Processing Single-Crystal Neutron Time-of-Flight Laue Data in DIALS

David McDonagh[1], David Waterman[2]

[1]STFC Rutherford Appleton Laboratory, Didcot, OX11 0FA, England
[2]CCP4, Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot OX11 0FA, England

david.mcdonagh@stfc.ac.uk

DIALS
Diffraction Integration for Advanced Light Sources

Summary

- The DIALS project[1] provides an open-source, extensible framework to analyse and reduce diffraction patterns from a variety of X-ray and electron monochromatic sources
- This work extends DIALS to polychromatic sources, allowing for the processing of time-of-flight (ToF) neutron diffraction patterns obtained from the Single Crystal Diffractometer (SXD) at ISIS[2]
- Refinement, integration, visualisation, and user workflows have all been enhanced for users with ToF data, giving a common interface for users with neutron and X-ray data
- In addition to allowing neutron data to be processed in DIALS for the first time, this opens up the possibility of developing DIALS for other polychromatic sources, such as X-ray Laue crystallography

DIALS: https://dials.github.io/ | WIP fork: https://github.com/toastisme/dials

SXD

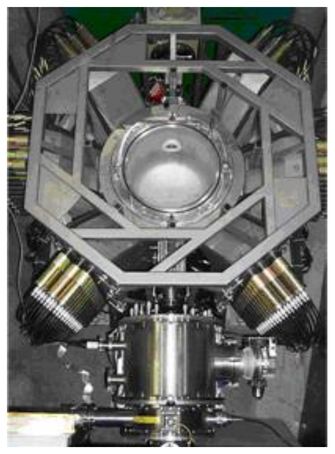


Figure 1: The SXD detector[2].

- SXD consists of 11 position sensitive detectors arranged in a bowl configuration
- A wide incident wavelength range of 0.2 – 10 Å requires the full treatment of each reflection's wavelength, rather than relying on wavelength normalisation
- Existing instrument-specific software exists as a gold standard for comparing to DIALS results
- Methods developed for this instrument are applicable to a variety of other ToF detectors (e.g. MaNDi), and those in development (LMX, NMX)

Methods

Spot Finding and Indexing

- Bragg peaks are identified by first locating strong pixels using a threshold algorithm, and then connecting these across spatial and ToF dimensions

$$pixel > min\ val$$

$$\left(\frac{\sigma^2}{\mu}\right) > G\left[1 + \sigma_b\left(\frac{2}{N-1}\right)^{\frac{1}{2}}\right]$$

variance; gain; mean; std. deviations; num. local pixels

$$pixel > \mu + \sigma_s(G\mu)^{\frac{1}{2}}$$

std. deviations

- Indexing can be carried out using 1D or 3D FFT-based methods, or a real-space grid search[3]

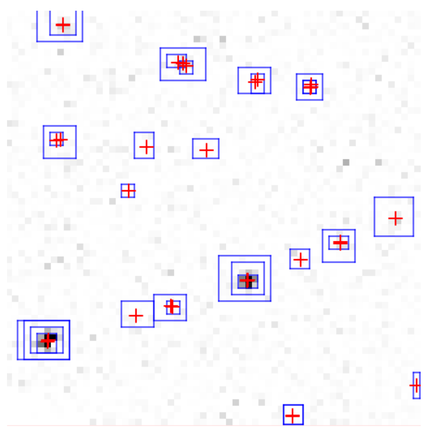
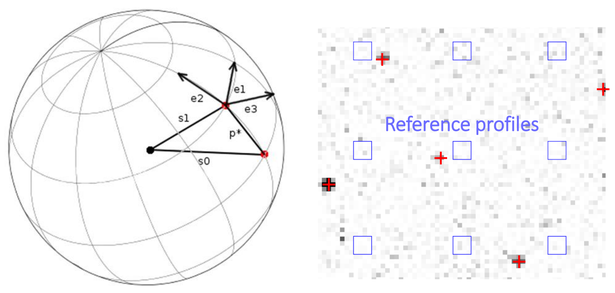


Figure 2: Spots identified from NaCl on a single panel of SXD, using the DIALS extended dispersion find spots algorithm. Centroids are shown as red crosses, and shoeboxes are shown in blue. The ToF dimension has been summed to give a 2D image.

Refinement and Integration

- DIALS follows a general global refinement approach using the entire dataset, prior to integration, minimising instability of refining different parameters, and allowing for maximum parallelisation
- Building on current rotation scan[4] and stills[5] refinement algorithms in DIALS, refinement specific to ToF data has been developed, allowing for model minimisation with respect to each reflection wavelength
- The profile fitting integration approach taken by XDS[6] has been adapted to ToF data by treating the Ewald sphere of each reflection separately (Fig. 3)



$$e_1 = \frac{\boldsymbol{S} \times \boldsymbol{S_0}}{|\boldsymbol{S} \times \boldsymbol{S_0}|} \qquad e_2 = \frac{\boldsymbol{S} \times \boldsymbol{e_1}}{|\boldsymbol{S} \times \boldsymbol{e_1}|} \qquad e_3 = \frac{\boldsymbol{S} + \boldsymbol{S_0}}{|\boldsymbol{S} + \boldsymbol{S_0}|}$$

Figure 3: Each strong spot is mapped to its own coordinate system along its Ewald sphere (left). A grid of reference profiles (right, blue) is generated based on a weighted sum of observed spots (right, red), which are then used for fitting predicted peaks in reciprocal space.

Visualisation

dials.geometry_viewer

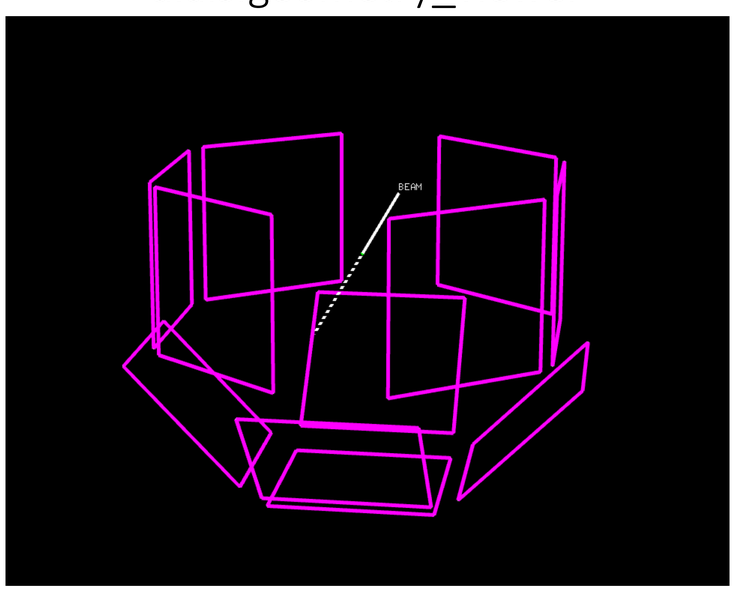


Figure 4: A given experiment is designed as a format class in the dxtbx software package[7], which can be visualised using the DIALS geometry viewer. Here the 11 SXD panels are shown in purple.

dials.image_viewer

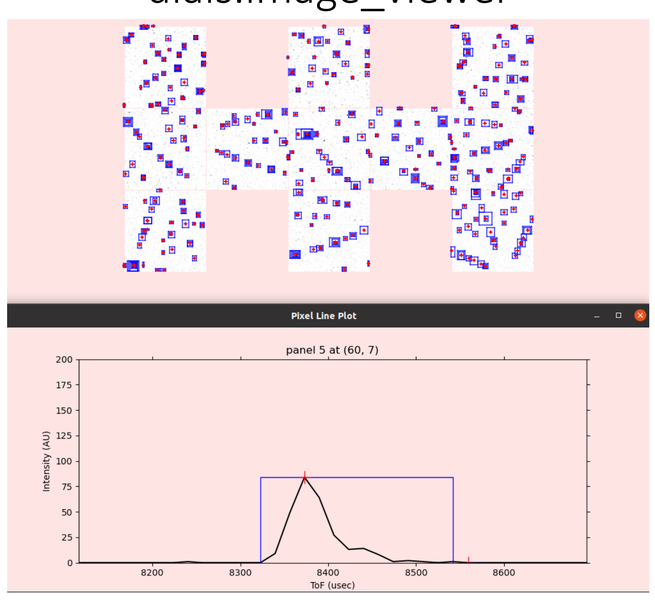


Figure 5: To investigate the quality of a given dataset the DIALS image viewer can be used to visualise diffraction patterns. A 2D projection of each SXD panel is shown, flattening the detector around the bottom panel seen in Fig. 4.

dials.reciprocal_lattice_viewer

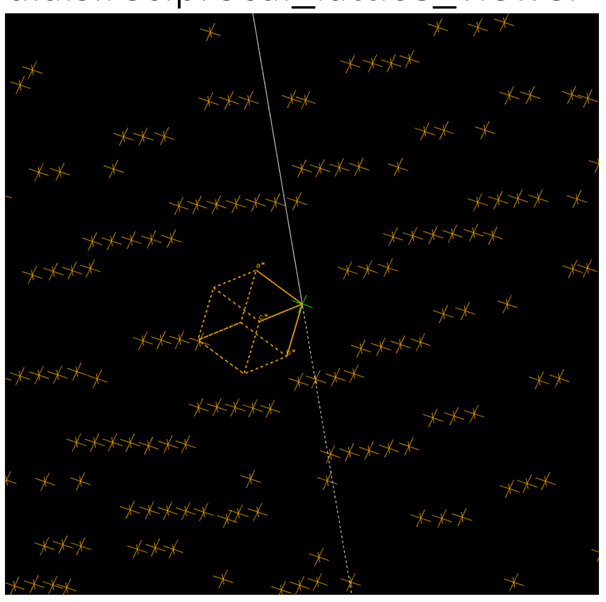


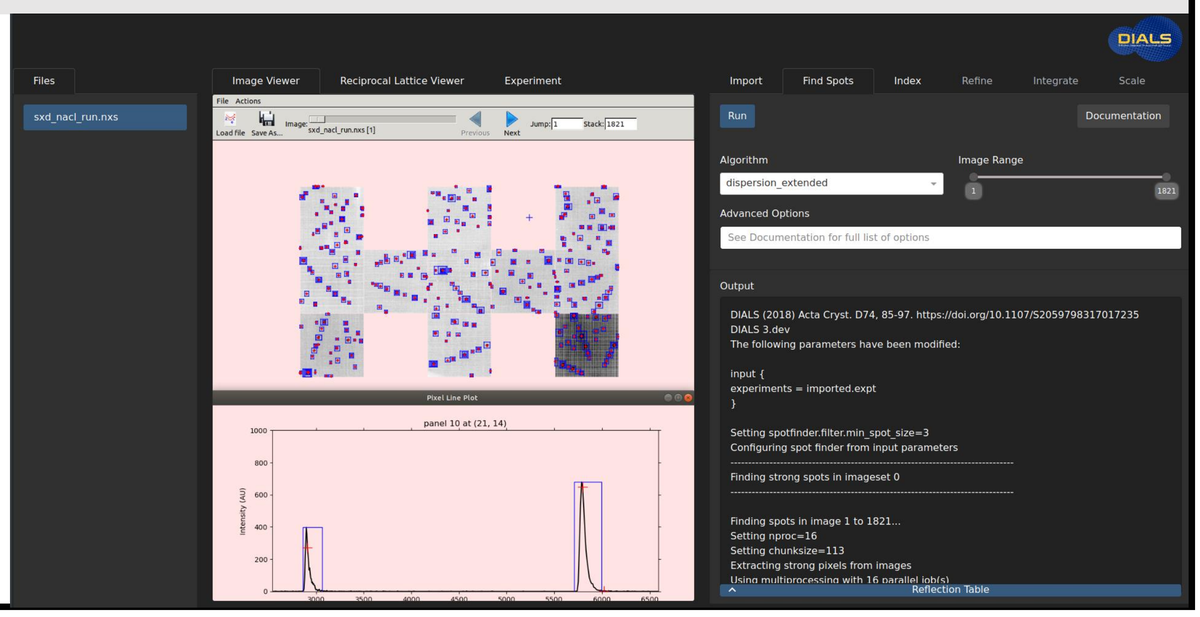
Figure 6: Once spots have been identified (or calculated), the DIALS reciprocal lattice viewer can be used to show the results mapped to reciprocal space. Spots can be filtered by panel, and whether or not they have been indexed.

Workflow

- To facilitate streamlined user workflows a lightweight, browser-based GUI has been developed for processing neutron data in DIALS (right), giving users the option to carry out the reduction process in a single window, without using the terminal
- Interfaces between DIALS and other neutron-specific software packages have also been developed, allowing users to combine software packages in their pipelines

Spot finding → Indexing → Refinement → Integration

DIALS → MANTID → DIALS → MANTID



References

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Acknowledgements

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