EMICOLGFB.DOC

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A. INTRODUCTION

EMICOLGFB is the second of two major programs in the icosahedral image reconstruction process that are used to produce a 3D map from image data. EMICOLGFB computes little g's from the big G's stored in the output data file from EMICOMATBG (or EMICOBG) (DEFAULT filename = BG.DAT) and then computes a Fourier Bessel transformation of the little g's to produce the three-dimensional density map of an icosahedral particle in the "standard" 2-fold setting (see [TSB.DOC]EMICO_SYS.DOC).

This program is now used in place of the programs, EMICOLG and EMICOFB and is run immediately after EMICOMATBG (or EMICOBG).

B. PROGRAM INPUT

1. INPUT FILENAME (A; DEFAULT = BG.DAT)
2. NANNULI,RADIUS,STEP_SIZE,LG_DUMP,FIVEFOLD (2I,F,2I)
   If LG_DUMP=1, then write out LG.DAT file
   If FIVEFOLD=1, then only write out top-half of 5F view for 3D MAP
3. 3D MAP OUTPUT FILENAME (A; DEFAULT = ICOS2F.MAP)
4. HEADER FOR 3D MAP (18A4)

1. INPUT FILENAME (A; DEFAULT = BG.DAT)

Enter the name of the file in which the big G output from EMICOMATBG (or EMICOBG) is stored.

2. NANNULI,RADIUS,STEP_SIZE,LG_DUMP,FIVEFOLD (2I,F,2I)

NANNULI is the cut-off radius (in annuli) in transform space. The maximum value, MAX_NANNULI (a value passed from

EMICOMATBG/EMICOBG) is the DEFAULT, but this may be reduced to compute the 3D reconstruction at lower resolution.

RADIUS is the number of radial steps in real space, i.e. the outer radius of the reconstruction in pixels (no limit). A DEFAULT is calculated on the basis of parameters passed from EMICOMATBG/EMICOBG [(ICO_DIAM - 1) / 2], where ICO_DIAM is the original boxed particle diameter in densitometer pixels. For example, if ICO_DIAM = 99 pixels, then the DEFAULT RADIUS would be 49 pixels.

STEP_SIZE is the size of each radial step in pixels (DEFAULT = 1.0). Thus, it is the size of pixels in the reconstruction RELATIVE to the pixel size in the original scanned image.

LG_DUMP is a switch, which, if set = 1, generates a binary output file of the little g data (DEFAULT FILENAME = LG.DAT).

FIVEFOLD is a switch, which, if set = 1, only calculates and writes out the top(near) half of the 3D density MAP in the five-fold view. Choosing this option may be very useful for producing preliminary maps where you just want a quick look at the MAP to see if it is correct. Invoking this option saves a tremendous amount of program I/O, since, for very large MAPs, much of the elapsed time is spent on I/O rather than CPU.

EMICOLGFB traps for improper values of NANNULI, RADIUS, and STEP_SIZE. For testing or preliminary reconstructions, RADIUS should be reduced from the DEFAULT value and STEP_SIZE increased (so that the product of these two parameters stays constant) in order to speed up program execution. For computing a "final" reconstruction, the MAP has the best appearance when it is calculated with a fine step size, i.e. with RADIUS twice or more than the DEFAULT setting and STEP_SIZE half or less of the DEFAULT setting. Under these conditions however, the program takes considerably longer to finish and may require enormous amounts of scratch and 'permanent' disk space. Typical, final reconstructions used to generate nice surface-shaded renderings are computed with RADIUS = ICO_DIAM and STEP_SIZE = 0.5.

NOTE: When RADIUS is set larger than the DEFAULT and STEP_SIZE is not reduced in proportion, meaningless density points outside the boxed boundary will be generated in the 3D MAP.

3. 3D MAP OUTPUT FILENAME (A; DEFAULT = ICOS2F.MAP)

Specify the name of the file to store the 3D MAP.

4. HEADER FOR 3D MAP (18A4)

   The header is used to identify the 3D MAP data. The DEFAULT header text is "ICOS2F.MAP: 3D Reconstruction of icosahedral particle in standard 2-fold".

C. PROGRAM EXECUTION

Normal operation of EMICOLGFB leads to a 3D that MAP contains the entire icosahedral particle viewed down the 2-fold axis in the standard orientation: the three mutually perpendicular two-fold particle axes are aligned with a Cartesian (XYZ) MAP coordinate system (NCOL columns in the X direction; NROW rows in the Y direction; NSEC sections in the Z direction).

NOTE: This program is generally run in BATCH mode. The following is an example batch job command file

D. EXAMPLE EMICOLGFB BATCH JOB

```
!       COMMAND FILE FOR RUNNING EMICOLGFB
!
!       THE INPUT ARE AS FOLLOWS:
!
!       1. INPUT FILENAME (A; DEFAULT = BG.DAT)
!       2. NANNULI,RADIUS,STEP_SIZE,LG_DUMP,FIVEFOLD (2I,F,2I)
!          IF LG_DUMP=1, THEN WRITE OUT LG.DAT FILE
!          IF FIVEFOLD=1, THEN ONLY WRITE OUT TOP-HALF OF 5F VIEW
!       3. 3D MAP OUTPUT FILENAME (A; DEFAULT = ICOS2F.MAP)
!       4. HEADER FOR 3D MAP (18A4)
!
$ DEFINE SYS$EMSCRATCH "JUSTEM2:[SCRATCH.TSB]"
$ SET DEFAULT JUSTEM2:[SCRATCH.TSB]
$ RUN SYS$EXELIB:EMICOLGFB.EXE
BABE3:[TSB.TEST]BG.DAT
60, 60, 1.0, 0, 0
reo.map
Large reo map computed with EMICOLGFB
$ WAIT
$ EXIT
```

E. PROGRAM NOTES

EMICOLGFB lists several parameters at the terminal (or in the *.LOG file):

NANNULI = Cut-off radius (in ANNULI) in transform space. Usually equals MAX_NANNULI (set in EMICOMATBG), but may be made smaller to reduce resolution.

FFT_STEPSIZE = width of each transform annulus, in transform pixel units (TPU), given by:

$$\frac{(\text{ICO\_IDIM}*\text{RSCALE})}{(\text{ICO\_DIAM}*\text{ICO\_NSAMP})} \text{ TPU}$$

MAX_BESSEL_ORDER = The highest Bessel order used in the computation of the layerplane data.

STEP_SIZE = Size of each radial step (i.e size of each pixel in the reconstruction relative to the original pixel size in the digitized particle image.

ICO_DIAM = Original particle diameter (in densitometer pixels). This also equals ICO_NSAMP times the reciprocal of annuli spacing in EMICOMATBG (ICO_NSAMP/FFT_STEPSIZE).

RADIUS = Number of radial steps (pixels) in real-space for the reconstruction. The particle diameter = (2*RADIUS + 1).

RESLUTION = Reconstruction resolution (in units of pixels in the original digitized image).

NCOL = Dimension of 3D MAP (# of pixels/row). Also equal to NROW (# of pixels/column) and NSEC (# sections in the MAP).

EMICOLGFB first computes one half of the icosahedral particle, viewed in a five-fold orientation (5-fold axis coincident with the Z axis and one, perpendicular 2-fold axis coincident with the Y direction), from the little g's. The little g's are only computed for Bessel orders that are multiples of 5. The density map is calculated a section at a time in unique 2pi/5 (= 72 degree) sectors. Each sector is subdivided in cylindrical coordinates (RHO(r,phi)) since the little g's are computed in polar form. The polar section is interpolated to produce a Cartesian section (MAP(x,y)).

After all sections are computed (the number of them = RADIUS+1), the half-particle 3D MAP is rotated so that the old Y

direction (2-fold) becomes the new Z direction and a 3D MAP of the entire particle is temporarily stored (in core memory if avaiable or on scratch disk). The MAP in this orientation has two other mutually perpendicular 2-fold axes in the XY plane of the central section, but not coincident with the X and Y directions. A final transformation rotates the particle into the "standard" orientation so the three mutually perpendicular 2-fold axes coincide with the X, Y, and Z directions (ROWS,COLUMNS, SECTIONS) of the 3D MAP.

The program produces a 3D MAP with strict 522 symmetry. Symmetry about the 3-fold axes is not enforced in the curent version of the program, but may be enforced by use of EMICOSYM (to give 532 symmetry).

The program performs many calculations in core memory if it is available, thus cutting down some of the I/O overhead and increasing execution speed. If memory is unavailable, computations are performed with the use of scratch space. In order to run this program efficiently, it may be necessary to ask your friendly VAX/VMS system manager to set up your account with the following job parameter limits:

```
Wsquo:     8000
Wsextent: 36000
Pgflquo:  40000
```

These settings may not be ideal, but they do seem to work fine for running the routine on the Purdue ALPHAVAX 4000-300 with 512 Mbytes core memory.

F. ADDITIONAL NOTES

1. Use EMICOROT to obtain 3D MAPS of the icosahedral particle in any equatorial setting (THETA=90.0 degrees).

2. Use option "X" of EMMAP to project the 3D MAP in any view orientation or EMICOPRJ to project the 3D MAP in any equatorial view (THETA=90.0 degrees).

G. FLOW CHART FOR EMICOLGFB PROGRAM