

# EMICOPFT.DOC

(last update May 27, 1992)

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### A. INTRODUCTION

EMICOPFT computes projections (PRJs) and/or polar Fourier transforms (PFTs) of the projections of a three-dimensional, icosahedral particle reconstruction. These are used as reference data in the program EMICOPFTCC to help determine initial refinement parameters ( $\theta, \phi, \omega, x, y$ ) for raw image data. Use of EMICOPFTCC provides an alternate to the normal common-lines routines (EMICOFV, EMICOORG) which have routinely been used to prepare data for refinement using EMICOGRA and EMICOGRA2. The use of reconstructed density data should provide more powerful constraints in the initial data refinement because of its higher signal-to-noise ratio. This, of course, assumes that the model (reconstruction) used is approximately correct.

Please note that the data output by EMICOPFT has a file format different from the common formats (IMG, MAP, SF, FFT, etc.) and therefore cannot be examined or analyzed with standard routines such as EMMAP, etc. Use EMICOPFTDSP to display either PFT or PRJ data on the graphics devices. EMICOPFTCC is used to compute initial  $\theta, \phi, \omega, x, y$  parameters.

### B. PROGRAM INPUT

1. INPUT FILENAME FOR 3D MAP (A FORMAT)
  2. PRJ/PFT OUTPUT OPTION (I FORMAT)
    - 2A. FILENAME FOR STORING PROJECTIONS (IF OPTION < 2) (A FORMAT)
    - 2B. FILENAME FOR STORING POLAR FFTS (IF OPTION > 0) (A FORMAT)
  3. DELTA\_THE, DELTA\_PHI (<CR>=1.0, 1.0) (2F FORMAT)
  4. RAD\_MIN, RAD\_MAX, RAD\_STEP (<CR>=1.0, MAX\_RADIUS, 1.0) (3F FORMAT)
  5. NCOL2 (<CR>= NCOL) (I FORMAT)
- 
1. INPUT FILENAME FOR 3D MAP (A FORMAT)  
-----

This specifies the file that contains the three-dimensional reconstruction.

2. PRJ/PFT OUTPUT OPTION (I FORMAT)

-----  
<CR> = Compute projections only.  
1 = Compute projections and polar FFTs.  
2 = Compute polar FFTs only.

2A. FILENAME FOR STORING PROJECTIONS (IF OPTION < 2) (A FORMAT)

-----  
Name of file to contain PRJ output.

2B. FILENAME FOR STORING POLAR FFTS (IF OPTION > 0) (A FORMAT)

-----  
Name of file to contain PFT output.

3. DELTA\_THE,DELTA\_PHI (<CR>=1.0,1.0) (2F FORMAT)

-----  
These specify the theta and omega angle step sizes taken over the icosahedral asymmetric unit. THETA and PHI values start at 69.0 and 0.0 degrees, respectively. For DELTA\_THE and DELTA\_PHI = 1.0, 374 PRJs and/or PFTs are calculated.

4. RAD\_MIN,RAD\_MAX,RAD\_STEP (<CR>=1.0,MAX\_RADIUS,1.0) (3F FORMAT)

-----  
The projected map data are converted from Cartesian to polar form. You are allowed to select an annular portion of the projected data by specifying the lowest (RAD\_MIN: DEFAULT=1.0) and highest (RAD\_MAX:DEFAULT=(NCOL/2)) radii to include in the calculations. RAD\_STEP (DEFAULT=1.0) sets the radial step interval and hence determines the number of annuli in the PFTs.

RAD\_MIN is normally left = 1.0 and RAD\_MAX is usually set to a value that is clearly outside the particle boundary (often much smaller than NCOL/2, especially if you boxed the original particle images conservatively with EMIMGBOX). Use RAD\_MIN > 1.0 if you suspect that the projected data at higher radii will give a more sensitive measure of the orientation parameters.

5. NCOL2 (I FORMAT)

-----  
This sets the desired box size of the projections (DEFAULT = NCOL). The only time you may want to change NCOL2 from the DEFAULT is if you want to display an entire asymmetric unit on the

graphics device with EMICOPFTDSP. If NCOL2.NE.NCOL, EMICOPFTCC will not work correctly.

### **C. EXAMPLE EMICOPFT BATCH JOB**

```
$ SET DEF BRAGG3:[SCRATCH]
$ DEFINE ACS_ACIP S1
$ RUN BERNAL2:[TSB.EXE]EMICOPFT
BERNAL2:[TSB.VIRUSES.SV40]TILT0.MAP
2
SV40_TILT0.PFTS
SV40_TILT0.PRJS
1.0, 1.0
1., 38., 1.
85
$ EXIT
```

### **D. FINAL NOTES**

1. Check [TSB.FOR]EMICOPFT.BCH for an example BATCH command file used to run EMICOPFT.
2. A Vaccelerator version ([TSB.AEXE]A\_EMICOPFT.EXE) runs much faster than the BRAGG version. It runs without apparent error on ACCEL1; ACCEL0 has not been tested and may work especially if your 3D data set is not too large.

## E. FLOW CHART FOR EMICOPFT PROGRAM

\*\*\*\*\*

\* MAIN \*

\* (EMICOPFT.FOR) \*

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```

*
*-- PIRADDEG
*
*-- MAP_OPEN -- |-- STRING_UPPER
*                |-- FILE_CHECK
*
*-- MAP_FILL_3D |-- PIRADDEG
*                |-- MAP_CLEAR
*-- MAP_PRJ ----- |-- MAP_PRJ_XZ --- MAP_CLEAR
*                |-- MAP_PRJ_AXIS - MAP_CLEAR
*                |-- MAP_PRJ_ALL -- MAP_CLEAR
*
*
*-- MAP_SYM_CAVG -- MAP_STATS
--*
*
*-- MAP_SYM_RAVG -- |--
MAP_SYM_GRID
*-- PRJ_OUTPUT -- |-- MAP_SYM -- |-- COPY_R4          |--
MAP_STATS --*
*
*-- MAP_TRP      |-- MAP_STATS -- MAP$STATS --
MAP_OPENSER
*
*-- MAP_POLAR ----- |-- MAP_CLEAR
*                |-- MAP$POLAR --
MAP_POLAR_GRID
*-- PMAP_FFT -- FOURT -- L6TO9
*
*-- PFT_OUTPUT
```