Chapter 8

XDFFT - A Fast Fourier Transform program

8.1 Overview

XDFFT is a 3-D fast Fourier Transform program operating over the whole unit cell, and using the algorithm and code of Ten Eyck [1]. It includes a peak searching routine, and is adapted from the GX programs FFT and SEARCH [2]. Since the calculation time scales as ***NlogN*** rather than ***N²***, it is at least an order of magnitude faster than a corresponding calculation using XDFOUR. It will probably be most useful for determining the extrema of the residuals after refinement, or the extrema of the deformation density. The value of F(000) is taken from `xd.fou`, and is included in the Fourier summations, ensuring the electron density is on a correct scale.

8.2 Files used and created by XDFFT

Input: `xd.mas, xd.res` (or `xd.inp`), `xd.fou`
Output : `xd_fft.out, xd_fft.cif` (also `xd_fft.grd, xd_fft.pks`)

8.3 Input instructions for XDFFT

8.3.1 SELECT

SELECT *fobs *fmod1 fmod2 (*)snlmin *snlmin* **(*)snlmax** *snlmax* **(*)sig** *sigcut* **(*)phase** *phasecut*

fobs, fmod1, fmod2

The selection and treatment of these coefficients for the Fourier calculation is exactly as described for XDFOUR (see Chapter 7). The default calculation is a difference Fourier. If a difference Fourier is selected, then the program writes out a CIF called `xd_fft.cif`, containing the maximum and minimum and RMS residual densities.

snlmin *snlmin* **snlmax** *snlmax*

These options define the sin(theta)/lambda range for which Fourier coefficients are included in the calculation. The default values are *snlmin* 0.0, *snlmax* 2.0. Note that the specified ranges are *only* applied if the corresponding items are starred - otherwise the default ranges are used.

sig *sigcut* **phase** *phasecut*

These options define cut-offs for which Fourier coefficients are included in the calculation. Only those reflections with $F/\sigma(F)$ > *sigcut*, and with $|F_c|$ > *phasecut* $|F_o|$ will be included. The default values are *sigcut* 3.0, *phasecut* 0.0. Note that the cut-offs are *only* applied if the corresponding items are starred - otherwise the default cut-offs are used.

SELECT gridsize *grdsize* **scale** *scale* **npeak** *peaks* **nhole** *holes* **(*)neutron (*)gridf (*)peakf**

gridsize *grdsize*

The grid spacing in Angstroms. The default value is 0.2 Å. The maximum number of grid points in any direction is 200. If the chosen grid spacing results in more than 200 points along any axis, the spacing is automatically increased by the program.

scale *scale*

The electron density scale factor. Currently not in use

npeak *peaks* **/ nhole** *holes*

The number of peaks and holes required in the peak searching routine. Default values are 10 for both. Input atomic positions are read from the `xd.res` (or `xd.inp`) files, and all details and interpretation of the map is listed in the file `xd_fft.out`. The peak searching algorithm uses a 19-point interpolation, giving a more accurate location of maxima and minima.

neutron

If this item is starred, then holes will also be included in the peaks interpretation. The default is not to include holes in the interpretation.

gridf

If this item is starred, then an XD gridfile `xd_fft.grd` is written. Users should note that the planes are always calculated along the *y* direction, with the *z* direction varying fastest, which is different from XDFOUR. Since this file can be very large and is probably of little use, the default action is not to write a gridfile. All atoms in the unit cell are included in the header, though not necessarily as complete molecules.

peakf

If this item is starred, the peaks selected by the search routine are written to the file `xd_fft.pks`.

Bibliography

1. L. F. Ten Eyck. *Acta Cryst.* **A29**, 183-191 (1973).
2. P. R. Mallinson, K. W. Muir, *J. Appl. Cryst.* **18**, 51-53 (1985).