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Chairman's Message

The past year has seen many important developments for CCP13. Three appointments have just been made to fill the posts funded by the recent BBSRC/EPSRC grant. In addition to Matthew Rodman, who continues his joint CCP13/NCD appointment based at Daresbury Laboratory, we welcome Jane Crawshaw, as well as Rajkumar Ganeshalingam (Raj) and Andrew He to the project. Jane is based at Cambridge and involved principally in the development of software for the analysis of synthetic polymer systems. Both Raj and Andrew are at Imperial College, with Raj having a particular involvement in data extraction procedures and Andrew taking on the task of molecular modelling for biological systems. It is also a great pleasure to welcome the involvement of David Dover in CCP13 modelling activity. The appointment of new staff has also allowed a redistribution of some of the administrative tasks - the workload associated with the organisation of the annual meeting, Fibre Diffraction Review and web site has gradually increased over the years and in recent times have all been shouldered by Matthew. As part of this, it is planned that the bulk of the work associated with the production of Fibre Diffraction Review will shift to Imperial College.

With the new personnel in post, CCP13 is poised to deliver high quality software solutions that will be badly needed by the Fibre Diffraction and Non

Crystalline Diffraction (NCD) communities as the field continues to expand. This growth is self evident: at the same time as rapid developments in biochemistry, molecular biology, and polymer chemistry are producing new types of problem, major developments in instrumentation are widening the scope of experimental methods and therefore the range of samples that can be studied. For synchrotron x-ray studies, in addition to beamlines 2.1, 16.1 and 14.1 at the SRS, the ESRF microfocus beamline ID13 can be used to study fibres as small as ~2mm diameter, while the high flux beamline ID2 provides for simultaneous low and high angle fibre diffraction experiments. At the Institut Laue Langevin (ILL) the EPSRC has just funded a major development for high-angle neutron fibre diffraction on instrument D19, opening up completely new areas. In parallel with this, an initiative for the preparation of deuterium labelled samples has occurred at the ILL with the award of a major grant (funded through Keele) from EPSRC for the support of a number of flagship projects (including three neutron fibre diffraction projects) that will exploit a new Deuteration Laboratory at the ILL & the EMBL Grenoble Outstation. The future also promises further major development with the construction of DIAMOND and also of the second target station at ISIS.

The implications of these developments for CCP13

are very significant. Not only are there continuous requirements for CCP13 to maintain compatibility with the various data formats that arise from the different facilities, but as the range of experiments extends, there is also a clear need for data extraction software to be able to cope with many different types of sample disorder. In addition to the "standard" cases (eg solutions/amorphous polymer, crystalline diffraction, continuous diffraction), there exist many situations where complex types of sample order/disorder make data extraction protocols more difficult. Examples include diffraction from "doubly oriented" samples (see previous issue of Fibre Diffraction Review) or other situations where diffraction may contain complex mixtures of crystalline and continuous diffraction (see paper by Millane et al, this issue). On the molecular modelling side it is unlikely that the needs of CCP13 will be accommodated by any single modelbuilding/refinement package. For some problems it is clear that programs such as SHELX are very effective. For others, programs such as X-PLOR are more suitable - fibre diffraction functionality has already been built into a modified version of X-PLOR and will be carried through to an analogous version of CNS. At the same time the linked atom least squares (LALS) programme is being rebuilt to include a user friendly front end - with the particular involvement of David Dover.

Over and above the scientific issues that form the main brief of CCP13 activity, the technical plan for the CCP13 software is to move towards a single Java based interface that will permit an easy route from data extraction through to model building and refinement. The large increases in computing power that we all now take so much for granted mean that the development of such an interface for CCP13 should not be restricted to Unix based platforms and that considerable emphasis should be placed on making all programs operable on standard Windows and Macintosh desktop/laptop machines.

It has been very pleasing to see the steady build up of activity within the CCP13 community over the last four years or so. The last CCP13 conferences at St. Andrew's, Sheffield, and Stirling Universities have been very well attended (with steadily increasing numbers of overseas delegates), with extremely interesting programmes. At the time of writing, the number of registrations for the next meeting at Keele makes it look as though the same will be true in June 2002. See you there!

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