

CCP13 Program Updates

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Richard Denny

Biophysics Section, Blackett Laboratory, Imperial College,
London SW7 2BZ &
CCLRC Daresbury Laboratory, Warrington WA4 4AD.

LSQINT

A flexible orientation distribution function (ODF) has been built into the spot profile calculation which has meant that a single profile type now supersedes the four profile types previously available. The ODF has the form,

$$N(\phi) = \frac{k}{\left[1 + 2 \left(\frac{1 - \cos \phi}{\tan^2 \frac{1}{2} \Delta \phi} \right) (2^{1/m} - 1) \right]^m}$$

where k is a normalising constant, $\Delta \phi$ is the width of the distribution and m is a shape factor. The function is similar to a Pearson VII: when $\Delta \phi$ is small, if $m = 1$, the ODF is approximately Lorentzian but as m increases, the ODF becomes more Gaussian in character.

The facility has been added to fit intensity on an image arising from more than one lattice. This is useful when two uncorrelated structures contribute to the same diffraction pattern.

The program FTOREC has long been able to output images remapped into polar coordinates in reciprocal space as well as an estimate of the standard deviations arising from the quadrant folding of the diffraction pattern. LSQINT is now able to use both these files: patterns can be fitted in polar coordinates and the standard deviation file can be used to calculate weights to be used in the fitting procedure. Other modifications include minor bug fixes and the correction of the helical selection rule facility which enabled the number of sampling points on a layer line to be limited by taking into account the helical symmetry.

Graphical user interfaces

Users of software have become accustomed to the pleasing simplicity of using flexible, intuitive and

robust graphical user interfaces (GUIs) for all types of application. Two CCP13 programs, FIT and FIX, seemed to merit the work involved in developing GUIs as their use involves an important interactive element.

The GUIs have been developed using the Motif widget set and the UIM/X interface builder which provides a rapid way of outlining the look of a GUI and many facilities for producing and maintaining the considerable quantity of code required for the modern GUI.

FIT and XFIT

XFIT is the name of the interface program which communicates with FIT (see figure 1) although FIT can still be run in the conventional manner. An "Auto" feature has been added to FIT (which is reflected in XFIT). This enables the user to fit a large number of sequential frames of data without further interaction, having obtained a satisfactory fit to the initial frame. The program proceeds by using the final parameter set for the previous frame as the starting set for the current frame. If the goodness of the fit worsens greatly between consecutive frames, the automatic run is interrupted and the user is asked if the current frame should be reassessed in the interactive mode, the automatic run continuing thereafter. Currently, XFIT is only available at Daresbury to NCD users but it will shortly be available via the CCP13 WWW pages.

FIX and XFIX

Similar in manner to XFIT, XFIX is an interface program designed to communicate with FIX (see figure 2). However, all the graphical functions concerned with analysing the image now reside in XFIT, so that FIX cannot be run independently in its most recent version. New features added to FIX include the capability to produce radial and azimuthal scans of the image which can then be processed in the peak fitting facility of the program. This facility uses many of the interfaces developed for XFIT. XFIX will shortly be made available to NCD users at Daresbury.

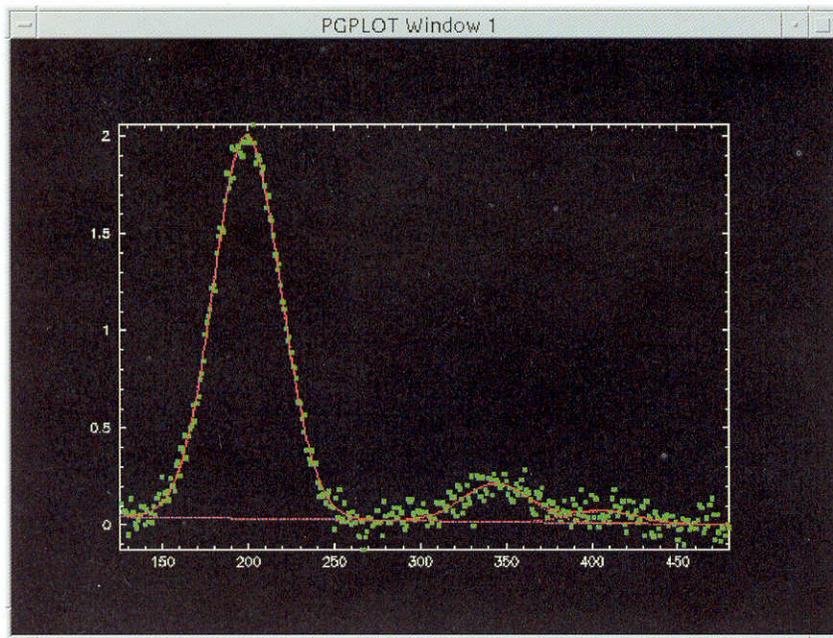


Figure 1: The Setup interface, PGPLOT graphics window and Confirm Action dialogue box. displayed while running XFIT. The Setup interface is used to modify parameter values, apply constraints to parameters (through the use of the option menus associated with each parameter in the fit) and to step through the fitting procedure. In the example shown, the widths of the three Gaussian peaks are constrained to be equal, removing two parameters from the fit. If the final solution is unsatisfactory, it is always possible to try again.

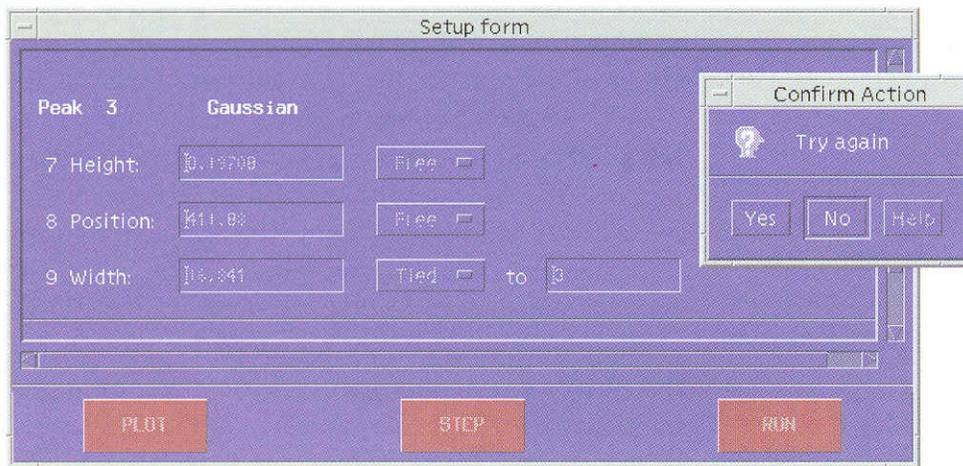


Figure 2: The XFIX interface is shown demonstrating the scan facility (scans are labelled 1 and 2 on a blue background) and the Object Editor. The scans can be integrated across their radial or azimuthal ranges and processed using the peak fitting option. The editor interface has been used to select two points (normally labelled with a black background but highlighted with red). The two selected points could then perhaps be used to estimate the rotation of the pattern.

