CCP13 program developments

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FIT: Curve and peak fitting

Introduction The facility to fit positions, widths and heights of a number of possibly overlapping peaks on top of a variable background can be particularly useful for studying time series of diffraction data. With this type of application in mind, a program, FIT, has been written which uses GHOST graphics and accepts OTOKO-style input. A new version of this program, XFIT, is under development which utilizes a Motif-based graphical user interface and a plotting widget developed at Daresbury.

Peak shapes Currently, two peak types are available: Gaussian and Lorentzian. Options can be activated when the pointer is in GHOST window; to change the peak type to Gaussian press <g>, to change to Lorentzian, press <c>. Voigt and Pearson VII will soon be implemented.

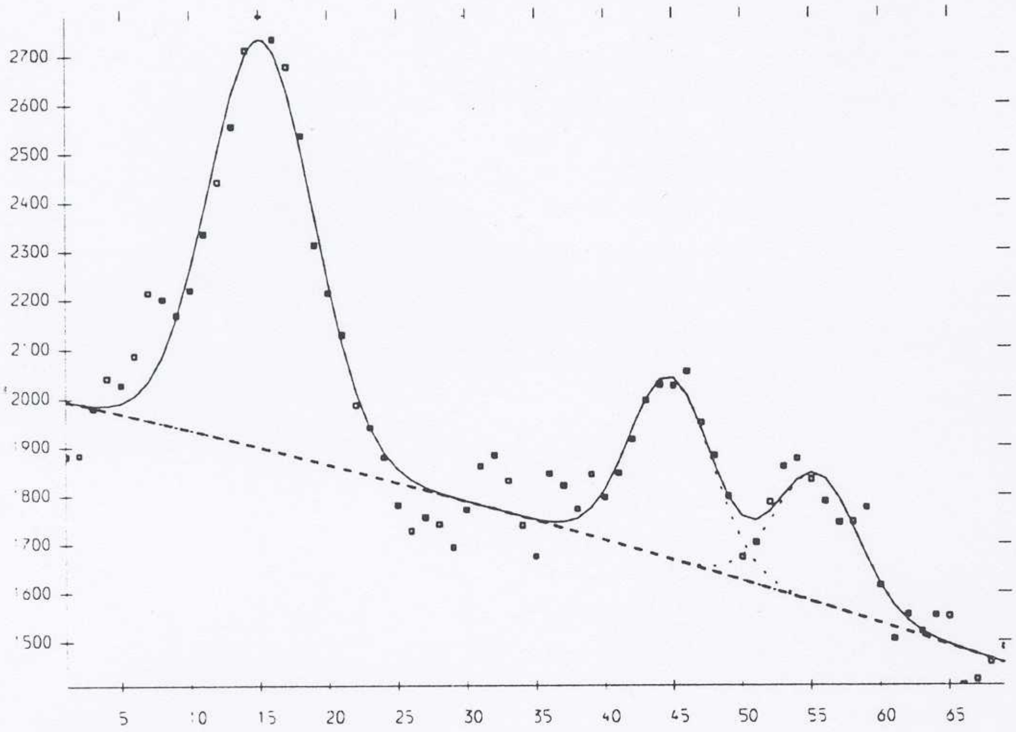
Background curve The background can be described by a polynomial of degree n where $n \leq 4$. This is chosen by pressing the appropriate number when the focus is in the GHOST window.

Selection of initial parameters The cursor and left mouse button are used to determine the starting point for the non-linear least-squares fitting. The horizontal position of the pointer determining the X-coordinate of the peak and the pointer's height above the base line of the plot determining the width of the peak. When fitting a time series, the initial parameters are determined by the fitted parameters from the previous frame. Alternatively, initial parameters for the whole series can be input from an OTOKO file describing a previous run.

Constraints Once the initial parameters have been chosen, it is possible either to set the value of a parameter, thereby removing it from the fit, or the value of a parameter can be constrained to be equal to the value of another parameter, removing a degree of freedom from the fit. For example, one might wish to ensure that the widths of two peaks were equal but that the width was refined along with the other parameters.

Output There are three forms of output from FIT, hardcopy output of the GHOST graphics as shown in figure 1, a list of the fitted parameters in an ASCII log file and OTOKO-style output suitable for examining the time-courses of background and peak parameters.

Fig. 1. Result of line fitting with three Gaussians and a cubic background in FIT. The small squares are the data points, the solid line is the total fitted curve and the dashed lines are the background and individual peaks.



DCV: Main beam deconvolution for small angle diffraction patterns

Introduction A large focus presents certain difficulties when processing fibre diffraction patterns. A problem common to all diffraction patterns is that the smearing produced by the focus makes it difficult to identify close-lying diffraction peaks and a loss of information occurs. The smearing out of layerlines in this fashion also causes the disorientation of the fibre pattern to be under-estimated (when the beam is broad in a direction perpendicular to the layerline) which in turn causes a systematic under-estimation of integrated intensity with resolution. Bragg-sampled patterns introduce the further problem of properly Lorentz correcting the data. There are two obvious approaches to this problem: either to attempt to deconvolute the beam profile from the entire diffraction pattern or to convolute the predicted diffraction spot shapes with the beam profile when fitting the pattern. In the program DCV the former approach is adopted in the hope that intensity peaks that may not have been predicted will be made more apparent although this maybe a somewhat optimistic viewpoint.

Preparation of the image Regions of the image which are not required for processing (e.g. the backstop, or unexposed areas around the perimeter of the scanned image) can be masked out in the program. Some estimate of the standard deviation of each pixel value is also necessary. This is taken to be dependent only on the pixel value in a relation of the form

$$\sigma_k = \sigma_{min} + \alpha\sqrt{D_k}$$

where σ_k is the standard deviation associated with the k^{th} pixel and D_k is the value contained in this pixel. If one does not have this degree of knowledge about the recording medium, the values of σ_{min} and α can be estimated by fitting a low order polynomial through regions of the image where the intensity varies slowly. Clearly, an image of the undiffracted beam will be required. This is trimmed and normalized by the program for use in the deconvolution process.

The deconvolution method The approach taken is similar to that for reconstructing images from blurred pictures. A linear equation is used to relate the blurred image $\{F_k\}$, to the ideal, point-focus image $\{f_j\}$,

$$F_k = \sum_j R_{kj} f_j$$

These F_k can then be compared with the data, D_k by use of a χ^2 statistic. The approximations are made that the angular divergence of the beam is small and that the shape of the beam profile does not vary over the image. The first assumption means that the only effect of the beam profile is to provide weighted shifts of the origin of reciprocal space rather than changes in its orientation. The second assumption causes the matrix which describes the beam profile, formed by the R_{kj} to be of the Toeplitz type which reduces the amount of storage necessary to contain mapping information. This limits the applicability of the program to small angle patterns.

In order to decrease the value of χ^2 relatively rapidly from the starting value, a conjugate-gradient method is until χ^2 is approaching M, the number of pixels. Henceforth, the maximum entropy algorithm of Skilling & Bryan (1984) is employed to remove structure in the conjugate-gradient solution which is not required by the data.

Deconvolution of 2–D Gaussian profile from simulated data In order to test the program, simulated data was produced using the NOFIT option in the program LSQINT. This was then convoluted with a Gaussian profile to produce an image reminiscent of part of a bony fish muscle diffraction pattern recorded on station 2.1 at the SRS. Figure 2 shows these starting patterns along with the solution obtained after 1000 iterations of the conjugate gradient minimization and 500 cycles of the maximum entropy algorithm.

The simulation had no noise added to it, but differences between figure 2(a) and 2(c) can occur due to the accumulation of roundoff errors or the premature termination of the minimization of χ^2. So that the a solution could be reached after a reasonable time, σ_{min} was set to 0.5 and α to 0.025. The presence of "flares" on some of the equatorial reflections despite 500 cycles of entropy maximization is somewhat worrying. A criterion for convergence of the algorithm at the appropriate value of χ^2 is given by

$$TEST = \frac{1}{2}\left|\frac{\nabla S}{|\nabla S|} - \frac{\nabla \chi^2}{|\nabla \chi^2|}\right|^2 < 0.1$$

for linear problems, where S is the entropy of the solution relative to some prior distribution (Skilling & Bryan, 1984). The value of $TEST$ achieved here was 0.117, indicating that yet more maximum entropy cycles are required.

Conclusion In principle, as long as one can obtain an accurate representation of the main beam profile and the characteristics of the recording medium are known, then it should be possible to obtain a maximum entropy reconstruction of the desmeared image for small-angle scattering experiments. However, recent attempts with real data have not led to a solution which a desmeared pattern might be expected to look like. In these trials, the main beam profile was recorded after scattering through a blank cell and attenuation through a semi-transparent backstop. A better method may be to use less attenuation and a much shorter exposure time for an otherwise unobstructed main beam as the use of a correct beam profile is critical in obtaining a useful deconvoluted image.

References

Skilling J. & Bryan R.K. (1984). *Mon. Not. R. astr. Soc.* **211**, 111–124.

Beam Profile Deconvolution

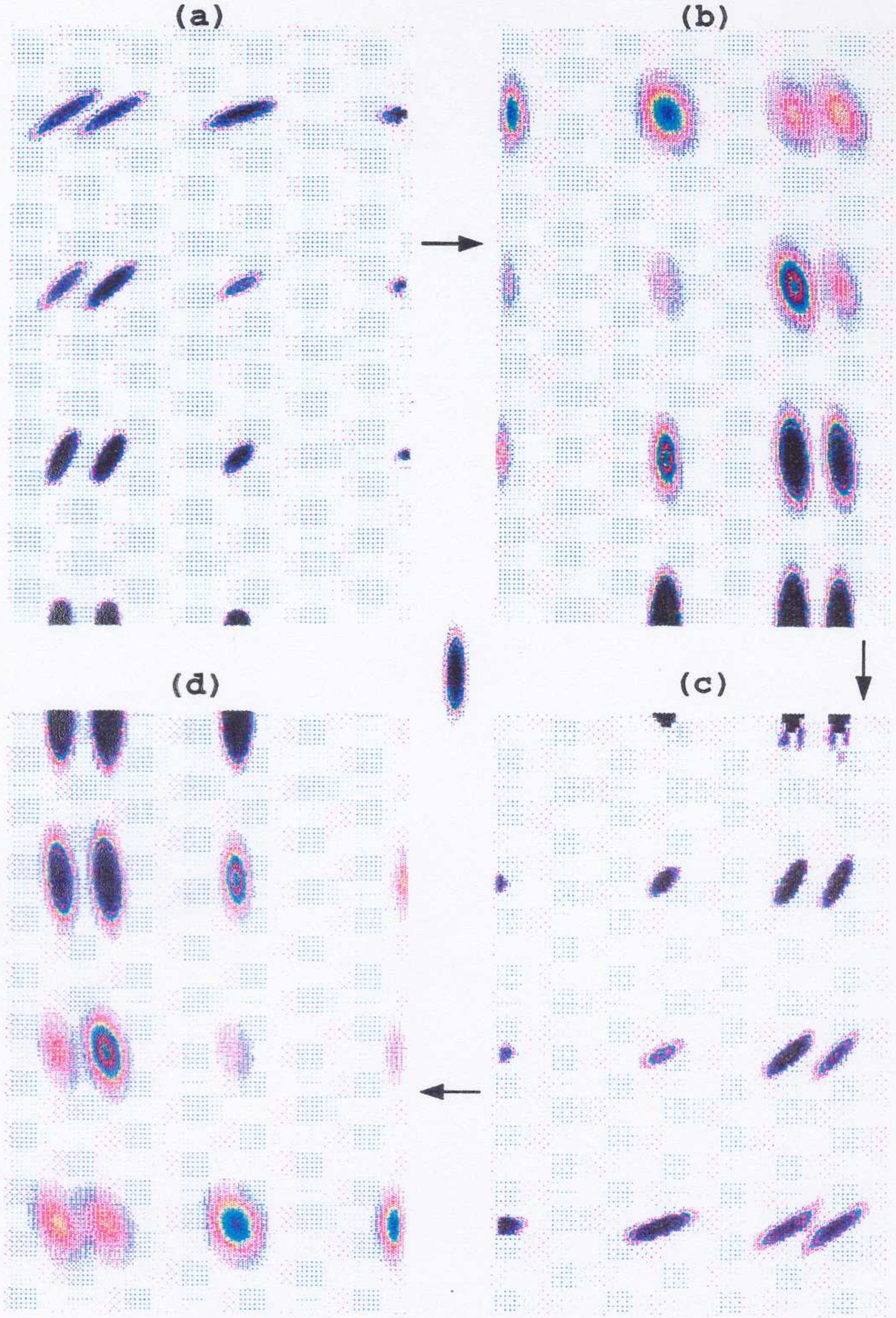


Fig. 2. The simulation used to test the deconvolution program. (a) shows a quadrant of a diffraction pattern simulated with the NOFIT option of LSQINT. (b) is (a) smeared out with the central beam profile. (c) is is the output from the deconvolution program and (d) is (c) re-smeared with the beam profile.