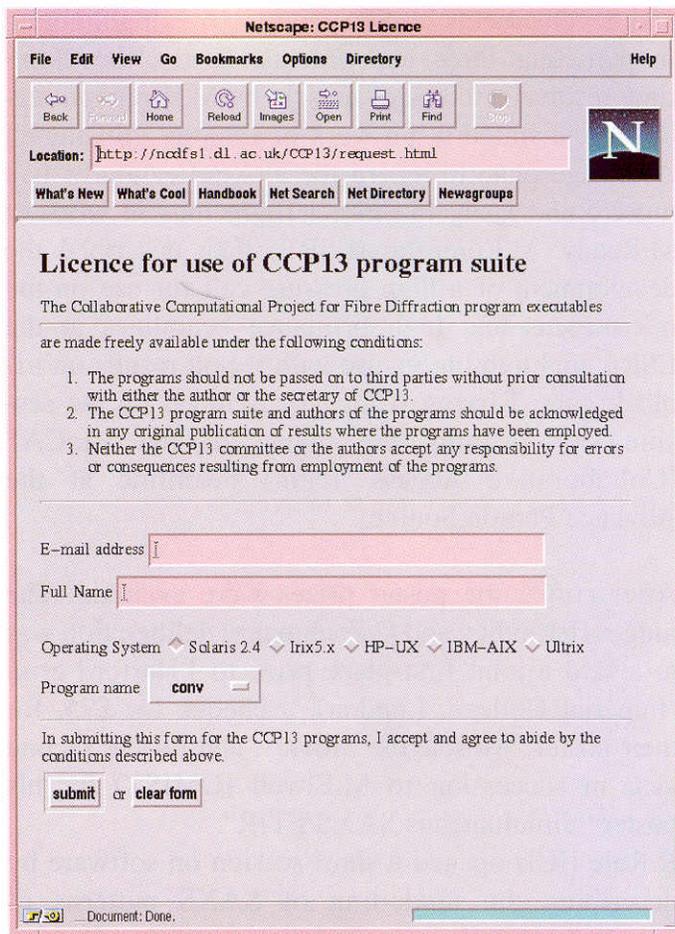


**Figure 1** The CCP13 WWW home page displayed with the Netscape program.



**Figure 2** The CCP13 WWW License and program retrieval request form. Look out for three forthcoming forms within the workshop96 index to register yourself for the CCP13 workshop 7-9th May, to submit an abstract and apply for a bursary.

## CCP13 Program Updates

### Richard Denny

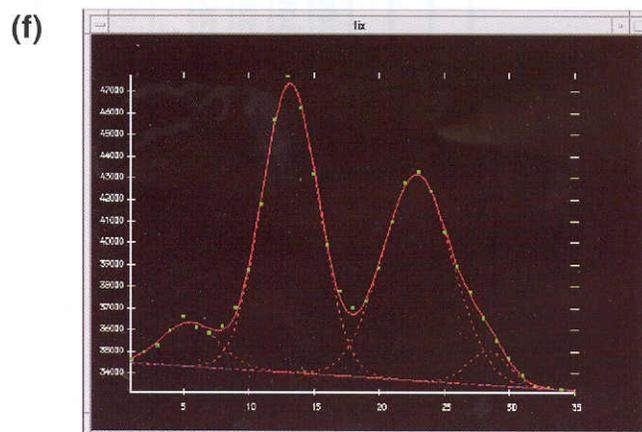
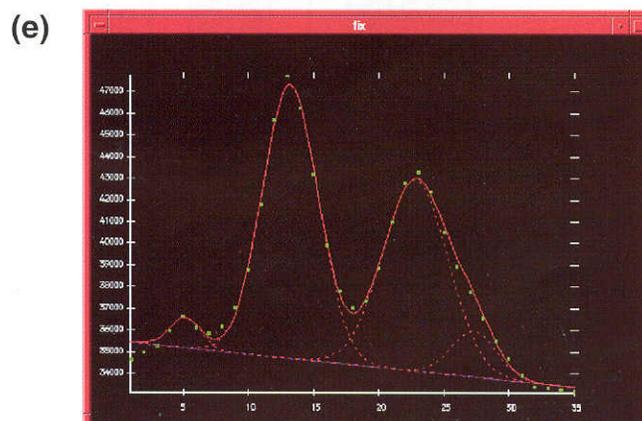
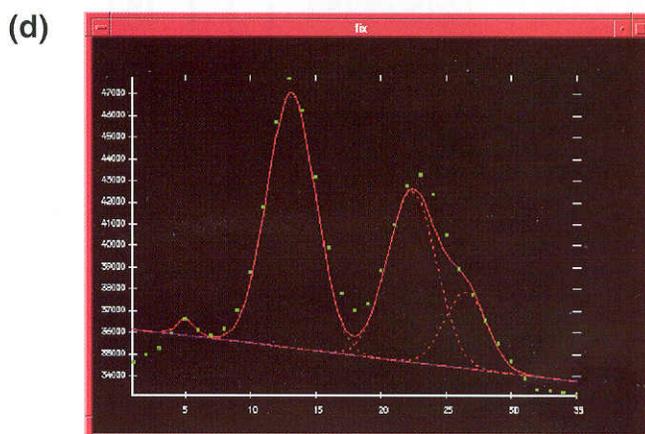
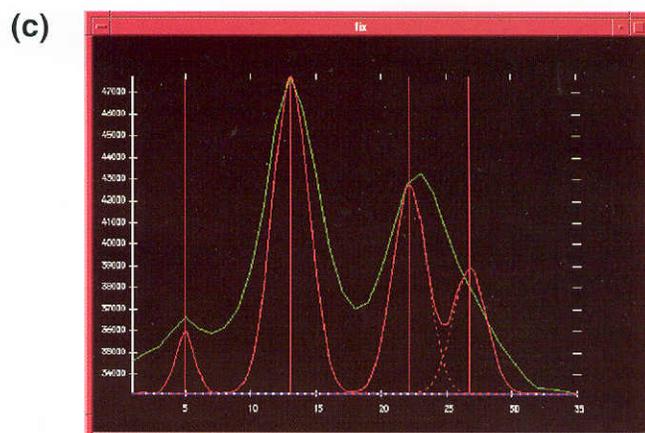
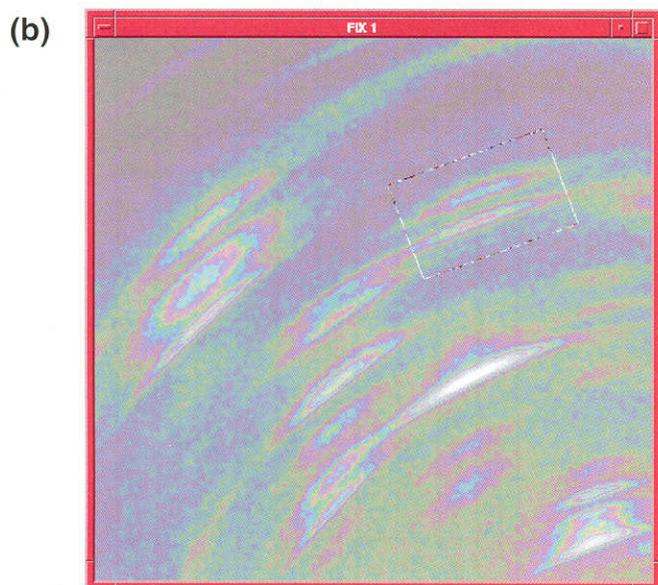
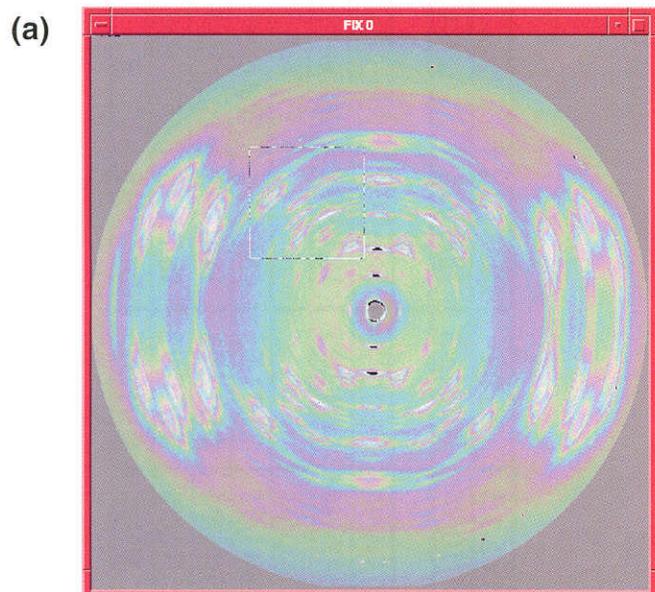
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**FIX** Updates include the use of backing store to restore window contents after exposure events and a refresh command to repaint images where the lines, crosses, etc. drawn by FIX are unwanted. The thresholds for an image can now be modified at any time, not just when the image is first generated. A thickline command has been added for integration of data in rectangular regions in general orientations. The collapsed data which results from the integration can then be fitted in the normal way with the line command (see figure 1). The line fitting routines are now common with those used in FIT so that development will be common to both programs.

**FIT** Five peak functions are now supported: Gaussian, Lorentzian, Voigt, Pearson VII and the Debye formula for diffraction from chain molecules. Simple lattice constraints can now be enforced on the positions of peaks for tetragonal or hexagonal lattice types where the  $l$  index is constant. General cubic indices will be allowed for in the near future. Also, simple limits can be placed on the range of a parameter during refinement. It is also now possible to step through the refinement algorithm, one iteration at a time, changing the value of any parameter when desired. Versions of the routines used in FIT have now been written which utilize PGPLOT line graphics for portability to machines which do not have the GHOST80 graphics library installed. This is an interim measure while a graphical user interface is developed.

**LSQINT** This program is in genuine need of updating as many modifications have been tacked on for different users. Work is currently in progress to replace the four available profile types with a single,

**Figure 1** An illustration of the use of the `thickline` command in `FIX` and the subsequent line fitting using the `step` option. (a) shows a window containing the diffraction pattern from the A form of DNA. A rectangular region has been selected for enlargement using the `box` command. In (b), the window displays the enlarged section in which a rectangular region has been selected for integration across its width using the `thickline` command. Once the line fitting part of the program has been entered, an initial set of peak parameters can be chosen as shown in (c). In (d) and (e) the results of successive iterations of the fitting procedure are shown, generated by the `step` command. In (f), the final model, achieved after 7 iterations, is shown.



more flexible, form. The single precision least-squares fitting option will be removed, but an option to use a version of the maximum entropy fitting which is more economical with memory will be included. The ability to integrate intensity from multiple lattices introduces the possibility of more parameters into the cell and profile refinement algorithm so the downhill-simplex method used for the refinement will be replaced by a modified version which

partitions the parameters into groups based on the magnitude of their shifts. All mathematical routines and matrix operations will use the SLATEC and LAPACK libraries.