EMICOPRJ.DOC
(last update Dec 11, 1990)

CONTENTS

A. INTRODUCTION

EMICOPRJ projects the 3D MAP of an icosahedral particle in regularly spaced THETA,PHI orientations for one-half of the icosahedral asymmetric unit (in the range from THETA=69-90 and PHI=0-32).

This program, run after EMICOFB or EMICOSYM (etc.), is mainly designed to produce a database of projections of the 3D reconstruction for comparison with unprocessed particle data and the refinement of their orientations with EMICOORG. The original version of EMICOPRJ (which replaced the MRC program "ICOSPROJ") only projected along the equatorial direction (THETA=90). To obtain single projections of the reconstruction along ANY THETA,PHI,OMEGA view direction, use EMMAP (option "X").

B. PROGRAM INPUT

1. INPUT FILENAME (A)
2. OUTPUT FILENAME (A; DEFAULT=EMICOPRJ.MAP)
3. HEADER (18A4)
4. DEL_THETA,DEL_PHI (2F; DEFAULT=1.0,1.0)
5. NCOL2, NROW2 (2I; DEFAULT=NCOL,NROW OF INPUT MAP)

1. INPUT FILENAME (A)

   Name of the file containing the 3D MAP. For EMICOPRJ to work correctly, the 3D MAP MUST be in the standard two-fold orientation (described in [TSB.DOC]EMICO_SYS.DOC).

2. OUTPUT FILENAME (A; DEFAULT=EMICOPRJ.MAP)

   Name of the file where the projection output data is stored. Projections are stored as "sections" of a 3D MAP data file (in INTEGER*2 format).

3. HEADER (18A4)

   Use a header, for example, to identify the projection data.

4. DEL_THETA,DEL_PHI (2F; DEFAULT=1.0,1.0)

   These define the sampling intervals in THETA and PHI. The
defaults result in computation of 374 projection views. for
coarser sampling and a correspondingly smaller output file, set
DEL_THETA and DEL_PHI > 1.0. WARNING: Sampling at < 1.0 degree
intervals is currently not allowed to prevent generation of
exceedingly large output files. For particles whose diameter is
about 150 nm or less, 1 degree sampling usually suffices.

Klug & Finch (J. Mol. Biol. [1968] 31:1-12) give the convention
 for defining the orientation angles THETA and PHI.

5. NCOL2, NROW2 (2I; DEFAULT=NCOL,NROW OF INPUT MAP)

   These specify the pixel dimensions of each projection in X and
Y directions. The DEFAULT produces projections with pixels of
identical size as in the input MAP data. If NCOL2 or NROW2 are
not equal to NCOL or NROW, then the projection data are resampled
by bilinear interpolation.

C. PROGRAM EXECUTION

   You may wish to cut out or flatten known regions of noise in
THE 3D MAP before running EMICOPRJ. This helps increase the
signal-to-noise ratio in the projections and improves comparisons
with raw particle data. With 3D icosahedral data, one typically
flattens (sets density values = 0.0) outside a spherical envelope
using the "K" option of EMMAP. The radius of the envelope is best
determined by computing and inspecting surface-shaded
representations of the 3D density MAP (option "B" of EMMAP).

   EMICOPRJ only works on 3D MAP data that fit into core memory of
the computer. A version of the program to work with large data
sets (using scratch disk space) is NOT currently available.

D. FINAL NOTE

1. [TSB.FOR]EMICOPRJ.BCH contains an example BATCH job command
   file for running EMICOPRJ.

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=================================================================
The FORTRAN code for EMICOPRJ is in [TSB.FOR]EMICOPRJ.FOR.
This documentation is in [TSB.DOC]EMICOPRJ.DOC        11-Dec-90
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E. FLOW CHART FOR EMICOPRJ PROGRAM

```
*****************
*      MAIN       *
* (EMICOPRJ.FOR) *
*****************
        *
        *-- MAP_OPEN ----|-- STRING_UPPER
        *                |-- FILE_CHECK
        *-- MAP_FILL_3D                    |-- PIRADDEG
        *                                  |-- MAP_CLEAR
        *-- MAP_PRJ ----------------------|-- MAP_PRJ_XZ ---
MAP_CLEAR
        *                                  |-- MAP_PRJ_AXIS -
MAP_CLEAR
        *-- SCR_STORE - MAP_TRP           |-- MAP_PRJ_ALL --
MAP_CLEAR
        *
        *-- PRJ_OUTPUT
```