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)