Poster Presentation

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DIALS - a toolbox for diffraction data analysis

L. Fuentes-Montero¹, J. Parkhurst¹, G. Winter¹, D. Waterman², R. Gildea¹, A. Brewster³, J. Hattne³, N. Sauter³, G. Evans¹ ¹Diamond Light Source LTD, Oxfordshire, UK, ²CCP4, RCaH, STFC Rutherford Appleton Laboratory, Oxfordshire, UK, ³Lawrence Berkeley National Laboratory, Physical Biosciences Division, California, USA

DIALS is a collaborative initiative to produce an open source software toolbox encompassing all aspects of diffraction data analysis, with an initial focus on X-ray diffraction data from synchrotrons and free-electron lasers for macromolecular crystallography. DIALS [1] has been developed as a modular plug-in framework that permits flexibility not only in the development of new methods and algorithms but also in the application of these methods to data analysis. DIALS builds on the cctbx [2] in addition to its own dedicated tool-kits. We will present the ideas behind DIALS and give examples of its versatility in permitting the use of several spot-finding and indexing schemes, global refinement and both two and three dimensional integration methods.

[1] D.Waterman, G. Winter, JM Parkhurst, "et al", "The DIALS framework for integration software", CCP4 Newsletter on Protein Crystallography, 2013, 49, 16-19., [2] RW Grosse-Kunstleve, NK Sauter, NW Moriarty, "et al", "The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework", J. Appl. Cryst. 2002, 35, 126-136.



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