

# Poster Presentations

## [MS10-P22] 2D Algorithms in DIALS

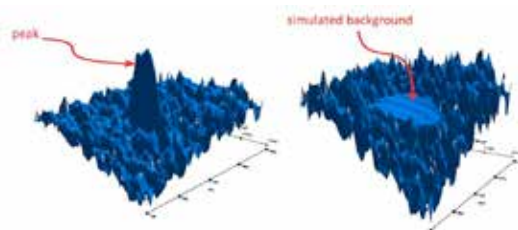
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<sup>1</sup>Diamond Light Source

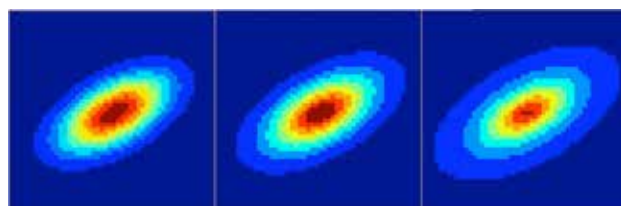
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The DIALS (Diffraction Integration for Advanced Light Sources) project [1] [2] aims to develop software tools for treating diffraction images and obtaining accurately the position and intensity of each Bragg reflection in a diffraction experiment. In this poster the algorithms used for treating 2D images are described. The DIALS team works in a wider range of algorithms including treatment of a 3D block made by several images, data format conversions and collaborating with the CCP4[3] team in refining the geometry of the cell and the diffraction experiment. The treatment of 2D images as part of DIALS framework is pluggable to the other algorithms by the same interface API used by the “3D block” algorithms. Peak search is performed by means of a four-step procedure: a) image smoothing; b) mask building through comparison of original and smoothed images; c) definition of peak boxes from the mask; d) determination of the “centre of gravity” of all the diffraction maxima. The background linked to a peak has been treated in several manners. The simplest treatment considers a (flat or inclined) plane background that is mathematically characterised from the area surrounding the considered diffraction spot. One of the procedures in DIALS models a curved surface that fits the shape of the background in the area surrounding the spot. The applied algorithm performs a Laplacian-inspired smoothed representation of the two-dimensional surface, first introduced by the application Esmeralda [4], developed at the Institute Laue-Langevin, Grenoble. The next image shows how this simulated background looks.



Calculation of the peak intensity can be made by simple summation or by “Modelling a Profile”. The procedure in DIALS that does “Modelling a Profile” starts by measuring the centre, height and widths of the considered peak and continues with the numerical refining of a 2D-domain pseudo-Voigt surface to the observed spot. The next figure shows an example of 2D peak evolving from Gaussian to Lorentzian shape.



[1] G. Winter *et al.*, - <http://dials.sourceforge.net/>

[2] R. W. Grosse-Kunstleve *et al.* - “The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework,” *J. Appl. Cryst.*, vol. 35, no. 1, pp. 126–136,( 2002)

[3] M. D. Winn *et al.* - "Overview of the CCP4 suite and current developments. Copyright © International Union of Crystallography. *Acta Cryst.* **D67** , 235-242 (2011) [4] L.Fuentes-Montero *et al.* <http://lauesuite.com/>

**Keywords:** 2D diffraction patterns; background modeling; automated peak search;