EMICOORG.DOC

(last update Dec 17, 1990)

CONTENTS

A. INTRODUCTION

EMICOORG refines the phase origin of an icosahedral particle. The program (or EMICOORG2 for several particles) is normally run as an interactive job after EMICOFV and before running EMICOGRAD. This program is adapted from the original MRC routine REFNORIG.

B. PROGRAM INPUT

1. INPUT IMAGE FILENAME (A)
   1B. IMG_NUM (I) (FOR BYTE-PACKED IMAGE FILES)
2. ICO_IDIM,RES_MIN,RES_MAX,NBAND,FMIN (I,2F,I,F)
   (DEFAULTS: RES_MIN = 1.0, RES_MAX = ICO_IDIM/4, FMIN = 1.0)
3. THETA,PHI,OMEGA (3F)
4. FFT_ORIGX,FFT_ORIGY,DX,DY,NX,NY (4F,2I)
5. NCYCLES,FACTOR,DEL_ANG (I,2F; DEFAULT = 7,0.67,0.0)

1. INPUT IMAGE FILENAME (A)

   Input to EMICOORG is in the form of IMAGE data (either as INTEGER*2 or BYTE-PACKED: see [TSB.DOC]EMPROGS.DOC for information about the different types of IMAGE data storage used at Purdue). If the file is contains byte-packed data, then you must enter the storage number for the IMAGE in the file.

   1B. IMG_NUM (I)

       IMG_NUM refers to the storage position of the IMAGE data
       for byte-packed format data.

2. ICO_IDIM,RES_MIN,RES_MAX,NBAND,FMIN (I,2F,I,F)

   ICO_IDIM is the size of the FFT. The only allowed values for

ICO_IDIM are 128, 256, 512 or 1024.

The radial area of the transform used extends from RES_MIN to
RES_MAX. See [TSB.DOC]EMICOFV.DOC for a complete description of
how to estimate what values should be used for these parameters.
The DEFAULTS for RES_MIN and RES_MAX are 1.0 and ICO_IDIM/4
respectively. The origin search is divided into NBAND annuli of
width (RES_MAX-RES_MIN)/NBAND. RES_MIN is the inner radius (in
TPU) of the band of data thought to be correlated icosahedrally.
This parameter should be carefully chosen as described in the
documentation for EMICOFV. The residuals at the end of the
calculation are displayed for each of the NBAND bands and
compared to the average RMS and phase errors in the initial search
area.

FMIN establishes an amplitude threshold and is used as
described in detail in [TSB.DOC]EMICOFV.DOC.

3. THETA,PHI,OMEGA (3F)

   THETA,PHI,OMEGA are the current values of the three orientation
angles for each particle image (obtained from a previous run of
EMICOFV or EMICOGRAD).

4. FFT_ORIGX,FFT_ORIGY,DX,DY,NX,NY (4F,I: DEFAULT = see below)

   FFT_ORIGX,FFT_ORIGY specify the pixel coordinates of the center
of the Fourier transform phase origin search. The lower left
corner of the boxed particle image is considered to have X,Y
coordinates = 0.0,0.0. If no values are specified for FFT_ORIGX
and FFT_ORIGY, then the center of phase origin search is set at
coordinates (NCOL-1)/2 and (NROW-1)/2 (the center of the boxed
area).

   DX and DY specify the initial search increments in pixels
(DEFAULT = 0.5,0.5).

   NX and NY set the number of grid points for the search in the X
and Y directions (must be less than 52: DEFAULT = 11,11).

5. NCYCLES,FACTOR,DEL_ANG (I,2F; DEFAULT = 7,0.67,0.0)

   NCYCLES sets the number of times the search grid is contracted
and phase residuals calculated for each particle (no limit). With
each new cycle, the window and step size is reduced by the factor
FACTOR unless a phase minimum is identified at one of the edge
values in the search window, in which case the scale is left

unchanged for the next cycle. At the end of NCYCLES, the best phase origin is identified.

   FACTOR determines the amount by which the window size of the phase origin search is reduced during successive refinement cycles. DX and DY are decreased by FACTOR unless the best point is at the edge of the current search window.

   DEL_ANG is the step size for a limited search over orientation angles. This option is rarely used since it dramatically increases
the run time of the program (27 times slower!).

C. PROGRAM EXECUTION

   The program begins by setting the search window size equal to DX*(NX-1) by DY*(NY-1) pixels (DEFAULT = 0.5*10 by 0.5*10 = 5.0 by 5.0 pixels). Thus, with the DEFAULT values, the search window covers phase origins from FFT_ORIGX-2.5 to FFT_ORIGX+2.5 and FFT_ORIGY-2.5 to FFT_ORIGY+2.5.

D. FINAL NOTE

1. FFT_ORIGX and FFT_ORIGY can also be refined or estimated with the programs EMCORORG and EMICOORG2.

E. FLOW CHART FOR EMICOORG PROGRAM

```
*******************
*     MAIN        *
*  (EMICOORG.FOR) *
*******************
      *
      *-- ICO_ROTMAT
      *                          |-- STRING_UPPER
      *-- IMG_OPEN ---------|-- IMG_PACK_BIMGCOM_CLEAR
      *                          |-- FILE_CHECK
      *-- IMG_PACK_GETRANGE
      *
      *-- IMG_PACK_FIND - IMG_PACK_NRECS
      *
      *-- IMG_FILL
      *
      *-- IMG_PACK_FILL - IMG_PACK_NRECS
      *
      *-- IMG_FFT_FILL - FFT_CLEAR
      *
      *-- FFT_2D - FOURT - L6TOL9
      *
      *-- RETURN_TO_UNIT_TRIANGLE ---<see below>
      *
      *-- FFT_TO_ATBT - PIRADDEG
      *
      *-- ZMINC - LINFIT
      *                          |-- PIRADDEG
      *-- ICOORG ----------|-- ICO_COMLIN
                                 |-- ICO_INTERP


      *                                |-- POLAR_TO_COSINES
      *-- RETURN_TO_UNIT_TRIANGLE --|-- VECMUL
      *                                |-- GOOD - GEOMETRY_INIT -
GENROT - DMATMUL
      *                                |-- EQUIVALENT_VIEW ---<see
below>


      *                          |-- PRINT_MAT ---------|--
ROTMAT_TO_AXIS
      *                          |-- POLAR_TO_COSINES   |--
COSINES_TO_POLAR
      *                          |-- VECMUL
      *-- EQUIVALENT_VIEW --|-- COSINES_TO_POLAR   |-- NORM
```

```
        *                      |-- ANGLE_TO_PMAT -----|-- DOT
        *                      |-- POLAR_TO_ROT_MAT    |-- CROSS
        *                      |-- TRANSPOSE3          |--
COSINES_TO_POLAR
        *                      |-- MATMUL              |--
POLAR_TO_ROTMAT
        *                                             |-- VECMUL
```