EMMAP3DT.DOC

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A. INTRODUCTION

EMMAP3DT is used to calculate 3D structure factors from a 3D MAP. These structure factor data can then be manipulated in programs like EMSF and can be back-transformed to 3D MAP data with EMSF3DBT, for example to magnify small regions of a 3D MAP (*i.e.* create data with very high pixel resolution for producing nice shaded-surface renderings in ROBEM). Note that some of these features are being added directly into ROBEM with the goal of being able to produce such renderings at near interactive speeds!

EMMAP3DT evolved from Lynn Tenn Eyck's "FFTBAK" P1 Fourier transform program and is adapted to the Purdue EM processing system. The program accepts as input a PIF format 3D MAP and now outputs structure factor data in PIF format.

In older versions of EMMAP3DT, the dimensions of the input 3D MAP had to obey certain restrictions: the x-dimension (NCOL) of each section of the input map had to have an EVEN number of sample points and none of the dimensions (NCOL,NROW,NSEC) were allowed to have prime factors greater than 19. EMMAP3DT still has these restrictions but the program handles the “work” for the user internally. Hence, the user (YOU!) no longer has to pre-trim the input 3D MAP to meet these restrictions before running EMMAP3DT (hooray, hooray!).

EMMAP3DT is fairly simple to run and can probably be run interactively with most size maps (probably 201^3 or smaller). The majority of time is spent on I/O (reading in the 3D MAP data and writing out the SF data). Hence, when this routine and its companion, EMSF3DBT, are implemented in ROBEM, the calculations should be lightning fast! (promises, promises)

B. PROGRAM INPUT

1. 3D MAP input filename (A)
2. PIXSIZ, RES_LO, RES_HI, SCALE_FAC (4F)
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Detailed descriptions of program input:

1. 3D MAP input filename (A FORMAT)

Enter the name for the file that contains the input 3D MAP. The program expects as input a map with Z-sections, in which X varies most rapidly (rows) and Y most slowly (columns).

2. PIXSIZ, RES_LO, RES_HI, SCALE_FAC (4F)
DEFAULTS: 1.0, 1000., 2.0001, 1.0

PIXSIZ is the dimension of each voxel in the 3D MAP. PIXSIZ may be defined in any units you choose (Å, nanometers, pixels, yards, etc.) but you **MUST BE CONSISTENT** and use the **same** units to define PIXSIZ, RES_LO and RES_HI. RES_LO and RES_HI define the lower and upper resolution limits, respectively, of the structure factor data to be calculated. RES_LO is generally entered as the DEFAULT (1000.0) to assure that all low resolution structure factor data, including the h,k,l=0,0,0 reflection, are computed. RES_HI must be **larger** than 2.0*PIXSIZ or the Nyquist limit (two-pixel resolution) would be violated (a definite no no). The DEFAULTS for PIXSIZ and RES_HI are 1.0 and 2.0001*PIXSIZ. This value for RES_HI should be treated as an **absolute lower limit**, which, if used, is likely to be an unrealistic value for 3D MAP data which normally have VOXELS that are at least two or three times smaller in dimension than the resolution limit of the data.

The number of structure factor data computed, and hence, time of execution of the program, varies inversely with RES_HI. The lower RES_HI is (*i.e.* to output data at a higher resolution limit), the longer it takes EMMAP3DT to complete and the amount of data output increases as does the size of the disk file.

SCALE_FAC is a scale factor (DEFAULT = 1.0) by which the structure factor data (A and B parts) are multiplied to expand or contract the dynamic range of the data.

3. SF output filename (A FORMAT)

Enter a filename for storing the 3D structure factor data. Currently the program automatically stores the data in PIF (BINARY) format. The program UNICONV will eventually be updated by RWA to

allow users to output SF data in an ASCII format (takes more disk space but can be edited). EMPROGS.DOC describes the SF data and how they are stored. (This is incorrect. Need to ask RWA where such information is kept.)

4. SF output file header (80A1 FORMAT)

Enter any header information (up to 80 characters) you like here. This information is stored in the header record of the SF data file.

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The FORTRAN code for EMMAP3DT is in DEXTRO3:[TSB.FOR]EMMAP3DT.FOR.
Documentation at http://bilbo.bio.purdue.edu/~baker/programs/programs.html
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C. FLOW CHART FOR EMMAP3DT PROGRAM