Contribution ID : **85** Type : **Presentation**

Computing at the service of crystallography

Thursday, 13 August 2015 12:30 (0:30)

Abstract content

Diamond Light Source (DLS) is a synchrotron facility conceived for macromolecular crystallography (MX) and biopharmaceutical research as its main purpose. Modern MX experiments are generally implemented as variants of the crystal rotation method, using 2D detectors. 2D diffraction images corresponding to several angular positions are collected at a rate of one scan every five seconds. Each scan contains 180 to 720 images of 2463 x 2527 pixels. Before the next shoot, all these images need to be processed nearly in real time. To achieve this DLS has servers with automated parallelized software that are launched automatically with the experiment. When the user launches one diffraction scan, as soon as the experiment finishes the computer connected to the instrument sends a signal and transmits the data to the servers. The servers process the data in a few seconds and return the solved structure to the instrument's computer. In DLS, several software packages are developed to be used in combination with other third party programs to achieve a high level of automation. All software packages developed at DLS with scientific purpose are open source, as it is the best way to produce software by collaboration between academic institutions. The most remarkable software packages developed at DLS are: DAWN - to be used in the instrument as a front end to the user and as a visualization GUI tool; GDA - to connect DAWN with the instrument's firmware or prepackaged program coming with the instruments; DIALS - to process 2D diffraction images, among other third party integration software. Particularly, the DIALS project is a collaborative effort aimed to be "future proof", extensible and reusable package. DIALS is based and depends on the well known CCTBX package. DIALS is being packaged as a large module which is part of CCTBX and also as part of the CCP4 package. The aim of DIALS is not only to be an integration program, but also to be a framework and a toolkit useful for both, users and programmers for developing new algorithms for integrating 2D diffraction images.

Summary

Primary author(s) : Dr. FUENTES-MONTERO, Luis (Diamond Light Source)

Co-author(s) : PARKHURST, James (Diamond Light Source); Dr. WATERMAN, David (STFC Rutherford Appleton Laboratory); Dr. GILDEA, Richard (Diamond Light Source); Dr. GERSTEL, Markus (Diamond Light Source); Dr. WINTER, Graeme (Diamond Light Source); Dr. GWYNDAF, Evans (Diamond Light Source)

Presenter(s) : Dr. FUENTES-MONTERO, Luis (Diamond Light Source)

Session Classification : Thursday II