Poster

Automating the 3DED/MicroED data processing at Diamond Light Source's Electron Bio-Imaging Centre

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Three-Dimensional Electron Diffraction (3DED) is an emerging and useful technique for solving molecular structures of small and biological macromolecules from nanometre-sized crystals. We present our automated data processing workflow for 3DED datasets collected at Diamond Light Source's Electron Bio-Imaging Centre. The processing pipeline includes data collection, data analysis, metadata gathering, file conversion, and finally data processing using the Xia2/DIALS package [1]. Our main goal is to reduce the workload of electron diffraction scientists, but also to enforce good standards already used in macromolecular crystallography (MX). For example, all the collected 3DED datasets are automatically converted into NeXus data format [2] which is considered a Gold Standard for MX. This standardized data format allows for all the relevant metadata about the experiment to be kept together with diffraction images. We also discuss some of the methods we developed for data analysis, in particular methods used to determine the position of the electron beam on diffraction images. Our automated solution not only enhances the productivity of diffraction researchers but also facilitates the exploration of complex biological and material systems through 3DED.

[1] Winter et al. (2018). Acta Cryst. D74, 85-97.

[2] Waterman et al. (2023). Structure 31, 1–8.