References:

[1] Wolfram Research, Inc., (2018). Mathematica, Version 11.3. Champaign, IL, 2018.

[2] C. P. Brock, International Tables for Crystallography 5th Edition, 8 Volume Set, Wiley, 2016.

[3] Schoonjans, T., Brunetti, A., Golosio, B., del Rio, M. S., Solé, V. A., Ferrero, C. & Vincze, L. (2011). Spectrochimica Acta Part B: Atomic Spectroscopy, 66(11), 776 – 784.

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MS41-O4

Using DIALS with DUI

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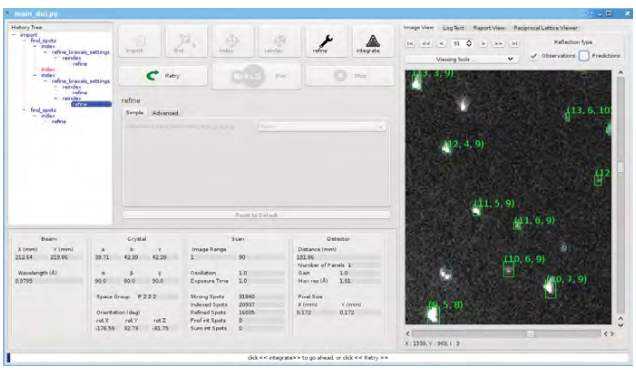
The DIALS User Interface (DUI) is a graphical user interface that is designed to make data processing with DIALS[1] more user-friendly and efficient. A key feature is a full history tree that keeps track of all steps of processing. Every position in the tree represents the execution of a DIALS command line with full record of the user-supplied parameters, and the results, which can be inspected with several visualisation tools. At any step, the user can either fork, proceed to the next command or navigate to another step without loss of information. This ability to keep track of different branches of data processing gives the user freedom to explore different hypotheses, such as the space group of the crystal.

The output and visualization tools in DUI are conveniently arranged in tabs that update their content when the user navigates the tree, allowing rapid comparisons to aid decision-making. Each tab provides a different view on the state at that position of the tree, from detailed log file output of the DIALS program and graphical reports to an interactive image viewer and a 3D reciprocal lattice viewer.

The image viewer has been redesigned for DUI to provide responsiveness alongside various image overlays that give information about the spots and experimental models. The reciprocal lattice viewer complements this by providing a view of reflection positions in reciprocal space. Together these tools provide a powerful means for identifying problematic cases that may not be so readily apparent from the graphs and statistics in the report and log files.

DUI is intended to be intuitive and immediately useful across a wide range of user expertise. Beginners learning about the integration process with DIALS will benefit from the ease-of-use of the GUI and the visualisation tools. Experts retain full control of the underlying DIALS programs and can use the history tree to test different ideas quickly.

In this presentation these features of DUI will be demonstrated with a rotation dataset from a macromolecular crystal. DUI is distributed to users as part of CCP4 7.0[2].



References:

[1] G. Winter et al. Acta Cryst D Struct Biol 74, 85-97 (01 Feb 2018). [PMID:29533234] "DIALS: implementation and evaluation of a new integration package"
[2] M. D. Winn et al. Acta. Cryst. D67 , 235-242 (2011) "Overview of the CCP4 suite and current developments" [doi:10.1107/S0907444910045749]

Keywords: data integration,graphical user interface,data processing,software,DIALS,CCP4,

MS41-O5

Crystallographic Computing Schools - training future software developers

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At the IUCr General Assembly and Congress in Geneva in 2002, several people were appointed to the IUCr's Commission on Crystallographic Computing ("CompComm"); a major part of their remit was "to do something rather than nothing".

It was recognised by CompComm at the time that there was no formal provision to apply the science of Crystallography to new software, particularly in small molecule and powder methods; all freely available software was developed either in existing groups or by people working independently who began with knowledge of either crystallography or programming (but rarely both).

The major result from the work of CompComm's new blood in Geneva was the Siena Crystallographic Computing School which was held before IUCr XX in 2005. Developers of major crystallographic software packages across the science (powder, small molecule and macromolecular) gathered together to interact with and pass on their knowledge to the next generation [1]. Since then, with the exception of 2014, CompComm has run these events before every IUCr General Assembly and Congress; the next is planned to take place in the Czech Republic in 2020.

In 2013, SIG9 of the European Crystallographic Association (ECACOMSIG, the Special Interest Group in Crystallographic Computing) held a similar event before ECM28 in Warwick [2]; part of the rationale was to "fill in the two years when no IUCr CompComm event took place". This has now been repeated in every non-IUCr year since then, and the fourth took place in Mieres, south of Oviedo this week.

I will discuss how the Schools are organised, how we fund them and how we try to make sure that they are relevant to as many students as possible.

References:

[1] https://www.iucr.org/resources/commissions/crystallographic-computing/schools/siena-2005-crystallographic-computing-school
[2] http://sig9.ecanews.org/sig9_warwick.html

Keywords: training, workshops, software