FIBERD

v3.0

1. Introduction

Fiberd provides a collection of optimized Fourier-Bessel transform, syntheses and related routines essential for general fiber diffraction computing. In particular, Fiberd can be used to compute structure factors, electron density and intermediates such as G and g. Angular convolution is built in to allow quick diffraction simulations. For related theories, please refer to

- W. Cochran, F. H. C. Crick and V. Vand (1952). Acta Cryst. 5: 581-586.
- A. Klug, F. H. C. Crick and H. W. Wyckoff (1958). Acta Cryst., 11, 199-213.
- R. Chandrasekaran and G. Stubbs (2012). International Tables for Crystallography, Vol. F, 583-592.

2. Input and output format

PDB: atomic coordinates. http://www.wwpdb.org/docs.html
MRC: 3-D electron density, nearly identical to CCP4. http://situs.biomachina.org/fmap.pdf
SMV: 2-D diffraction image, also known as ADSC. http://fiberdiffraction.org/software/fmt/smv.html
LGG: Gs and gs. http://fiberdiffraction.org/software/fmt/lgg.html

3. Program summary

For a quick usage summary please run fiberd on command line without argument. The routines are named x2y, where x is the input and y is the output. For example, c2G takes c (atomic coordinates) from a PDB file, computes and outputs G (Fourier–Bessel structure factors) to a LGG file. All routines require an input file, an output file, and options that describe helical symmetry, computation limit, etc.

3.1. Symbols and abbreviations

R, ψ, Z:	polar coordinates in reciprocal space
r, φ, z:	polar coordinates in real space
C:	helical repeat distance in angstroms
T, U:	defining helix symmetry: T sub-units in U turns of a repeat
L, N:	layer line number and Bessel function order that satisfy the selection rule L = TN + UM
F:	structure factors, $F(R, \psi, Z)$
I:	diffracted intensities, I(R, L)
G:	Fourier–Bessel structure factors, $G_{N, L}(R)$
g:	a complex function that is to e as G is to F, $g_{N, L}(r)$
c:	atomic coordinates
e:	electron density

3.2. Routine summary

The syntax for all routines is the same: *fiberd x2y options*, where the options include input and output files, helical parameters, and computation limit parameters. An option inside [] is optional.

```
c2G PDBin LGGout T U C resolution                [ Nmax      ]
e2G MRCin LGGout T U C resolution                [ Nmax      ]
g2G LGGin LGGout T U C resolution                [ Nmax      ]

c2I PDBin SMVout T U C resolution alfa           [ Nmax dlow ]
e2I MRCin SMVout T U C resolution alfa           [ Nmax dlow ]
G2I LGGin SMVout T U C resolution alfa           [ Nmax dlow ]

c2e PDBin MRCout T U C resolution turn vxsz      [ Nmax dlow ]
G2e LGGin MRCout T U C resolution turn vxsz rmax [ Nmax dlow ]
g2e LGGin MRCout T U C resolution turn vxsz      [ Nmax      ]

G2g LGGin LGGout T U C resolution rmax           [ Nmax dlow ]
e2g MRCin LGGout T U C resolution                [ Nmax      ]
```

Parameter description

`resolution`: high angle resolution cutoff, Å
`dlow`: low angle resolution cutoff, Å. defaulting to indefinite if not specified or specified as negative
`alfa`: degree of fiber disorientation, º
`vxsz`: voxel size for electron density, Å
`turn`: number of turns to output for electron density
`rmax`: max radius of the molecular model, Å
`Nmax`: max Bessel function order to be used in computation.
defaulting to `2·PI·rmax·Rmax/0.825` if not specified or specified as negative

3.2. Notes

For command line consistency all routines ask for T and U, but not all need them. For e2* routines, if T and U are specified as 1, Fiberd will attempt to guess the helical symmetry.

c2I provides a faster, simpler but a bit less accurate alternative for DISORDER. Disorientation in c2I is evaluated with angular convolution (Makowski, J. Appl. Cryst. 11:273-283, 1978), instead of full spatial integration as done in DISORDER (Holmes and Barrington Leigh, Acta Cryst. A 30:635-638, 1974; Stubbs, Acta Cryst. A 30: 639–645, 1974).

G2g is useful for processing data from WCEN and RADFN to obtain radial density distributions.

I2G is not implemented in fiberd. Extracting Fourier–Bessel structure factors from diffracted intensities is the job of WCEN and RADFN.