s9.m30.p1 **Treatment of Non-merohedral Twins.** Regine Herbst-Irmer, *University of Göttingen, Department of Structural Chemistry, Tammannstr. 4, D-37077 Göttingen, Germany. E-mail: rherbst@shelx.uni-ac.gwdg.de*

Keywords: Twin; Non-merohedral; Data processing

In contrast to twinning by merohedry the reciprocal lattices of the different domains of non-merohedral twins do not overlap exactly. So only part of the reflections are affected by the twinning. This will often become apparent during data collection. If both twin domains are similar in size, there are often problems with the cell determinations and usual automatic indexing programs fail. But nowadays there are several programs that can deal with such kinds of problems, e.g. *GEMINI* [1], *DIRAX* [2], *CELL_NOW* [3]. With these programs it is possible to find two (or even more) orientation matrices that lead to the same cell constants. With these matrices it is possible to integrate the data. In principle two different procedures are possible. The simpler one would be to integrate with all orientation matrices separately in different runs. This leads to three kinds of reflections: the reflections with no overlap, the reflections with an exact overlap, and the reflection with a partial overlap of a reflection of a second domain. The non-overlapped reflections are not affected by the twinning. The exactly overlapped reflections should be used in the refinement. They determine the fractional contribution of the twin domains. For the partially overlapped reflections only part of the reflection of the second domain is integrated and the degree of overlap is not known. So the treatment is difficult and often they are omitted. A second better way of integration is to use all orientation matrices in one step. Then the whole intensity of every reflection is integrated and we only have non- or exactly overlapped reflections. This procedure is possible with newer versions of the *SAINT* program [4] and with *EvalCCD* [5]. Normal scaling and absorption correction programs are not able to handle such data sets. Therefore the program *TWINABS* was developed [6]. Refinements with data sets generated by different integration processes will be compared. Taking non-merohedral twinning into account is only possible using a special data file that distinguishes between non-overlapped and exactly overlapped reflections [7].

[1] Sparks, R. (1999). *GEMINI*, Bruker AXS Inc. Madison.
[2] Duisenberg, A.J.M. (1992). *J. Appl. Cryst.*, **25**, 92-96.
[3] Sheldrick, G.M. (2003). *CELL_NOW*, University of Göttingen.
[4] Bruker (2001). *SAINT*, Bruker AXS Inc. Madison.
[5] Duisenberg, A.J.M., Kroon-Batenburg, L.M.J. & Schreurs, A.M.M. (2003). *J. Appl. Cryst*. (2003), **36**, 220-229.
[6] Sheldrick, G.M. (2002). *TWINABS,* University of Göttingen.
[7] Sheldrick, G.M. (1997). *SHELXL-97*, University of Göttingen.

s9.m30.p2 **High Performance Computing and Grid Applications in High Throughput Protein Crystallography.** R. M. Keegan, D. Meredith, G. Winter and M. D. Winn, *CCLRC Daresbury Laboratory, Warrington, WA4 4AD, U.K. E-mail: m.d.winn@dl.ac.uk*

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We present details of work being carried out to aid the development of high throughput protein crystallography through the use of high performance computing and Grid technologies. We focus upon the speedup of data collection processes and of certain structure solution steps, and upon remote access to high-performance compute resources.

Recent advances in data collection, such as the use of robotic sample changers, mean that large numbers of crystals can be screened and/or have datasets collected. Feedback regarding the quality of data collected is essential for efficient operation, and the speed of data processing programs can become limiting. To address this, we have developed parallel versions of the programs MOSFLM and SCALA, using a scripting approach for the former and parallelising the source code of the latter. We have also investigated the use of cheap Beowulf-type compute clusters, and clustering tools such as queuing systems.

Developments in automated systems for structure solution are well suited to the utilisation of HPC and Grid technologies. A parallel version of the molecular replacement code BEAST for running on a Beowulf type system has been developed, and has been shown to scale well with the number of processors. Access to high-performance compute resources has been achieved through the use of web-services and Grid-enabled web-portal technologies. These technologies facilitate the remote submission and monitoring of computationally intensive jobs in a secure, platform independent environment.