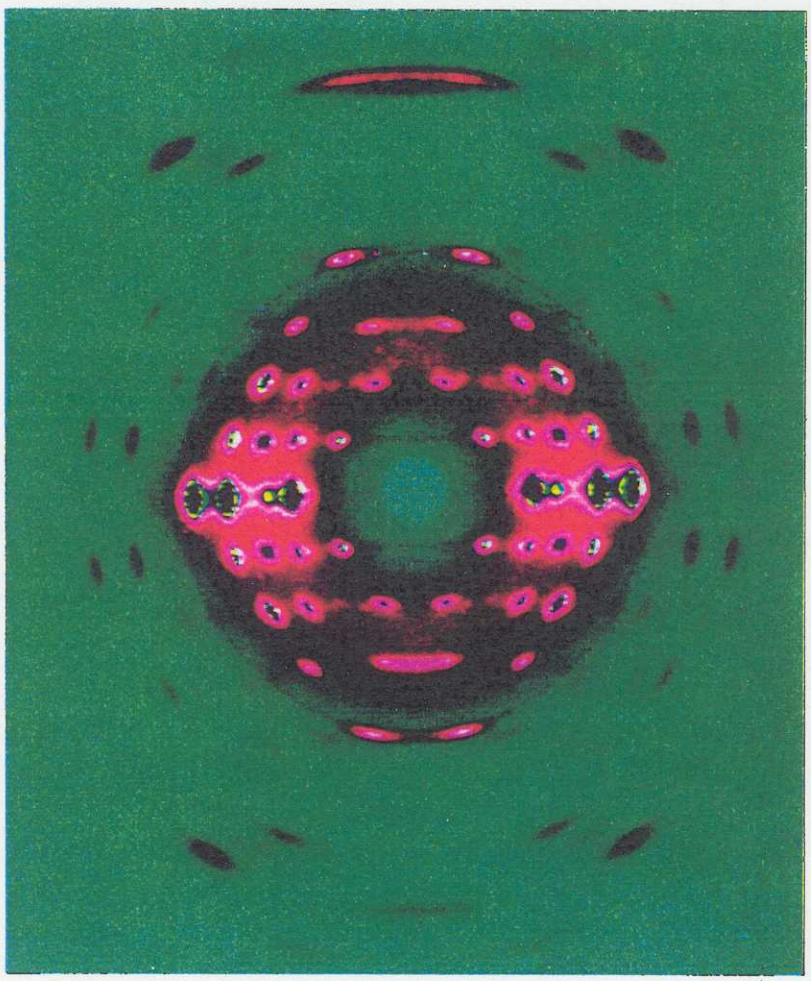
THE CCP13 NEWSLETTER

Software Development for Fibre Diffraction



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STEERING PANEL

The current membership is: Dr. John Squire (Chairman; 1996), Dr. Geoff Mant (Secretary; 1996), Dr. Richard Denny (CCP13 'RA'; ex officio), Dr. Mike Ferenczi (1995), Dr. Trevor Forsyth (1995), Dr. Keith Meek (1995), Dr. Manolis Pantos (1996), Dr. Robert Rule (1997), Dr. Tony Ryan (1997).

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CHAIRMAN'S MESSAGE

This is the second of the annual CCP13 NEWSLETTERs. The articles in the Newsletter detail the progress in developing fibre diffraction software in the past year, some ideas about the direction that CCP13 should take in the future, an overview of aspects of synthetic polymer science that CCP13 could and should address and reports of fibre diffraction meetings, especially the CCP13 Annual Workshop held in Daresbury in May 1993.

Reminder - What is a CCP?

CCP stands for Collaborative Computational Project. CCP13 is currently funded by the UK Science and Engineering Research Council via its Science Board Computing Committee (Computing Science Initiative) and is one of 12 current CCPs. These are:

CCP1	Electronic structure of molecules
CCP2	Continuum states of atoms and molecules
CCP3	Computational studies of surfaces
CCP4	Protein crystallography
CCP5	Computer simulation of condensed phases
CCP6	Heavy particle dynamics
CCP7	Analysis of astronomical spectra
CCP9	Electronic structure of solids
CCP11	Biosequence and structure analysis
CCP12	Novel architecture computers in Fluid Dynamics
CCP13	Fibre diffraction
CCP14	Powder diffraction

The general policy on CCPs and the evaluation of their progress etc is considered by the CCP Steering Panel, currently chaired by Dr. Julia Goodfellow, Birkbeck College, London, UK). The Steering Panel comprises all of the CCP Chairmen and various observers.

Note that with the restructuring of the Research Councils, some CCPs currently funded by SERC may not remain there, in its new guise as the EPSRC, but may be funded wholly or partly by the new BBSRC.

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.

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 FIBRE suite of programs would be much appreciated and will, of course, permanently carry the authors' attribution.

IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS - THIS CCP IS FOR YOU - PLEASE HELP TO MAKE IT WORK!

REPORT ON THE 2nd CCP13 WORKSHOP

The Second CCP13 Workshop was held at the Daresbury Laboratory on May 14th and 15th, 1993 and attracted nearly 40 participants, including visitors from Australia, Canada and France. The scientific content of the Workshop was of a high standard throughout, the level of discussion was good and the organisation by Daresbury Laboratory staff was excellent. Our thanks are due to them for enabling the meeting to run so smoothly.

ELECTIONS It is important for the health of CCP13 that it is entirely democratic and open in its structure and operation. Elections were therefore held at the Workshop for the positions of Chairman and Secretary. In addition, owing to the retirement of two of our founder Committee members, Professor Joan Bordas and Dr. Paul Durham, whose services and input have been much appreciated, two Committee vacancies needed to be filled. In the election, Dr. John Squire and Dr. Geoff Mant were confirmed as Chairman and Secretary respectively, and it was left to the Committee to identify two synthetic polymer scientists to appoint to the Committee in order to strengthen what was accepted as a very important aspect of CCP13 activities. Subsequently Dr. Robert Rule (ICI, Runcorn) and Dr. Tony Ryan (UMIST) were appointed by Chairman's action. Current Officers and Committee members with their period of office are given on Page 1.

SCIENTIFIC SESSIONS The Workshop started on the Friday with a presentation by Joan Bordas of the plans for the future of Synchrotron Radiation Science in the UK. In particular, for this fibre diffraction community, he described the properties of a new medium energy source (*Diamond*) that had been presented to SERC as a replacement for the SRS at about the turn of the century. This machine would be of substantially higher brilliance than the SRS, although not as high as the ESRF, but it would have total fluxes comparable to ESRF for certain applications and would satisfy the volume of work expected from UK users, who would only expect to obtain a modest amount of time at ESRF for particular, specialist applications. Richard Denny, the CCP13 Research Assistant, then outlined his initial developments of fibre diffraction software and his plans for the future. An outline of the current state of CCP13 software is given elsewhere in this Newsletter. There followed an interesting series of talks on recent results and analysis of muscle and DNA diffraction data: Mike Ferenczi on recent work on single muscle fibres studied with sub-millisecond time resolution, Barry Millman on studies of whole muscle carried out at CHESS, Joan Bordas on recent time-resolved diffraction data from active, shortening frog muscle, Nick Berovic on some problems that had been found using multiwire detectors, Jeff Harford on recent millisecond time-resolved diffraction results from contracting fish muscle and modelling of these results to produce Muscle-The Movie, and Watson Fuller on the location of water and ions in DNA and on time-resolved transitions in some synthetic polymer systems. The Friday session closed with an enjoyable social gathering over drinks, followed by Dinner in the Daresbury restaurant.

On Saturday, two talks were on results from collagen fibrils: Andrew Hammersley on software development for analysis of collagen diffraction patterns, Veronica James on the observation of very long spacings in some collagen preparations. Hind AL-Khayat gave a talk on actin filament structure which showed the increasing relevance of low-angle X-ray diffraction to the determination at high resolution of sub-domain movements within known molecular structures and both that work and the collagen studies pointed towards the partial overlap of the interests of CCP13 and CCP4 in Protein Crystallography. Robert Rule gave a presentation on small-angle scattering from synthetic polymers, which also served to illustrate not only some of the kinds of polymer structure being studied (oriented semi-crystalline polymers, phase-separated systems) but also novel experimental approaches (e.g. simultaneous SAXS, DSC studies etc.). The session concluded with an overview by Rob Lewis of the properties of different X-ray detectors, especially the image plate systems that are becoming increasingly popular. After lunch there was a general discussion concerning the future development of CCP13 and also the next 'renewal' grant application that needs to be submitted to SERC in January 1994. The main conclusions are presented elsewhere in this Newsletter.

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In summary, the Workshop provided not only an excellent environment for fibre diffractionists to meet and to share common problems, but it provided a good forum for presenting new software developments, new results and new hardware. The main disappointment was in the small number of synthetic polymer scientists at the Workshop. The area of synthetic polymers is seen by the Committee as central to the activities of CCP13, and it is hoped that in the future this Workshop will be seen by the polymer community to be an excellent place to discuss the development of new ways of both stripping and modelling polymer diffraction data.

REPORT ON THE 2ND WORKSHOP ON FIBER DIFFRACTION FROM BIOLOGICAL MACROMOLECULES

The CCP13 Chairman (John Squire) and Research Assistant (Richard Denny) were privileged to attend the Second Fiber Diffraction Workshop held in McCormick's Creek State Park at Spencer, Indiana from June 13th to 16th, 1993. We were joined by one other UK participant, Watson Fuller (Keele University). This really was a 'Workshop', with about 15 participants in total and a few days in which to discuss fibre diffraction problems in some detail. These Workshops were the brain-child of Gerald Stubbs (Vanderbilt University) and the main organiser of this one was Rick Millane (Whistler Center for Carbohydrate Research, Purdue University). On Monday 14th, the Workshop comprised talks on general fitting of fibre diffraction patterns (Richard Denny, Imperial & Daresbury and Thomas Hendrixson, Purdue), high resolution analysis and phasing of polysaccharides and viruses (Gerald Stubbs), modelling of disorder (Bill Stroud, Purdue) and molecular dynamics computations (Hong Wang & Gerald Stubbs). Gregory Kishchenko (Florida State University) presented analysis of M13 phage at 7 Å resolution, and discussed a new, high accuracy, method of determining specimen to film distance directly from the observed diffraction data. After lunch there was a roundtable discussion on specimen preparation. After a free afternoon in which to enjoy the scenic McCormick's Creek State Park and after Dinner, there was a 'special' talk by Watson Fuller on 'Complementary neutron and X-ray fibre diffraction of DNA and synthetic polymers'.

Tuesday morning saw talks on actin filament structure and regulation (John Squire, Imperial), the structure of Alzheimer β-amyloid fibres (Dan Kirschner, Harvard Medical School) and on the influence of side-chains, ions and water molecules on the rheological properties of calcium welan (Akella Radha, Purdue). After coffee were three talks by people from the Whistler Center on the roles of sodium ions and water molecules in the stability of the Poly d(A).Poly d(T) helix (R Chandrasekaran) and on the polysaccharides araban (Min Zhang) and mannan and related polysaccharides (Rick Millane). A roundtable discussion on data collection followed after lunch, and, after dinner, John Squire gave a 'special' talk on "Muscle - The Movie: An approach towards the first ever 3-D movie of molecular activity in an intact cell". Wednesday morning comprised a roundtable discussion on phasing and refinement and the Workshop closed with a short business meeting.

Though the participants were small in number, the meeting was of a high scientific standard and was informative and stimulating; it emphasised common problems, it reinforced the desirability of cooperating on the development of fibre diffraction software and it enabled the participants to get to know each other in a relaxed environment. Roll on Workshop number three!

THE 1993 ALPBACH EMBO WORKSHOP ON: 'COILED-COILS, COLLAGEN AND CO-PROTEINS'

This meeting was organised in Alpbach, Austria in September, 1993 both as a means of bringing together scientists working on related fibrous biological structures (e.g. muscle proteins, intermediate filaments, collagen) and also as an opportunity to honour two outstanding fibre diffractionists; Bruce Fraser and Tom MacRae. Their classic book 'Conformation in Fibrous Proteins' has been an invaluable source for many fibre diffractionists and their general contribution to the field has been enormous. The EMBO Workshop was well attended (about 65 scientific participants), it was thoroughly enjoyable scientifically, the Hotel was excellent and the surrounding scenery - typical Tyrolean hills, valleys and mountains - was superb. The next such Workshop is planned for 1997!

Integration of fibre diffraction patterns: FTOREC and LSQINT

Richard Denny

Introduction

The aim of these two programs is to provide an automatic method for integrating intensity on fibre diffraction patterns. The programs are in fact extensively rewritten and augmented versions of programs written to analyze diffraction patterns from Pf1 virus by Colin Nave, Richard Bryan and Ian Clifton, packaged to allow refinement of cell and intensity profile parameters and processing of multiple data sets.

The programs are well suited to the analysis of "simple" patterns in which the diffracted intensity of interest is either all Bragg sampled or all continuously distributed along layer lines, although it is hoped that in some cases the background subtraction methods built in to the program LSQINT will be sufficiently sensitive and well-conditioned in order to provide a method for separating continuous from Bragg sampled intensity, leaving the continuously distributed intensity intact for further analysis. The assumption of a "simple" diffraction pattern allows effective integration of intensity by prediction of the positions and profiles of sampling points (either intervals along a layer line or Bragg peaks) and then fitting this linear model to the observed pattern once the background has been subtracted or if a suitable function for the background can be included as part of the model.

FTOREC

The program FTOREC provides a means of transforming data from detector space to reciprocal space, but currently assumes the user has prior knowledge of the centre and rotation of the diffraction pattern and the tilt of the specimen. The backstop can be masked out to prevent this region from being fitted in LSQINT and other more general areas using a combination of the BSL functions .MSK and .ADD. By default, the pattern is transformed and quadrant folded with optional corrections for film absorption.

LSQINT

Fitting of the data is performed on the reciprocal space output from FTOREC. The first stage of the program is to generate intensity profiles for the sampling points defined by the input lattice parameters. There may be only one parameter defining the c-axis repeat for one-dimensionally crystalline specimens or six for fully crystalline examples. The profiles of the sampling points are described by up to five parameters for the fully crystalline case or two for the one-dimensional case. The two which are always required are the reciprocal particle length and disorientation (arcing). Bragg sampled patterns require one more parameter to define the reciprocal particle diameter and optionally another two terms giving a quadratic dependence of spot width with reciprocal space radius. At this stage, an image can be computed for comparison with the transformed

data consisting of equally weighted sampling points smeared out with the given intensity profile parameters. This gives the user an immediate appreciation of the closeness of the input cell and profile parameters to the true values.

Once the user has arrived in the right ball park, it is safe to continue with background subtraction and fitting. There are four background subtraction methods available in LSQINT, three of which require information generated by the profile calculation. It is probably safest, therefore, to start with the option which does not assume any knowledge of the sampling point profiles.

Background subtraction methods

1. A method devised by Paul Langan is used to subtract background when no knowledge of the positions and intensity profiles of the sampling points is to be assumed. A notional aperture of user-defined dimensions is centred on a pixel in the diffraction image. The pixel values that fall within this aperture are sorted into ascending order and a user-defined interval of this sorted list are averaged to calculate the background value for the central pixel of the aperture. This process is repeated for every pixel in the image so that a complete (smoothed) background image is formed. In order to trap excessively high background, the calculated values are compared with the circularly averaged background, which is determined by iterating the procedure of averaging pixel intensities in resolution bins and then rejecting (high) outliers. The number of iterations and the definition of an outlier are again under user control.
2. A similar notional aperture can be used in conjunction with a least squares fit of background and all sampling points whose intensity profiles impinge upon the aperture to estimate the height of the background at the central pixel. In this scheme, the background across the aperture is initially assumed to be a horizontal plane and the height of this plane is fitted along with the relevant peaks. The aperture is then translated by half its width (or half its length when it comes to the end of a raster) in order to build up a grid of known background values. Cubic spline interpolation is then performed over this grid in order to complete the background image for the first cycle. The next iteration will construct a background over each aperture position, not using a plane but with the surface formed by the interpolated background. The background is then re-fitted using this surface, and the relevant peaks, scaling the height of the central pixel of the aperture in the fit. This procedure can be repeated as many times as is desired but it is important to remember that the usefulness of the fit will depend on having good estimates of the intensity profiles and that too many iterations may allow the background to accumulate a linear combination of the intensity profiles.
3. If the background is sufficiently smooth, a simple linear function can be used to fit it simultaneously with the peak fitting. The function currently employed for this

purpose is:

$$Background = \sum_{i=0}^{3} A_i D^i + B_i \cos 2(i+1)\phi$$

where $D = \sqrt{R^2 + Z^2}$ and $\phi = \arctan(R/Z)$.

4. During the intensity profile calculation, the profile of any sampling point is trimmed if the contribution of the outermost points is insignificant. This means that the significant extent of each sampling point is known and that the total area on the pattern impinged upon by profiles can be excluded from being considered as background. The remaining partial background image can then be interpolated to give a complete background image. If the interpolation gives rise to background values too far from the circularly averaged background (as defined in method 1), the values are replaced by the circularly averaged background at those points. The usefulness of this method is limited if there are large areas of the image where no background information is available.

Peak fitting

Once the background has been subtracted, the peaks defined by the input lattice and profile parameters can be matched to the image by a linear fit. This can be done either with a least squares method, or with a maximum entropy technique. Depending on the degree to which the sampling points have been smeared out, there may have been some information loss in the observed pattern compared to the ideal case of the squared molecular transform sampled by Dirac delta functions (in one or more dimensions). If this is the case, the matrix describing the linear transformation between the perfect sampling and the observed pattern will be singular and no direct inverse transformation will be available. Even if this is not the exactly the case, the large number of operations performed on the matrix using the limited precision available may cause it to appear almost singular. If a least squares fit is desired, it is almost always necessary to filter out the smaller eigenvalues of the normal matrix in order to eliminate the problems of singularity and construct the pseudo-inverse with only the surviving eigenvalues (and eigenvectors). This approach is suitable when the number of peaks to be fitted is around 500 if the fit is performed in double precision and works well for Bragg sampled patterns.

Alternatively, a maximum entropy criterion can be imposed upon the solution relative to some prior distribution with the constraint that the transformed solution agrees reasonably well with the data. This approach guarantees positivity of the solution and removes the problem of singularity by selecting that solution (out of a set of solutions which agree equally well with the data) which contains the minimum information content with respect to the prior distribution. The algorithm of Skilling and Bryan utilized in LSQINT, has the added benefit that it operates only on a subspace of low dimension of parameter space in any iteration, so that diagonalization of matrices is fast and the difficulties associated with roundoff error are reduced. For large problems, this algorithm is faster and more stable than least squares and is recommended for fitting intensity which is continuous along layer lines.

Cell and profile parameter refinement

Once a set of intensity values has been assigned to the sampling points by the fitting procedure, the cell and profile parameters may be refined. The maximum number of parameters that can be refined is eleven for a triclinic cell (five profile parameters along with the six cell parameters) but the number is usually less than this. A simple refinement algorithm, due to Nelder and Mead, which requires no derivative calculation has been employed as calculation of the profiles is fast compared to the fitting and background subtraction procedures. The user specifies the number of cycles of refinement, the initial shifts for the profile parameters and the reciprocal cell parameters and the tolerance used to define convergence. The refinement can then be used in tandem with the fitting procedure to provide an overall refinement scheme for intensities and the sampling point position and shape description.

Input and output

The action of both programs is decided by keyworded input from the user. The image file format used is the same as that used by BSL and OTOKO with the minor extension that input files for LSQINT require some reciprocal space mapping information written into the second header record by FTOREC. Intensity output files from LSQINT are formatted with seven columns:

$$h, k, l, R, M, I, \sigma(I)$$

corresponding to the indices and reciprocal space radius of the sampling point, the multiplicity, intensity and standard deviation. If the multiplicity is greater than one, the last reflection in the multiplet list is assigned the total intensity value. In addition to the formatted intensity output file, it is optional to output an image file containing two frames for every frame fitted. Odd numbered frames correspond to the calculated background while even frames represent a simulation of the fitted image from the addition of the calculated background and the smeared out fitted intensity values.

Availability

Executable files are available for SUN, HP and DEC platforms from /nfs/dls12/ccp13/CCP13 on any of the NCD nodes at Daresbury Laboratory. Documentation is in the doc subdirectory.

FIT2D

An alternative program is available for users who have a suitable version of the PHIGS graphics system. Written by Andrew Hammersley at the E.S.R.F., FIT2D also offers the facility to correct Molecular Dynamics image plate data for spatial distortion. Work is currently underway to port the program to use SunPHIGS and to make it available to NCD users at the SRS.

SUMMARY OF AVAILABLE SOFTWARE

Compiled by Dr. Geoff Mant

The following table lists mosts of the frequently requested DL supported programs, available as executable modules.
The dates refer to the last software update.

Program	Description	SunOS 4.1.x *	Irix 4 *	HPux	Ultrix
xotoko	1-D data manipulation	09/10/92	02/12/93	24/06/92	13/04/92
bsl	2-D data manipulation	02/12/93	02/12/93	27/06/92	13/04/92
v2a	vax to unix data conversion	06/08/91	24/06/92	27/06/92	13/04/92
a2v	unix to vax data conversion	19/01/93	-	-	-
otcon	ascii to otoko data conversion	17/02/92	-	-	-
reconv	otoko to ascii data conversion	05/02/92	-	28/06/92	-
tiff2bsl	image plate to bsl format	29/10/92	-	-	-
i2a	ieee to ansi data conversion (DEC only)	n/a	n/a	n/a	
ftorec	Image to reciprocal space transformation	17/05/93	10/01/94	17/05/93	17/05/93
lsqint	2-D integration & background subtraction	09/08/93	10/01/94	09/08/93	09/08/93
fdscale	scaling of intensities	06/07/93	10/01/94	06/07/93	06/07/93
fd2bsl	conversion of intensities to BSL format	03/08/93	10/01/94	03/08/93	03/08/93
u2v.exe	VMS record conversion (VMS only)	n/a	n/a	n/a	n/a

* Implementations for Solaris 2.3 and Irix5 should be available by mid 1994.
n/a is not applicable.

SOFTWARE DEVELOPMENT FOR SYNTHETIC POLYMER DIFFRACTION

Robert Rule, ICI Chemicals & Polymers, Runcorn, UK.

The aims and achievements of CCP13 have generally been perceived as being more relevant to the software needs of the Biophysics Community. However, the overall scope of the project is very much broader, and several opportunities exist for the development of software which is better suited to the requirements of diffraction or scattering from other Non-Crystalline materials. Amongst others, these include scattering from synthetic polymers, solutions, voids and liquid crystals.

In all of these areas, irrespective of the sample under investigation, the basic procedures for the reduction or correction of experimental data are identical:

(i) normalisation by ion chamber or semi-transparent beamstop methods,
(ii) nonuniformity (or detector response) correction,
(iii) removal of detector artefacts (e.g removal of TACs),
(iv) spatial distortion correction (for 2-D data).

Similarly there are several standard requirements for the manipulation or interrogation of data which are also met by the existing BSL and OTOKO programs. Thus, it is possible to redisplay the corrected data in the most appropriate form for the experiment in question (e.g. horizontal or vertical slices of 2D images, background subtraction, multiplication or division of images, exponentiation, straight line fitting and so on).

At this point, numerous approaches are taken to the treatment or analysis of the data: the integration of discrete reflections; the modelling of complete 2-D patterns; the fitting of 1-D patterns to a given theoretical form; the characterisation by inspection of kinetic phenomena such as phase changes and reactions. Naturally, much of this analysis is sample-dependent and is performed back at the home laboratory, often using software which has been developed in-house specifically for that purpose. However, it is recognised that CCP13 may be able to make a significant contribution to many of these activities, particularly through the development or collation of software that would be of general use in a particular subject area.

In the field of synthetic polymer diffraction, there are many common forms of data analysis which are not generally available (at Daresbury or elsewhere). In Wide Angle Scattering (WAXS), for example, it would be useful to have routines which provided a straightforward estimate of crystallinity, based on the fitted intensities of the amorphous and crystalline components of the diffraction pattern. Several established methods exist for this calculation [1,2] which could be applied directly to 1-D data from the INEL detector on the Daresbury SAXS/WAXS station 8-2. Further work would be required to provide similar estimates using 2-D images from, for example, the FAST detector soon to be installed on line 16-1 at Daresbury, from image plates, from multiwire area detectors or from CCD cameras.

Similarly, routines which allowed the calculation of an orientation parameter (e.g. $<P2>$) from 2-D WAXS patterns of oriented polymers and liquid crystal systems would also be generally useful. Furthermore, it may be helpful to investigate the packages (such as CERIUS) for simulating WAXS data. This assumes that the CCP13 suite will allow easy conversion of all 2-D datafile formats into BSL format, as described in the Newsletter of December 1992.

In small angle studies of polymers, similar generic approaches exist. A common form of analysis of SAXS data is the 1-dimensional correlation function [3,4] which is relevant to the lamellar morphology which exists in many semi-crystalline polymers and block copolymers. The correlation

function is able to provide a measurement of parameters such as the crystalline and amorphous layer thicknesses and the electron density difference between the layers. The 1-D correlation function could be calculated from data produced by OTOKO using extrapolation methods combined with a Fourier transform technique. Another useful development for interpreting SAXS data from polymers (and other materials) would be the introduction of experimental uncertainty measurements. This is not a straightforward task, but would enable error-weighted fitting of experimental data to models and would improve the general appreciation of data quality.

A further improvement for SAXS analysis of polymers would be the increased use of absolute intensities (or differential scattering cross-section per unit volume) rather than using arbitrary units. The availability of absolute scattering intensities [5] enables absolute electron density values to be determined and also provides an internal consistency check when fitting data to models such as the Debye-Bucche random two-phase model or Guinier's Law.

A recent development in data manipulation and display within the CCP13 package has been the incorporation of a circular integration routine for 2-D images. This enables the azimuthal variation in intensity to be plotted for a specified range of Q values. This is particularly valuable for oriented polymer specimens in both SAXS and WAXS.

It is hoped that CCP13 may be able to incorporate more of these broad ideas into standard software packages which are generally available. Suggestions for improvements in the general capabilities of data analysis or manipulation of 1-D and 2-D diffraction patterns are very welcome. In particular, the CCP13 Workshop in May is an ideal forum for discussing the scientific achievements as well as the software needs of all 'NCD' users, regardless of the nature of the materials which they study.

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CHAIRMAN'S NOTE

In order to promote the development within CCP13 of software which will be generally useful in the synthetic polymer field, an application to SERC to fund a young Research Assistant in this area is currently being made by CCP13. If successful, this appointment will be made in October 1994. Those interested in details of this position should contact the Chairman.

COVER ILLUSTRATION

Fibre X-ray diffraction pattern from an oriented sample of PEN [poly(ethylene-naphthalate)] recorded on beamline 7.2 at the Daresbury Synchrotron Radiation Source by A. Mahendrasingam as part of an ICI/ Keele University collaboration.

COMPUTING WITH PARALLEL VIRTUAL MACHINES

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A large number of scientific applications have now been implemented on parallel supercomputers of the multiple processor, distributed memory, shared bus kind. Access to such resources is limited to relatively a few sites. For many research groups the principal computing resource is a small number of workstations accessed by a small user population. Modern workstations can be quite powerful machines in their own right. Highly suitable as they are in providing high peak performance and graphics visualisation capability they are not always fully utilised. Consequently, "spare" capacity goes begging during idle periods.

Recent developments in harnessing the power of independent computers have resulted in the emergence of software tools which enable the parallel utilisation of workstation clusters of different configuration, type, or even manufacture. Such a software harness is the PVM package [1] which utilises a protocol for data and message passing between the workstations over the network. The individual workstations constitute the elements of the *parallel virtual machine*.

We have employed the PVM software to implement four programs of relevance to SAXS and fiber diffraction work. The first uses the Debye formula to compute the structure factor of a structure modelled by a number of spheres [2]. The CPU intensive part of the code computes the histogram of pair distances from which the structure factor as well as the pair correlation function, CF, and the radial distribution function, RDF, can be calculated as defined in [3]. Fig. 1 shows the computed SAXS, CF and RDF for a model of a gel network produced by program GRASP [4].

The second program calculates the mass projection of a model structure for a series of projection angles. It has been used in the past to produce mass projections of muscle fibre models [5]. It is now being modified to read coordinates of any structure produced by any model building program. The third computes the Fourier Transform of the mass projection series to produce the simulated X-ray diffraction pattern [5]. The fourth program is a new application under development for background subtracting experimental X-ray diffraction patterns and computing the area under diffraction peaks.

The first two programs have already been implemented on the Daresbury 64-node Intel iPSC/860 hypercube [5]. The principal restriction arose out of the limited memory on each processor (16MB), a significant handicap for processing large 2D images or for large sphere models. Workstations, on the other hand, are usually equipped with larger memory. This makes implementation significantly easier as there is no need to utilise temporary disk storage.

In all four cases we take the coarse-grain SIMD approach where identical copies of the compute-intensive code are executed on each workstation but operate on different data. In the first two cases the same dataset is read in by all the processing nodes but each processor operates on different subsets of the coordinates. In the last two cases each workstation processes different datasets. Communication overheads are small compared to the total processing time. Processing of the different chunks of data is independent of each other and no synchronisation is necessary at intermediate stages of the calculation.

The small communication overheads result in almost ideal performance, i.e., processing time is inversely proportional to the number of processors used. The slower processor determines the overall rate. We can run the programs in a mixed environment of SUN, SG and HP workstations. Even just a few nearly equally powerful machines can make a significant impact on turnaround time. PVM also allows execution of the same code on multiprocessor, shared-memory machines where parallelisation can be acheived by explicit compiler directives and, in cases where the problem is sufficiently small, even on a single workstation.

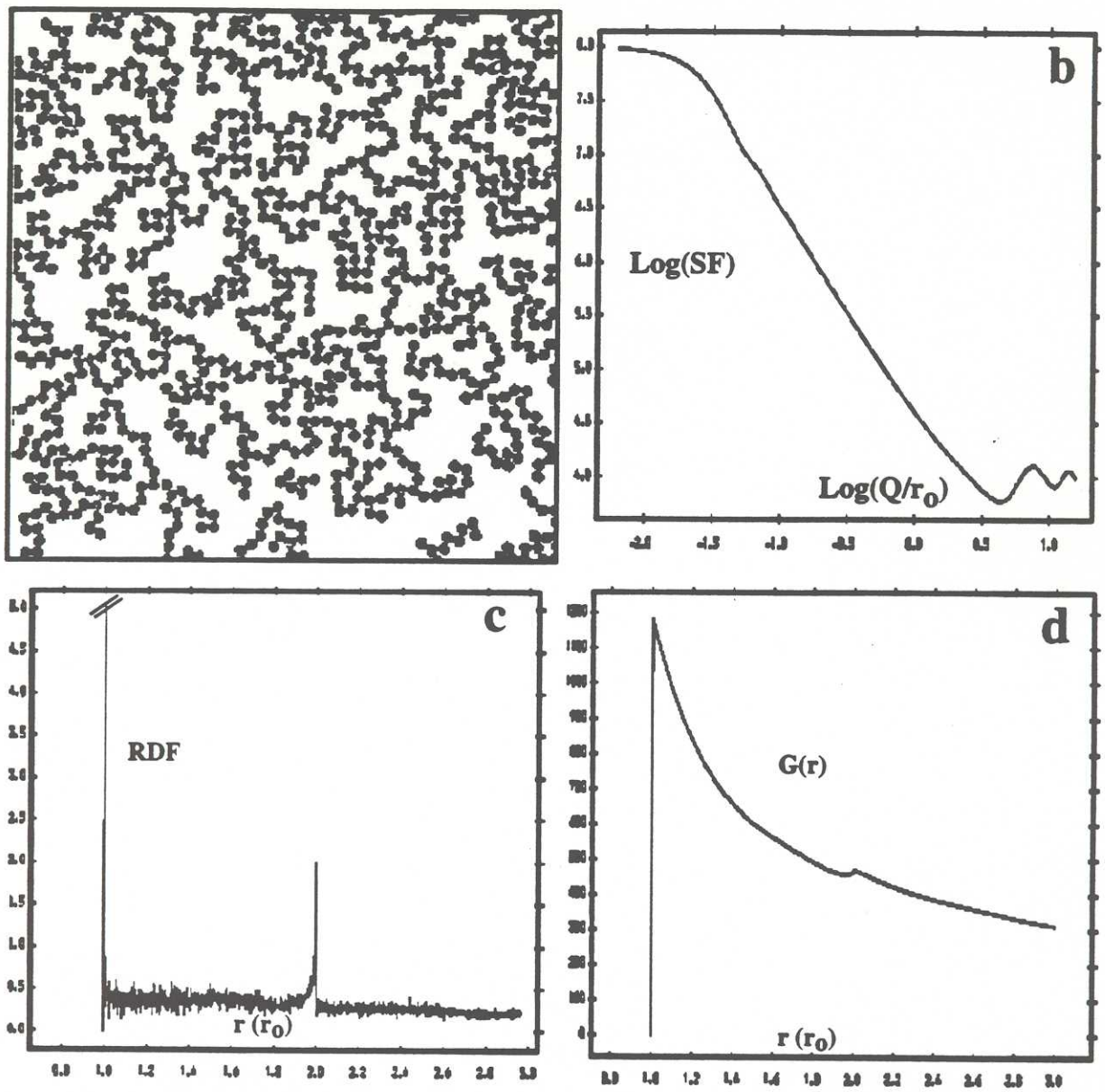

Figure 1. a) A section of a 2D model of a percolating gel network. The simulation conditions promote the growth of linear polymers with occasional branching. b) The SAXS structure factor in log–log plot for a system of 10000 particles in 2D at 40% vol/vol concentration. The slope of the linear section measures the fractal dimension of the system. c) The radial distribution function (peak at r=1 truncated) and d) the correlation function up to 3 particle diameters.

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1994 CCP13/NCD WORKSHOP

"Diffraction from Fibres and Polymers"

This Workshop will be held at Daresbury Laboratory on May 9-11, 1994. It is an extended Workshop to allow full discussion of NCD results, particularly synthetic polymer studies.

The Provisional Timetable is as follows:

Monday 9th May

11.00am	CCP13 Steering Committee meeting.
1.00pm	LUNCH
2.00 - 6.00pm	SESSION I: 'Synthetic Polymers'
6.30pm	DINNER in DL restaurant
8.00 - 10.00pm	Poster Session, Commercial Exhibits, Demonstrations.

Tuesday 10th May

9.00 - 1.00pm	SESSION II: 'Hardware; Sources and Detectors'
1.00pm	LUNCH and POSTER VIEWING
2.00 - 5.30pm	SESSION III: 'Software Developments and Results'
5.30 - 6.00pm	CCP13 General Business Meeting & Poster Prize Award
7.30pm	DINNER at LORD DARESBURY HOTEL

Wednesday 11th May

9.00 - 1.00pm	SESSION IV: 'Biological Systems; Collagen, Muscle, DNA'
1.00pm	LUNCH
2.00 - 4.00pm	SESSION V: 'Biological Systems; Membranes and Solutions'
4.00pm	TEA and CLOSE of MEETING

Note that it is hoped that each Session will be opened with a 'Plenary' Lecture by an eminent scientist, some of whom will be from overseas.

NOTES ON THE CCP13/NCD WORKSHOP

REGISTRATION FORMS for the Workshop are enclosed with this Newsletter.

Deadline for receipt of Abstracts: March 31st, 1994
Deadline for registration: March 31st, 1994

A POSTER PRIZE will be awarded for the Poster that the Judges like best. The judges will be selected from the distinguished speakers from overseas. Remember when making posters: to keep the wording to a minimum, not to try to say everything but to select a 'take home message' that you want the viewer to go away with, to keep the poster simple, to keep the lettering very large. You will be asked to stand by you poster for part of the Monday evening 'Poster Session'. It is hoped that there will be time for you to give a three minute (2 slide or overhead) summary of your Poster to generate people's interest in your work.

BURSARIES will be available for a number of students and young scientists to attend the meeting. Please apply to Dr. Geoff Mant with a legible Abstract (one side of A4 suitable for direct copying), a reason for requesting support, and (in the case of students) the signed approval of you supervisor. Sponsored students and young scientists will be required to bring a Poster and to supply an Abstract.

For further details of the meeting please contact Dr. Geoff Mant at the Daresbury Laboratory, Warrington, Cheshire WA4 4AD or telephone as below.

GEOFF MANT (0925 603169) JOHN SQUIRE (071-589 5111 x 6741)
MALCOLM IRVING (071-836 8851) GREG DIAKUN (0925 603630)
RICHARD DENNY (0925 603636 & 071 589 5111 x 6743)

1994 CCP13/NCD WORKSHOP

"Diffraction from Fibres and Polymers"

Monday 9th to Wednesday 11th, May 1994

DARESBURY LABORATORY

Following the success of the first and second WORKSHOPs of CCP13 in Fibre Diffraction, the Third Workshop is being organised at the Daresbury Laboratory in conjunction with the Non-Crystalline Diffraction (NCD) User community at Daresbury from Monday 9th to Wednesday 11th May, 1994. Application details are enclosed with this Newsletter.

It is very much hoped that you and your colleagues will be able to come to this meeting so that the CCP and NCD groups get full input from interested users. As before, the Workshop will consist of a healthy mix of technical and hardware discussion, software reports and presentations of recent results.

INVITED SPEAKERS INCLUDE

Bruce Fraser, Gerhard Zachmann,

The First and Second Workshops of CCP13 attracted several overseas participants, and it is hoped that the 1994 Workshop will attract many more.

JOHN SQUIRE (071-589 5111 x 6741) **GEOFF MANT (0925 603169)**
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