

Oral Contributions

[MS11-02] Dupond, Dupont ou Dupondt? Jumeaux ou sosies[1]? Dealing with extra lattices.

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Integration of diffraction images collected from merohedral twins is no more difficult than for single crystals - any problems can only be identified later in the processing, following the scaling and merging steps, and are dealt with in structure solution and refinement. Other multiple lattice experiments, in which the maxima from the different lattices are not perfectly superimposed, should be addressed at the integration stage. This other kind of problem includes data collected from pseudomerohedral and non-merohedral twins and also from samples that are best described as being composed of multiple lattices. In these multi-lattice experiments, there are three distinct classes of reflections, viz those that are not overlapped by spots from other lattices, those that are completely overlapped and those that are partially overlapped. This last type of observation is that which is most challenging to deal with properly.

We have implemented algorithms into the integration program *Mosflm* to index several lattices present in a single sample and improved its GUI *iMosflm* to present this information to the user clearly and straightforwardly [2]. More recently we have extended the functionality so that each lattice identified can have its parameters refined and then integrated to yield a reflection file. This is written in a modified MTZ format which includes extra information about the type of overlap of each observation. A new program *Feckless* has been written to process the MTZ file prior to the normal treatment with *Pointless*

and *Aimless* to give scaled and merged output. Modifications to the program *REFMAC* will allow these enhanced data to be used effectively in the refinement of macromolecular structures.

We will discuss these improvements to processing and present early results from their implementation.

[1] Hergé, *Le Sceptre d'Ottokar*, 1929, 3 *et seq.*

[2] Powell, H.R., Johnson, O. & Leslie A.G.W., *Acta Crystallogr., Sect. D: Biol. Crystallogr.*, 2013, **69**, doi:10.1107/S0907444912048524

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