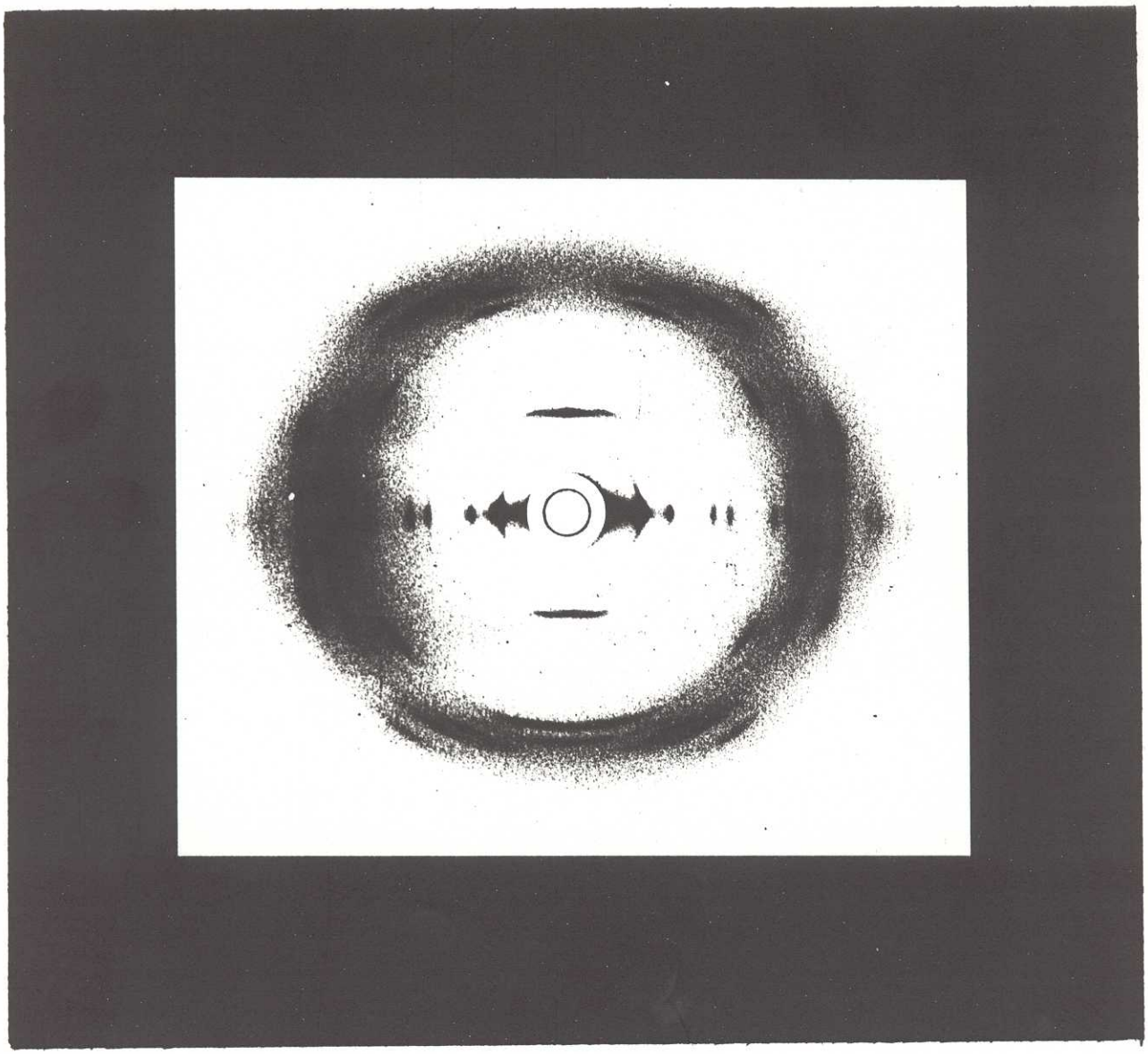
THE CCP13 NEWSLETTER

Software Development for Fibre Diffraction



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CCP13 OFFICERS 1992/1995

CHAIRMAN
NEWSLETTER EDITOR

DR. JOHN M. SQUIRE
BIOPHYSICS SECTION
BLACKETT LABORATORY
IMPERIAL COLLEGE
LONDON SW7 2BZ.

Tel: 071 589 5111 x 6741 (Sec)
071 581 5864 (Direct)
FAX: 071 589 0191
e-Mail: BIOPHYS@UK.AC.IC.PH.V1

SECRETARY

DR. GEOFF MANT
SERC DARESBURY LABORATORY
WARRINGTON
CHESHIRE WA4 4AD.

Tel: 0925-603 169
FAX: 0925-603 174
e-Mail: G.R.MANT@UK.AC.DARESBURY

RESEARCH ASSISTANT

DR. RICHARD DENNY
SERC DARESBURY LABORATORY
WARRINGTON
CHESHIRE WA4 4AD.

Tel: 0925-603 636
FAX: 0925-603 174
e-Mail: RCD@UK.AC.DARESBURY
(or at Imperial College - as for Chairman)

STEERING PANEL

The current membership is:

Dr. John Squire (Chairman), Dr. Geoff Mant (Secretary), Professor Joan Bordas (retiring 1993), Dr. Paul Durham (retiring 1993), Dr. Mike Ferenczi, Dr. Trevor Forsyth, Dr. Keith Meek, Dr. Richard Denny (CCP13 'RA'). Elections to replace retiring members will be held at the next annual workshop in May 1993 at Daresbury.

Contents:

CHAIRMAN'S MESSAGE

This is the first issue of what we hope will be an annual CCP13 NEWSLETTER. The articles in the Newsletter explain the purpose of CCP13, which started on 1st January 1992. However, it is worth emphasising its main objectives - namely to produce a generally accessible and useful suite of software for analysis and modelling of fibre diffraction patterns.

What is a CCP?

CCP13 is funded by the UK Science and Engineering Research Council via its Science Board Computing Committee (Computing Science Initiative) and is one of 11 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
CCP8	-
CCP9	Electronic structure of solids
CCP10	-
CCP11	Biosequence and structure analysis
CCP12	Novel architecture computers in Fluid Dynamics
CCP13	Fibre diffraction

The general policy on CCPs and the evaluation of their progress etc is considered by the CCP Steering Panel, chaired by Dr. Richard Catlow (Royal Institution, UK). The Steering Panel comprises all the CCP Chairmen and various observers.

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 could, for example, exist with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association. Others exist with the European Synchrotron Radiation Facility 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 -
THIS CCP IS FOR YOU - HELP TO MAKE IT WORK!

THE 1st WORKSHOP - BIRTH OF A NEW CCP

CCP13 in FIBRE DIFFRACTION

The first of what is planned to be an annual series of CCP13 Workshops on Fibre Diffraction was held at the Daresbury Laboratory on 15 and 16 May 1992. There were over 40 registered participants.

FRIDAY MAY 15th

In his introduction, the Chairman explained the purpose of CCP13 as follows:-

- To develop a suite of fibre diffraction programs for general circulation and implementation by CCP13 members.
- To inform CCP13 members of software developments in their area.
- To organise workshops on fibre diffraction (with a strong emphasis on teaching).
- To promote interaction and collaboration between UK fibre diffraction groups and to establish links with interested groups overseas (e.g. with ESRF, DESY, the fibre diffraction special interest group (SIG) of the ACA, the Photon Factory).

There followed two talks on the current status and future plans for fibre diffraction work at Daresbury (Joan Bordas) and at the ESRF (Christian Riekel), after which there was a session on high resolution fibre structures. Don Marvin (Cambridge) talked about recent results from filamentous bacteriophage, Ken Holmes (MPI, Heidelberg) talked about the actin filament structure and Watson Fuller (Keele) presented time-resolved diffraction work on DNA and on the polymer PEEK. Talks on methods during this session were given by Paul Langan (Keele) on the application of Patterson methods in DNA studies, Michael Lorenz (Heidelberg) on the new software package PROFIDA that was used to analyse with Ken Holmes the diffraction patterns from actin gels and Alex Stewart (Brandeis) on a possible file structure for the new 'FIBRE' suite of programs.

On the evening of the 15th, drinks and conversation were enjoyed in the evening sunshine overlooking the canal and looking towards western Cheshire. This was followed by an excellent dinner and a spectacular sunset!

SATURDAY MAY 16th

The Saturday session started with a series of talks on the current status of various area detectors of use to fibre diffractionists (apart from film!). Rob Lewis (Daresbury) spoke about the rapid progress being made with multiwire proportional counters, Chris Hall (Daresbury) discussed his comparisons of various commercial image plate systems, and Simon Hanna (Cambridge) described his application of CCD detectors to 'diffractometry' of oriented polymer specimens. The session was completed by a quick resume by Wojcieck Wolf (Daresbury) of how CCP4 in Protein Crystallography operates and what the CCP4 programs are.

After coffee there were a number of talks on low-angle fibre diffraction studies; Tim Wess (Edinburgh) spoke on collagen fibril structure, Jeff Harford (Imperial College) discussed recent time-resolved diffraction results from fish muscle and new methods for analysing the observed data and John Harries (Daresbury) presented work on frog muscle, including impressive new data from 'image plate' experiments. The session concluded with two talks on software. Geoff Mant (Daresbury) talked about the new BSL package, implemented for UNIX workstations, and Alex Stewart (Brandeis) discussed some new approaches to analysing muscle diffraction patterns.

After lunch there was a general discussion on how CCP13 should proceed. The Chairman reported that the CCP13 Steering Panel (see below) had set up a Working Group (Geoff Mant, Trevor Forsyth, Jeff Harford and Richard Denny [the CCP13 'RA']) to define as a matter of urgency a standard file format for FIBRE software. At the same time existing fibre diffraction software from different sources will be scrutinised and adapted, where appropriate, to form the core of the FIBRE suite. The first planned development of new software will be to write a program to fit asymmetric (i.e. non-circular) 2-D background scattering in fibre patterns for subtraction from 'useful' diffraction (sampled peaks, layer-lines, etc). At a later stage the modelled diffraction pattern would be refined together with a background to give an optimised fit.

At the end, the Chairman thanked Geoff Mant and the Daresbury office for all of their hard work in organising what was a very enjoyable and successful meeting. He also thanked Professor Joan Bordas for his support and all the speakers and session chairmen for their contributions.

ARE YOU INTERESTED?

CCP13 is open to anyone who is interested. If you want to join us to promote fibre diffraction and to help in your own data analysis then contact the secretary, Dr. Geoff Mant, at the SERC Daresbury Laboratory, Warrington WA4 4AD, Cheshire, U.K. [tel: 0925 603169], giving your name, address, telephone number and e-mail address. You will then receive all CCP13 information including the Newsletter.

Report from the meeting of the working party on 2nd June 1992.

DATA FILE FORMATS

Present: Geoff Mant, Jeff Harford, Trevor Forsyth, Richard Denny.

It was decided that most current data file formats could be accommodated if an ASCII header file of the BSL type was created containing information relevant to the data type being considered.

Arguments which are currently unused in the BSL header could convey such information as:-

(i) the "endian" of the machine the data file was written on,
(ii) the data type
(iii) whether or not the data is compressed,
(iv) the number of bytes at the top of the file corresponding to header information.

A program would be distributed for creation of the appropriate header files by the user. Renaming and concatenation of data files could also be incorporated into this routine. The current BSL file naming convention would be adhered to.

The defaults of the new descriptions would correspond to files currently accepted by BSL. Output file type would be at the discretion of the user.

The first data types to be supported would be:

0 32 bit real (default)
1 unsigned char
2 unsigned 16 bit integer

Later the following types could be included:

3 signed char
4 signed 16 bit integer
5 unsigned 32 bit integer
6 signed 32 bit integer
7 64 bit complex

Conversion programs would be supplied for data recorded on Fuji or Molecular Dynamics image plates as these are not accommodated for in this scheme.

Richard Denny

Report from the CCP13 Working Party on Monday, 3rd August 1992

GRAPHICS

Present: Geoff Mant, Trevor Forsyth, Richard Denny.

The aim of this working party was to identify the criteria for choosing between graphics libraries and to nominate some candidates for incorporation into the CCP13 program suite. The working party considered the following aspects of available packages:

(i) The chosen package should be both C and FORTRAN callable.
(ii) The package should drive XII, Postscript and tectronix devices.
(iii) The package should be portable among a diversity of machines.

Remaining questions are:

(iv) Should the chosen package be public domain or should users be expected to pay for licences?
(v) What level of plotting routine is required? For example, is contour plotting essential?

Two packages, Vogle and PGPLOT, were considered in this context.

Vogle is portable, public domain, it drives the appropriate devices and is both C and FORTRAN callable. However, it does not possess any higher level plotting routines. PGPLOT also drives the appropriate devices, has high level plotting routines but it is only (as far as we know) FORTRAN callable.

Opinions on aspects (iv) and (v) and any suggestions for graphics libraries from the fibre diffraction community would be appreciated.

Richard Denny

COVER ILLUSTRATION

High-angle fibre diffraction pattern from a liquid-crystalline gel of racemic poly-γ-benzyl glutamate in the α-helical form produced by swelling a dried oriented fibre in dimethylformamide. Although the main polypeptide structure is α-helical, the benzyl groups on the long side-chains interact specifically to form a regular structure with a different symmetry to the α-helical backbones. The strong inner meridional reflection at 10.6Å is from the side-chain structure. The diffraction pattern was recorded in about 1967 using an Elliott toroid camera on a Hilger microfocus X-ray generator. It displays many of the key factors involved in analysing fibre diffraction patterns: partial sampling, strong diffuse scattering, arcing of layer-lines. (Squire, J.M., Ph.D Thesis)

THE CCP13 RA, Dr. RICHARD DENNY - A PROFILE

Richard Denny graduated from Keele in 1986 in mathematics and physics. Postgraduate work was also carried out at Keele into structural transitions in the conformationally flexible DNA double-helix using X-ray fibre diffraction, under the guidance of Professor Watson Fuller.

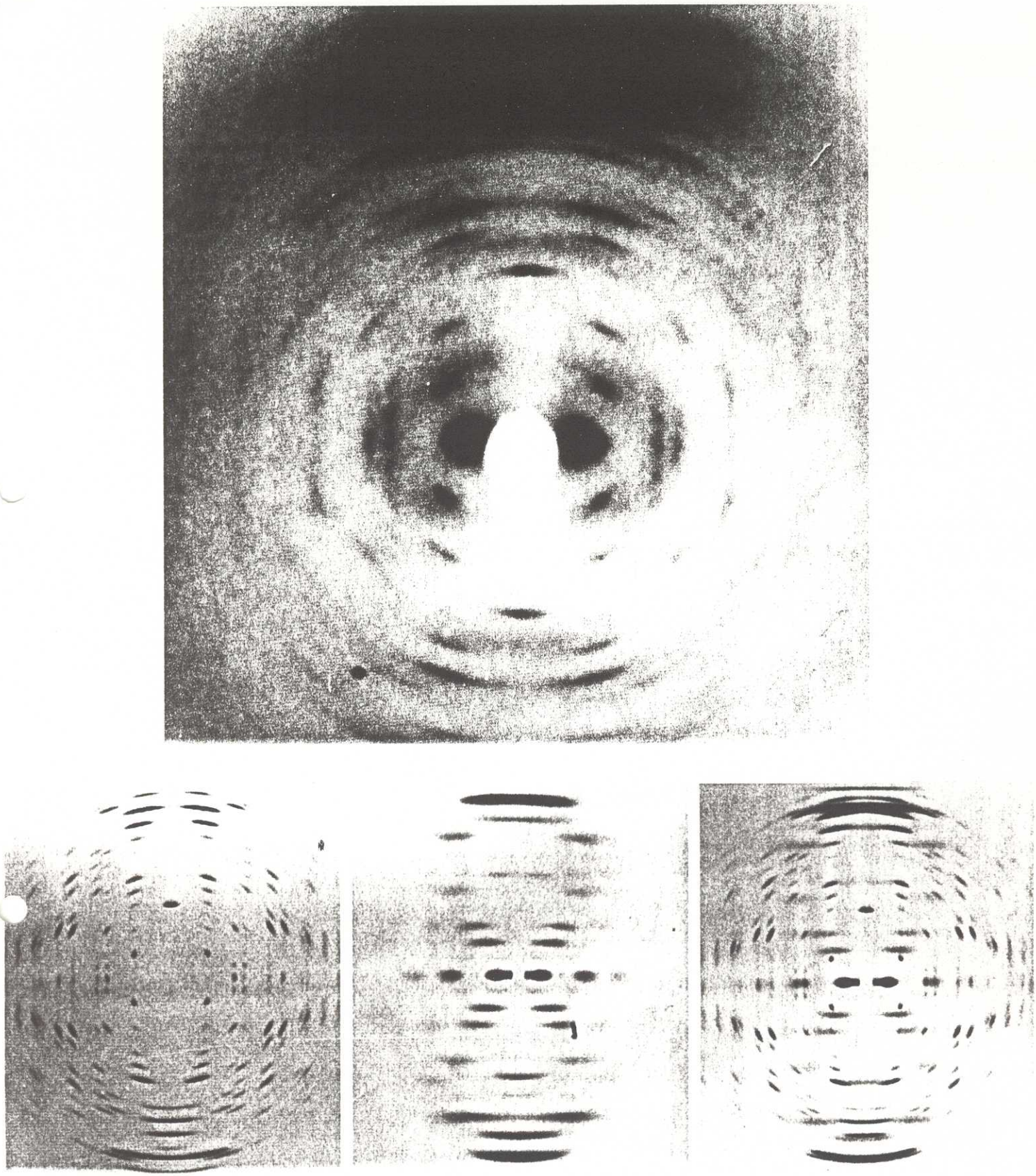
The main area of study was the S -> B transition where the DNA double-helix is thought to change handedness from left to right. One of the approaches adopted was to simulate fibre diffraction patterns using the two end point structures, incorporating various types of lattice disorder (see Figures on Page 9).

In October 1990, allegiance was switched within the Keele physics department, to the protein crystallography group run by Trevor Greenhough. Here, the majority of work involved carrying out and analyzing the results of multi-wavelength anomalous diffraction (MAD) experiments using CCP4 programs and a suite of programs specific to MAD data analysis supplied by Wayne Hendrickson.

Two systems were studied, oligopeptide permease A(oppA) and an 18 kDalton fragment of duck ovo-transferrin (dOT) using station 9.5 at the SRS. Other work has included conversion of the Laue integration program INTLAUE for use with image plates and the simulation of thermal diffuse scatter using correlations derived from molecular dynamics simulations.

Current work for CCP13 includes the modification and updating of a fibre diffraction package whose authors include Colin Nave, Richard Bryan and Ian Clifton. The package is designed to remove background and assign intensities to Bragg spots or evaluate continuously varying intensity along layer lines by a maximum entropy method, which depends on calculating expected profiles for spots or layer line broadening.

Richard Denny started as the CCP13 RA on October 1st, 1992 and currently spends Monday to Wednesday each week at Daresbury and Thursday & Friday at Imperial College, London. As the RA on this project, one of his briefs is to visit contributing Research Groups to get first hand experience of the problems that people are facing in their particular fibre diffraction studies so that the newly developed software package can be as useful as possible. Please contact him if you would like him to visit your Group.



The top photograph shows a frame recorded during time-resolved monitoring of the S to B transition in DNA. The predominant conformation appears to be S_{II}, but there is also strong equatorial intensity and other diffuse scatter not associated with S_{II}. Bottom left is a photograph of a pattern simulated from a model S_{II} structure. Bottom middle is a pattern simulated from a B model with slippage disorder and paracrystallinity (distortions of the 2nd kind). Bottom right shows the addition of these simulations in the ratio 50 B : 1 S_{II}.

THE CCP13 SUITE

The intention is that 1-D or 2-D data from a variety of detectors will be converted to a common format and processed using the "FIBRE" suite of programs in an X-Windows environment.

The software will enable such processes as:

[1] Dividing/ Adding/ Subtracting/ Scaling/ Rotating/ Straightening of images. (The Daresbury Program BSL does most of this already)

[2] EITHER (a) Allowing integration along a rectangular strip (for example, to give layer-line or row-line profiles) followed by background fitting and subtraction.

OR (b) Fitting a 2-D continuous anisotropic background function to the data (from specified background positions or using automatic methods) and then subtracting to give a background free 2-D image or layer-line and row-line profiles as in (a).

[3] Fitting observed patterns EITHER by peak fitting of selected 1-D traces (from [2]) OR by doing 2-D fitting with chosen 2-D peak shapes (from [2](b)).

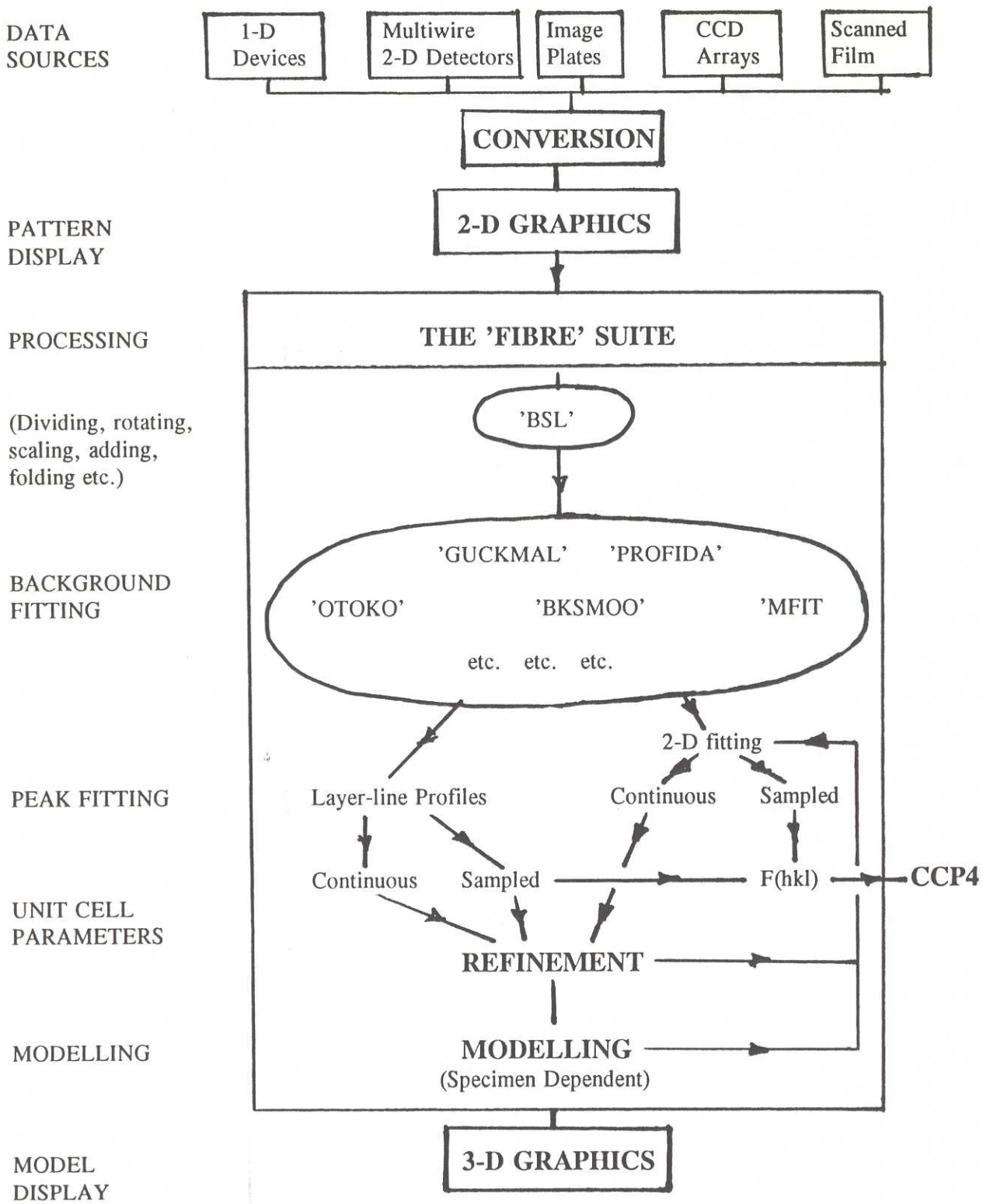
In either case the future intention is to allow background and fitted peak fitting to be optimised together.

[4] The resulting continuous layer-line profiles or F(hkl) values can then be modelled OR used for Fourier synthesis. In the case of F(hkl) values, the output data can be in the CCP4 standard MTZ format.

The flow diagram opposite provides an overview of the intended scope of CCP13 software development and its relationship to other software such as that of CCP4.

If you have any software that could be useful in such a scheme and you are prepared to make it available, please contact Geoff Mant or Richard Denny. Your authorship will be acknowledged in perpetuity within the program suite.

FLOW DIAGRAM OF THE CCP13 SUITE



CCP13 IN FIBRE DIFFRACTION

"Second Annual Workshop"

Friday 14th, Saturday 15th May 1993

DARESBURY LABORATORY

Following the success of the first WORKSHOP of CCP13, the Second Workshop is being organised at the Daresbury Laboratory on Friday 14th and Saturday 15th May, 1993. 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 gets full input from interested users. As before, the Workshop will consist of a healthy mix of technical discussion, software reports and presentations of recent results.

At the same time it is necessary to appoint replacements on the Steering Committee for Professor Joan Bordas and Dr. Paul Durham.

Note finally that the CCP is not an exclusively UK affair. The first Workshop attracted several overseas speakers, and it is hoped that the 1993 Workshop will attract many more.

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