

Chairman's Message

CCP13 News

As in previous years, 1998 has seen the Collaborative Computational Project in Fibre Diffraction (CCP13) go from strength to strength. As detailed elsewhere in this, the 7th issue of *Fibre Diffraction Review*, we had an excellent Annual Workshop in May, there were several visits to outstanding meetings and conferences by people sponsored by or associated with CCP13 and there were many interesting publications of work in which CCP13 software has played a central part. *Fibre Diffraction Review* is being incorporated as part of the CCP13 World Wide Web pages (as with the previous Newsletters: details elsewhere: see <http://www.dl.ac.uk/SRS/CCP13>) and it is also now recognised by libraries by having an allocated ISSN number (ISSN 1463-8401).

The Annual Workshop this year saw some changes in CCP13 personnel. Dr. Richard Denny, who was the CCP13 Research Assistant from its early days, was offered and accepted a permanent position at the CLRC Daresbury Laboratory. Richard has been absolutely central to the development and collation of the CCP13 software suite and, as many of you will know, his input and expertise have contributed a large part to the undoubted success of CCP13. Our congratulations go to him as do our very best wishes for success in his new job. However, I am delighted to say that Richard will still remain associated with CCP13. Dr. Geoff Mant has decided to step down as CCP13 Secretary, once again a role that he has carried out with great enthusiasm and skill since the start of CCP13 and to whom our thanks are due, and Richard Denny has agreed to take over from Geoff as the new CCP13 Secretary. Geoff will also remain in touch with CCP13 as a member of the CCP13 Committee ex officio. The loss of Richard Denny as the CCP13 RA obviously left a vacancy to be filled. We were fortunate in being able to recruit another recent PhD from Keele University, Dr. Mark Shotton. Elsewhere in this issue Mark gives a short biography of himself so that you can all get to know him and love him as in the case of Richard Denny! You can contact him at m.shotton@dl.ac.uk.

The original appointment of Mark Shotton was for a few months to the end of September 1998, because that was the termination date of the CCP13 grant from the BBSRC. An application to the BBSRC for

renewal of the grant for another three years was greatly aided by the decision of CLRC Daresbury Laboratory to part sponsor the Research Assistant position. The activities of CCP13 and its association with the Non-Crystalline Diffraction (NCD) community at Daresbury are closely linked and this sponsorship by Daresbury is a clear recognition of that. Fortunately the BBSRC application was successful and CCP13 is funded for another three years to September 2001 with Mark Shotton's appointment being extended to that date. As well as funding the Research Assistant and some much needed computing equipment, the new BBSRC grant helps to cover the costs of the Workshops and Newsletters.

At the Annual General Meeting of CCP13, formal elections to the Committee were made. The terms of office of Dr. Trevor Forsyth and Dr. Mike Ferenczi both concluded at the Annual Workshop this year but both members indicated their willingness to serve again if elected.

At the Annual General Meeting of CCP13 at the 1998 Workshop, I announced that I thought it to be timely and appropriate for me to step down as Chairman of CCP13 in the near future. I suggested that to make a smooth transition a new Chairman should be elected with a view to him/ her taking over from the time of the Annual Workshop in 1999. The CCP13 Committee considered the choice of successor and it was unanimously agreed that the name of Dr. Trevor Forsyth should be put forward to the AGM. This was done and at the AGM Trevor was duly appointed as Chairman-elect of CCP13. I have no doubt that Trevor's abilities and infectious enthusiasm for fibre diffraction research will ensure that CCP13 is in good hands and will fare well in the coming years. But no, you haven't seen the last of me yet! For the time being, at least, I will still be running the BBSRC grant and I will still edit *Fibre Diffraction Review*. Also at the AGM, Dr. Mike Ferenczi was elected to serve on the CCP13 Committee for another three year term.

We very much hope that you will come along to the 1999 Workshop (June 15-17, 1999) at St. Andrews University - details of which are given elsewhere in this issue. Among the eminent participants at the Workshop will be our host, the Principal of St. Andrews, Professor Struther Arnott, and also the

Principal of Stirling University, Professor Andrew Miller, both well-known fibre diffractionists. Remember not only that your poster could win a large cash prize (1st Prize - £100; 2nd Prize - £50), but also that abstracts will be included in the 1999 *Fibre Diffraction Review* - your work will automatically be available to a worldwide audience on the web. As usual, there will be bursaries available for students and young scientists to attend the 1999 Workshop. Details of all these are given at the end of the Newsletter.

CCP13, its Newsletter and its Friends Overseas

Your Contribution

Interested groups or individuals are invited to contact any of the officers of CCP13 to obtain information about CCP13 Workshops, software developments, software standards and so on. Offers of home-written software that could be incorporated into the new CCP13 suite of programs would be much appreciated and will, of course, permanently carry the author's attribution. Make sure that you are on the CCP13 mailing list and you will be kept informed.

International Cooperation

Although these CCPs are UK funded projects, there is a very strong interest in making them international

through cooperation with interested scientists in other countries. A natural link for CCP13, for example, exists with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association and possibly with some American synchrotron users (CHESS). Others exist with the ESRF at Grenoble and with the Photon Factory in Japan.

Newsletter Editorial Policy

Articles for inclusion in *Fibre Diffraction Review* are welcome by the Editor at any time, but preferably items for the December 1999 issue should arrive before the end of November 1999. It is hoped that *Fibre Diffraction Review* will become an annual 'essential' for fibre diffractionists. This is the place to advertise your fibre diffraction or NCD meetings, to report on new software or 'hot' results obtained using the CCP13 or other fibre pattern processing suites and to provide reports of meetings of interest, preferably together with one or two photographs. All technical articles will be scrutinised both for scientific content and presentational style by the Editor (or his nominee) together with at least one other member of the CCP13 Steering Panel. In this way we hope to maintain high standards. Remember that the Newsletter not only goes to other fibre diffractionists, but also to various members of the Research Council Secretariats and to other funding agencies.

Fibre Diffraction Featured on Covers of IUCr Publications

Fibre diffraction has recently received increased exposure in the crystallographic community, being featured on the covers of two IUCr (International Union of Crystallography) publications.

The May (Vol. 6, No. 2) 1998 issue of the IUCr Newsletter featured work from Keiichi Namba's laboratory (International Institute for Advanced Research, Japan) on the structure of bacterial flagellar filaments. This work (see *Nature Structural Biology*, 5, 125-129, 1998) describes X-ray fibre diffraction data from the left and right supercoiled states of the flagellar filament, and the 9Å structure

of the R-type filament. Bacteria swim using the rotating filaments, and bacterial motility involves switching between the left and right states. An editorial on fibre diffraction, as well as a report on the Third Fibre Diffraction Workshop, held in Kentucky in October 1998, appeared in the same issue.

The 1999 issues (Vol. 55) of *Acta Crystallographica Section A* feature work from Rick Millane's (Purdue University, USA) laboratory on diffraction by disordered polymer fibres. This work (see *Acta Cryst. A* 52, 812-829, 1996) describes theory and