

Tools for MicroED within the DIALS package

David Waterman¹

¹STFC

david.waterman@stfc.ac.uk

DIALS is an open source data processing package, consisting of command line programs and an extensible programming framework. DIALS is popular for macromolecular and small molecule X-ray crystallography, but the flexibility of its design also allows adaptation to other methods. In recent years, DIALS has been successfully employed to process single crystal electron diffraction data, particularly continuous rotation MicroED experiments. Relevant features and algorithms include plugins that allow importing of data in native formats, specialised spot-finding algorithms, automated rotation axis determination, indexing methods for snapshot ED patterns, refinement of beam drifts, combination of multiple incomplete datasets, and more. Some of these aspects will be discussed in detail during this talk.