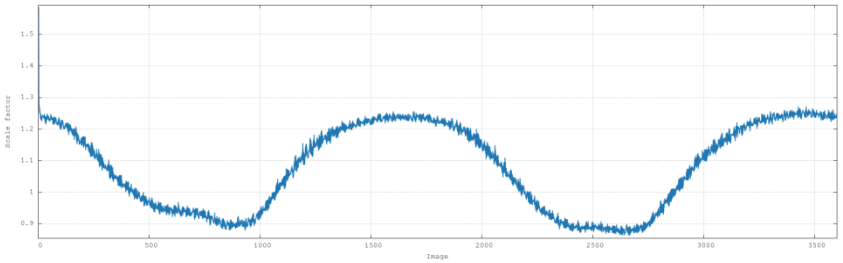
November 7th: Remote test on ESRF ID30B

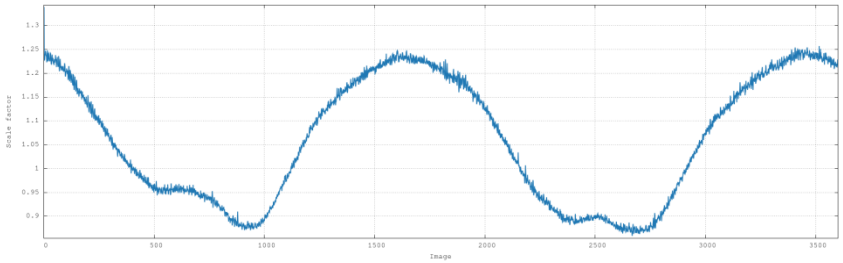




“Furriness” in image scale factors (50Hz pump, 50Hz frame rate)

Corrected on 21 November, just in time for the GSK experiment





“Furriness” in image scale factors (42Hz pump, 50/20 Hz frame rate)

22 November: Workflow-driven remote multi-orientation data collection with GSK

- Proprietary project.
- Thin monoclinic plates.
- Poor reproducibility of re-centring when recalled from “bookmarks” led to only one useful 3-orientation dataset (1.43Å, 38-fold redundancy)
- We need to add a fine-tuning re-centring step just before collecting each sweep
  - by manual intervention
  - by image processing from optical snapshots
  - by a mesh scan over a very small volume

ALBA visit 26-27 October 2018

- First contact with the MXCuBE environment on BL13
- Problems in driving Kappa and Phi from the execution queue
- However, 10-fold increase in scanning speed OK!
- First use (for GPhL) of tungsten pins as Translation Calibration test objects: superb!
- Fitting residual in TransCal ~ 10µ rms

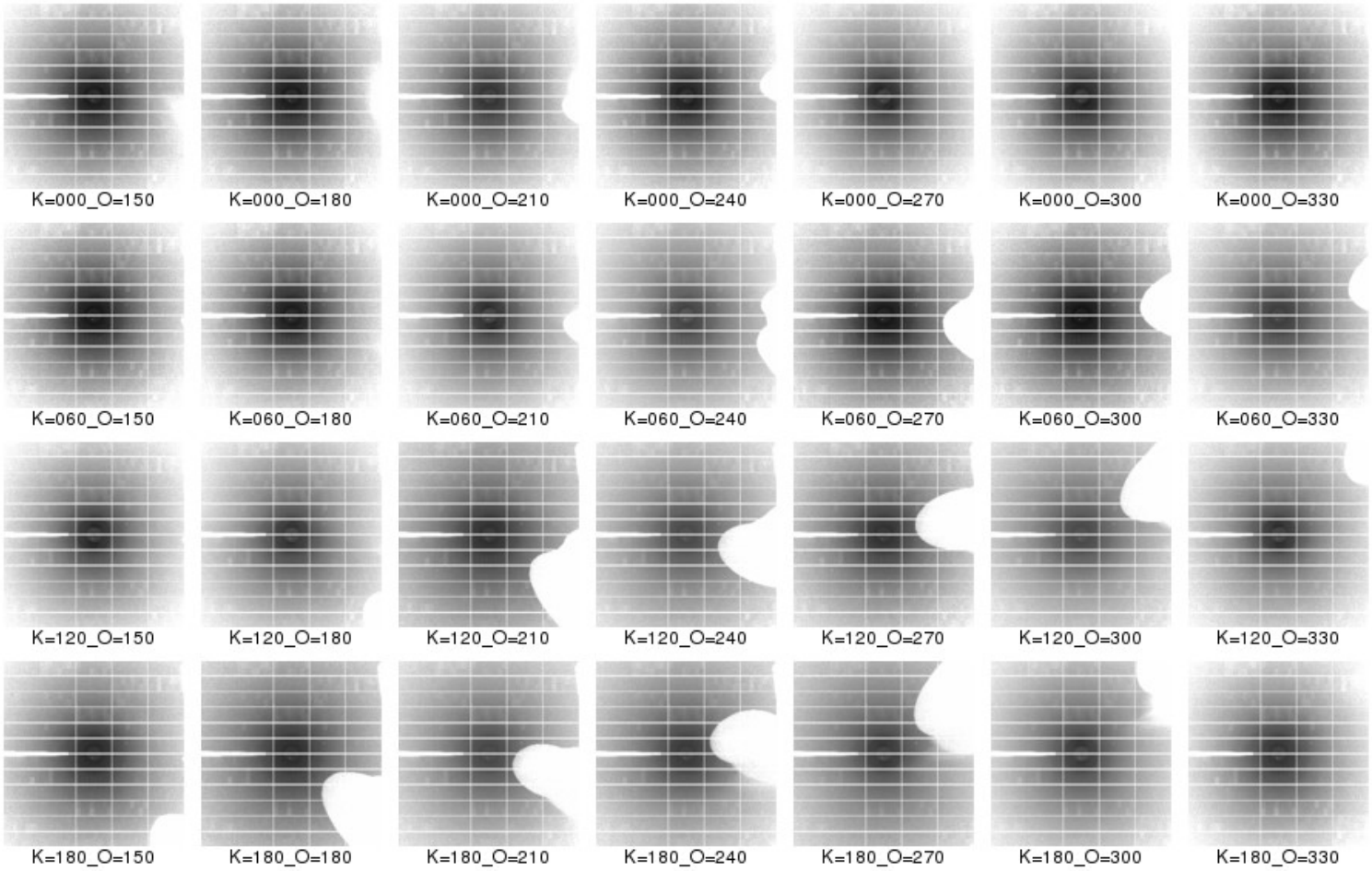
SOLEIL Proxima2 visit 21-14 January

- The MXCuBE integration worked well with only minor errors and tweaks, even though it had been upgraded and coded to the pre-refactoring master branch and only adapted to SOLEIL-specific code in a limited way beforehand.
- Proxima2 uses an original optical centring procedure.
- Unexplained movements of the centring test object were observed.
- Translation Calibration measurements could nevertheless be recorded: final fitting residual in Transcal ~15µ rms
- DiffractCal measurements were complicated by the fact that this was the first time we executed the corresponding workflow with an Eiger detector (HDF5 with multiple triggers, instead of mini-cbf).
- The data analysis for a short DiffractCal run is still ongoing.

ALBA visit 19-20 February 2019 (1)

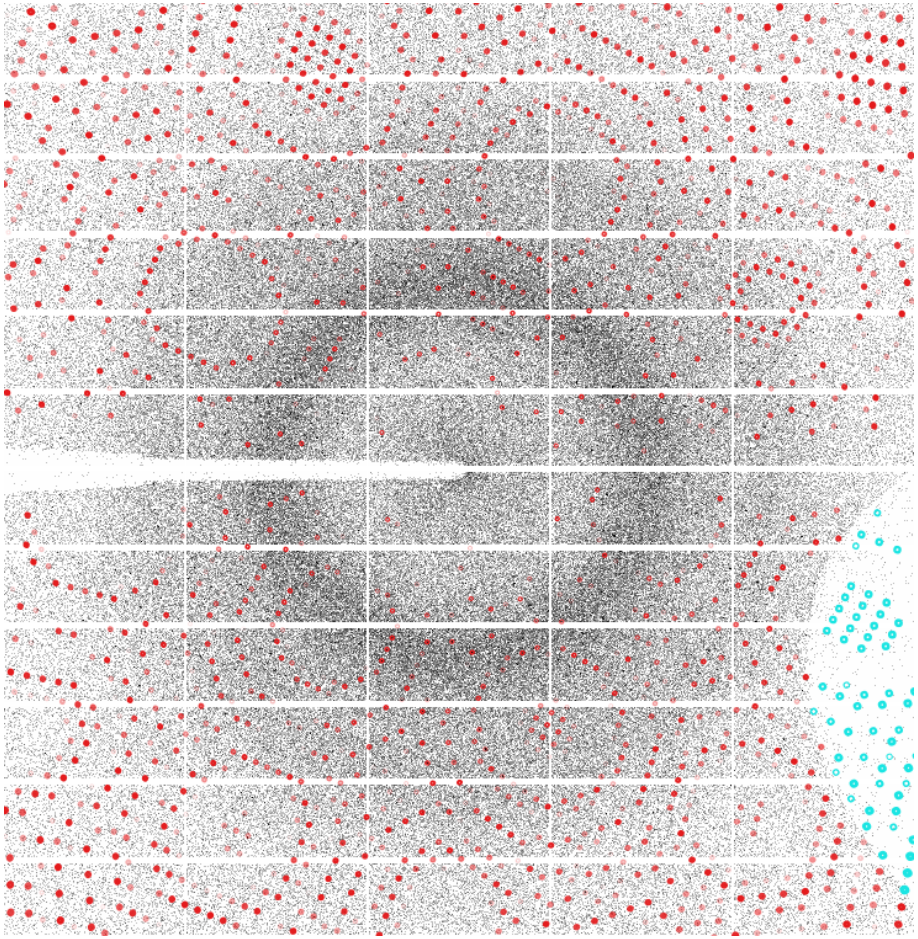
- Some synchronisation issues were identified in the motor movements requested by the GPhL calibration workflows.
- Nevertheless a new set of Translation Calibration measurements (with a tungsten pin) gave a fitting residual in TransCal of < 8µ rms – the best we have ever seen.
- A full set of DiffractCal measurements (22 sweeps) was collected and analysed.

ALBA visit 19-20 February 2019 (2)



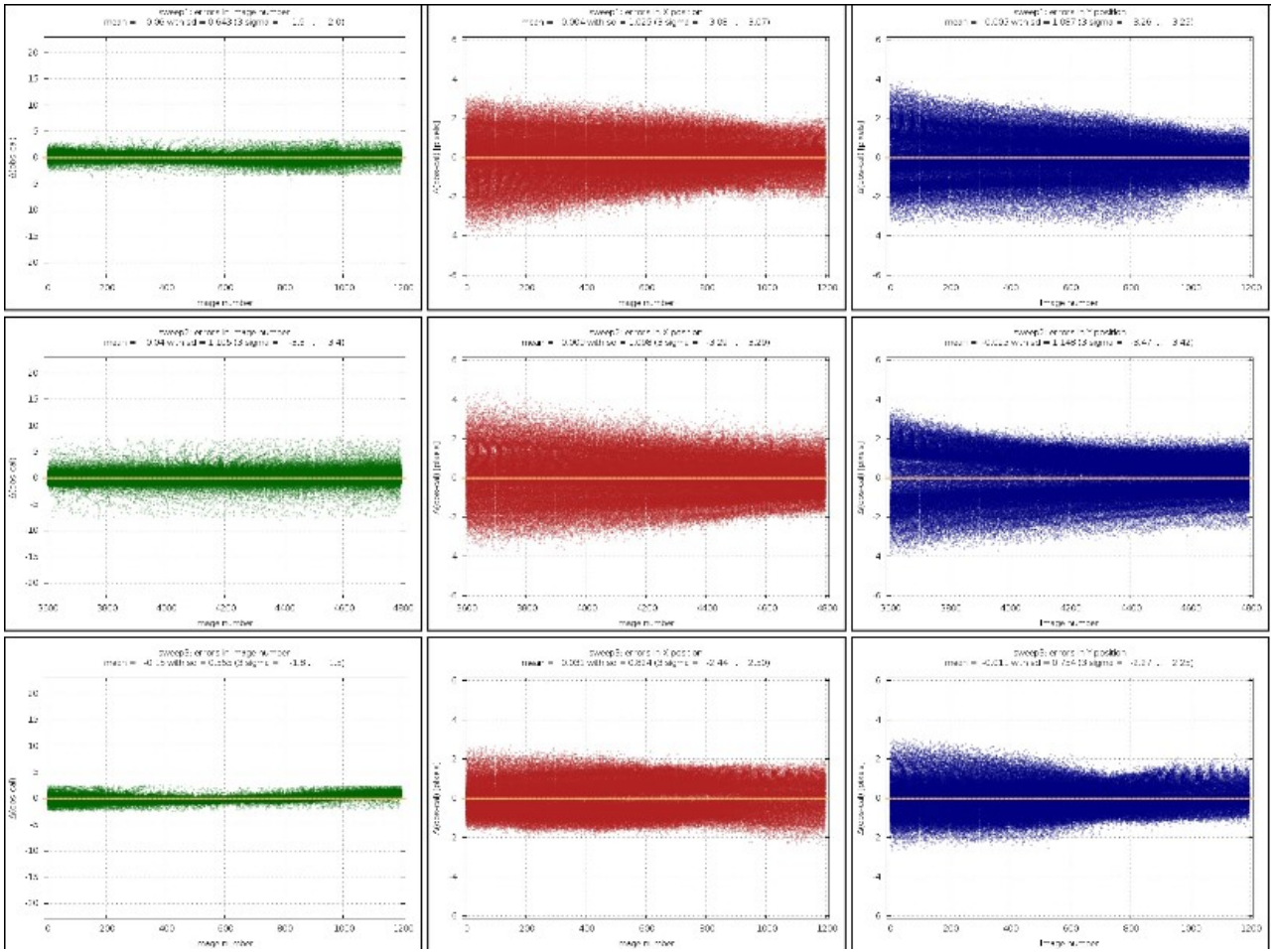
A “shadowing series” at distance=122mm

ALBA visit 19-20 February 2019 (3)



Validation of shadowing predictions

ALBA visit 19-20 February 2019 (3)



Excerpt of final analysis of DiffractCal data

Last but not least …

- Participation in all the monthly (sometimes twice monthly) developers' videoconferences.
- Rasmus's participation in the face-to-face developers' workshop (15-16 November 2018 at ESRF) and in the subsequent refactoring effort.

Acknowledgments

- Andrew McCarthy (ESRF ID30B)
- Roeland Boer, Jordi Andreu (BL13 ALBA)
- Bill Shepard, Martin Savko (Proxima2 SOLEIL)
- Bernard Lavault, Ralf Siebrecht (ARINAX)

- The MXCuBE developers