

Chairman's Message - from John Squire

Once again CCP13 activity over the last twelve months has been at a high level and significant new software developments have been made. One of the criticisms of our software in the past has been that, although it is clearly robust and effective, it is sometimes difficult to use especially for newcomers. For this reason tremendous efforts have been made, particularly by Andrew He and Ganeshalingam Rajkumar, to generate updated and more user-friendly versions of such key programs as XCONV, XFIX, FTOREC and LSQINT. These programs have also been implemented in WINDOWS and have been put together into a new integrated package called ICE (the Integrated CCP13 Environment) which also includes a new image handling package called the CCP13 Image Viewer (See He *et al.*, this volume, for a description of ICE). At the moment Image Viewer has a restricted range of image handling routines, but these are gradually being enhanced so that in the end all the early image rotating, centering, scaling, adding or subtracting procedures that are needed, for example, to enhance signal to noise, to subtract camera backgrounds, and to properly orient the recorded diffraction images before further pattern modelling and data reduction actually take place, should be relatively easily achievable. Finally, with regard to data reduction, all of the classic CCP13 packages are gradually being implemented in JAVA so that they become platform-independent.

Data reduction is clearly only part of the CCP13 remit and several new modelling programs have now been included, or are about to be included, in the CCP13 portfolio. Of particular interest here, especially for those either not familiar with the nature or origin of helical diffraction patterns or who are themselves teaching others about helical diffraction, is that there is a new program called HELIX which is a very user-friendly program that simulates helical diffraction patterns. Using HELIX, the effects of adjustments to different helical parameters can be easily and quickly tested. It is hoped that HELIX will be a useful didactic tool for fibre diffraction, but it also has use as a research tool, since simple trial structures can be generated and tested against observed diffraction data from an unknown structure as a preliminary filter prior to going into full modelling. This brings us to the need to have available fully rigorous and well-documented modelling programs. CCP13 has now implemented three such programs. One is the program LALS (Okada, K., *et al.* & Arnott, S. (2003: *Comptl. Biol. & Chem.* 27, 265-285) which can model and refine molecular structures to atomic resolution against high-angle fibre diffraction data. The second is the program MOVIE, which is fully described in the paper by AL-Khayat *et al.* in this Volume. MOVIE can take a known molecular crystal structure, can model it as a collection of spheres or with full atomic coordinates, and, if the structure can be broken down into discrete sub-domains, the full molecular and sub-domain positions can be parameterised and a simulated-annealing approach used to optimise the molecular configuration and shape against observed low-angle fibre diffraction data (see AL-Khayat *et al.*, this volume, where the myosin head in muscle is used as an example). The third package, called CalcTrans, is a simple but versatile program that takes in object positions in cartesian coordinates or cylindrical polar coordinates and computes the cylindrically averaged Fourier transform.

Apart from software development, CCP13 has an important role in helping to form a coherent and active 'non-crystalline diffraction' (NCD) community, both in the UK and abroad, and both our annual Workshops and the production of this Journal help to achieve this. In addition we welcome and very much congratulate our US colleagues who have been successful in setting up the National Science Foundation-funded *FiberNet* organisation (see article by Gerald Stubbs in this Volume). We very much look forward to working with and contributing to *FiberNet* in the next few years. Since its inception, an important activity of CCP13 has been to support solution scattering studies. However, despite the inclusion of several solution scattering papers in *Fibre Diffraction Review* over the years, this approach has probably appeared to have a relatively low profile compared with fibre diffraction itself. The CCP13 Committee are very keen to be able to represent the important solution scattering component of the NCD community and efforts are currently being made to form close links with solution scatterers and their software and to supplement this software where it is needed. We are also interacting fully with such organisations as CanSAS.

The Annual CCP13/NCD Workshop in 2003 was a splendid affair held at Fitzwilliam College in Cambridge and very ably organised by Jane Crawshaw to whom our thanks are due. A brief report on this very successful Workshop is given elsewhere in this Volume of *Fibre Diffraction Review*. The Workshop this year, this time being held in Grenoble, France, the first ever CCP13/NCD Workshop not to be held in the UK, is being organised by Trevor Forsyth with the support of ILL and ESRF. This welcome development illustrates the growing interactions between CCP13 and the European 'central facilities'. For many years we have appreciated the support of the CLRC Daresbury Laboratory which was instrumental in getting both CCP13 and our software development off the ground. Now our central facility links not only continue at Daresbury but are also spreading to the ILL and the ESRF in France, and to ISIS at the Rutherford Laboratory along with the newly emerging DIAMOND synchrotron at the same site. There is enormous synergy between the aims of the NCD activities at these facility sites and the activities of CCP13 and in the future it is hoped that we can be more involved with the whole data analysis procedure so that good software is available at each beamline for immediate data reduction and on-line evaluation of new data as it is being recorded. As an indicator of this need, a new grant application to our sponsors BBSRC and EPSRC has just been submitted for renewal of our support from October 2004. As an important part of the package presented in the new grant application, all of the central facilities mentioned above have made financial commitments to CCP13 staff support in the next grant period, as has the University of Cardiff which will host the CCP13 Workshop in 2005.

I look forward to seeing you all at the Grenoble Workshop in June, where, as well as excellent talks and posters, there will also be hands-on demonstrations of the CCP13 software together with an opportunity to visit the ILL and ESRF facilities. Why not bring your poster along to this meeting and try to win one of the prestigious cash Poster Prizes that are awarded each year.