

the end, the journal is nothing without your contribution as users. Please remember this for future issues – this is *your* journal and its success will help to ensure continued support of CCP13 from the BBSRC and from Daresbury Laboratory. Whether you are an industrialist, academic staff, or a postgraduate student, please consider submitting articles or reviews of your work to *Fibre Diffraction Review*. We cannot guarantee publication but I know that John will make sure that all articles are refereed well. If it is published, your article will land on the desks of just about everybody in the field.

Please *do* come to the Sheffield meeting in June and please *do* submit your work (whether as a review or otherwise) to *Fibre Diffraction Review*. Please also remember that in addition to the training sessions held at the main annual meeting, CCP13/NCD now runs separate software training workshops for newcomers to the software. Last year the first of these was held at Daresbury Laboratory and was

organised by Mark Shotton and Nick Terrill. About 17 people attended and the feedback was very positive. The timing and location of this training workshop makes it an ideal and cheap way for new students to familiarise themselves with the field. If you require any further information on CCP13 and NCD, remember the website at <http://www.dl.ac.uk/SRS/CCP13>. Also take the few minutes or so that are needed to subscribe to the CCP13 bulletin board (instructions for this at the website).

It just remains for me to thank all those involved for their efforts over the years and to welcome our new steering committee members, Keiichi Namba (Japan), Tom Irving (Illinois, USA), Gerald Stubbs (Vanderbilt, USA), and Rick Millane (Purdue, USA). We are delighted to have their input on the panel.

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## Meeting Reports

### CanSAS II, 16th May 1999, Brookhaven National Laboratory

On May 16th 1999, a workshop entitled “Data Handling for Small-Angle Scattering” a.k.a. “canSAS II” was held at Brookhaven National Labs as a prelude to the worldwide SAS 99 Congress. The workshop was chaired by John Barnes of NIST, (the chair of the IUCr Commission on Small-Angle Scattering who sponsored the workshop). “canSAS” stands for “Collective Aid to Nomadic Small-Angle Scatterers”. “canSAS I” was a workshop in Grenoble in February of 1998 attended mainly by “Instrument Responsibles”. canSAS II, in contrast, represented an attempt to bring data handling issues to the larger SAS community which was represented by about 90 attendees.

Wim Bras kicked off the workshop with an overview of the accomplishments of canSAS I and some of the issues raised at the time. More general talks were “Using Statistics to Assess SAS Data Quality” by John Barnes, “Resolution Issues in SAS” by John Barker also of NIST, and “Modeling and Goodness of Fit in SAS Data Reduction” by Jan Skov Pedersen, Risoe. The remainder of the talks and the subsequent panel discussion were aimed directly at

the concerns brought out in canSAS I, namely how can we make it easier for users to take home their data and interpret it once they get there? To this end Marc Malfois and Dmitri Svergun from EMBL, Hamburg talked about “sasCIF - A Proposed Standard for 1-D SAS”. Joachim Kohlbrecher, PSI, followed up with “One User’s Experience with Nexus” which dealt with the Nexus file format, a work in progress which proposes a standard file format for arbitrary SAS data based on HDF. Richard Heenan, of ISIS, followed up with “Existing Tools for SAS Nomads” which was a comprehensive overview of existing programs and their availability.

The remainder of the workshop consisted of a panel discussion moderated by myself (Tom Irving, BioCAT). The main issues that were discussed were:

- 1) How to make it easier for users to get access to their data.
- 2) Are we in a position to bless a “standard format” or formats?
- 3) Can we move towards a “gold standard” software package or packages?

The sasCIF ASCII format allows simple text tools to get at data. Although no-one could claim that there were any definitive answers to any of these questions, it was clear that there were some positive movements in that direction, however glacial.

Clearly portable, widely supported, self-describing file formats would assist users greatly with using data from a variety of facilities. There is still controversy whether the best approach is to develop and widely distribute routines for converting the formats used into one or more "standard formats" once they have been determined or to rewrite existing code to use the new formats? The advantage of the former is that it is less work for the programmers. In the discussions both sasCIF and Nexus appear to be viable candidates for "standard formats". ImageCIF (for 2-D) and sasCIF could fit naturally together and would be likely to get the stamp of approval from IUCr. It was resolved that new facilities should be encouraged to support one or both of sasCIF and Nexus and see which meets the needs best, as well as giving feedback data for the developers. Tom Irving, BioCAT, and Wim Bras, Dubble CRG, said they would endeavor to do so.

Can we move towards a "gold standard" software

package or packages? It was recognized that currently available packages are hard to find and documentation varies widely in adequacy still, despite many efforts by various people to improve this situation. The basic problem is that these outreach activities are generally too time-consuming for busy developers to support. The group was informed that the CCP13 project had recently taken SAS as part of its purview. It was suggested that Mark Shotton (the main CCP13 maintainer) should be invited to visit various facilities with established code bases to get a handle on the magnitude of the problem and see what can be done. People who would like to help in this way should contact Mark at m.shotton@dl.ac.uk. The workshop ended with a discussion of future canSAS meetings. There seemed to be a consensus that a "technical" canSAS meeting should be scheduled in 18 months or so. The next international SAS meeting in 2002 would be the next opportunity to communicate progress with the larger community of users.

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### **SAS99, XIth International Conference on Small Angle Scattering, 17th-20th May 1999, Brookhaven National Laboratory**

The XIth International Conference on Small Angle Scattering was held at the Brookhaven National Laboratory (BNL) on Long Island, New York in the USA. BNL was founded in 1947 on the site of the U.S. Army's former Camp Upton, by a non-profit educational consortium called Associated Universities, Inc. under contract to the Atomic Energy Agency. Brookhaven Science Associates now operate BNL for DOE, they are a partnership of the State University of New York at Stony Brook and the Battelle Memorial Institute.

The Brookhaven facility carries out basic and applied research in physical, biomedical and environmental sciences together with energy based technologies at its various centres of excellence. These include an Accelerator Test facility for High Energy Physics and accelerator research, an Alternating Gradient Synchrotron to provide protons for High Energy Physics, a High Flux Beam Reactor for neutron

experiments and The National Synchrotron Light Source with X-ray and vacuum ultra violet rings. They are in the process of commissioning RHIC, a Relativistic Heavy Ion Collider with a 3.8km diameter ring, used in the study of atomic particles.

With a meeting of this size it would be impossible to give justice to all the topics that were up for discussion so instead what follows are a few of the highlights.

One of the features of the meeting was the excellent work now being carried out at a number of third generation sources in the field of microfocus X-ray scattering. In particular Christian Riekell gave an excellent presentation on the recent advances in microfocus work carried out at the ESRF on beamline ID13. These included new developments in the field of microfocus collimation *e.g.* capillaries, mirrors and waveguides which can give useful X-ray