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MACROMOLECULAR CRYSTALLOGRAPHY DATA PROCESSING WITH DIALS

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Abstract

The DIALS project provides an open-source toolbox for single crystal diffraction image processing and analysis tasks. DIALS was originally developed as a collaboration between Diamond Light Source, the Lawrence Berkeley National Laboratory and CCP4 to address the needs of advanced light sources, where rapidly-developing technology and experimental methodology have changed the way modern crystallography is performed. The flexible and modular design of the toolbox combines established algorithms alongside novel methods, and provides interfaces at multiple levels of detail. This facilitates a wide scope of use cases, from automated data processing pipelines at synchrotron beamlines, through to user-driven operation of the software using a graphical user interface or a suite of command-line programs. At the lowest level, new software or specialist scripts can be produced by using DIALS as a Python library. Indeed, it is hoped that the open, collaborative nature of the project will inspire the next generation of scientists working on methods development. In this presentation, the main features of the DIALS package will be described, in particular focusing on its use for fast, high quality integration by 3D profile fitting in the context of synchrotron rotation experiments. Examples of some of the novel developments that have come out of the DIALS project will also be given, including algorithms for indexing multiple lattices, improved background determination for weak data collected on pixel array detectors, and clustering methods for multi-crystal data sets. Active areas of current development will be touched upon. These include better modelling for serial snapshot crystallography and adaptations for electron and neutron diffraction experiments.

About

Provides and supports an integrated suite of programs for determination of macromolecular structures by X-ray crystallography; aims to develop cutting edge approaches to experimental determination and analysis of protein structure; as a community based resource, supports the development and integration of novel software into the suite; serves the widest possible research community, embracing academic (not for profit) and for profit research. Offers education and training of scientists in experimental structural biology and encourages the wide dissemination of new ideas, techniques and practice.

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