
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

