

EMICOCOR.DOC

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A. INTRODUCTION

EMICOCOR cross-correlates different images to find their relative radial and amplitude scaling factors, as well as checking that the view parameters have been assigned according to the same hand. A residual is automatically calculated for each hand. This program, used after each particle origin and view has been refined with EMICOFV and EMICOORG, replace the original MRC icosahedral program XCORRLN.

B. PROGRAM INPUT

First enter the view parameters (THETA, PHI, OMEGA in degrees: from EMICOFV) for the reference particle and then for the particle which is to be fitted to the reference. Next enter the filename for the Fourier transform of the reference particle, and when prompted, enter the refined x,y origin (ORIGX1,ORIGY1) obtained in EMICOORG. The default value for ORIGX,ORIGY is the center of the original boxed image which is UNLIKELY to be the same as the value refined in EMICOORG.

Enter values for SCLMIN, SCLMAX and DELSCL which specify the range and step size of the set of radial scaling factors to be applied to radial distances in the transform of the second particle. The default values for these variables are 0.95, 1.05 and 0.005.

Enter values for RMIN and RMAX to specify the inner and outer radii of the area of the transform to be used for the cross-correlation. The default values for these variables are RMIN = 1.0 and RMAX = the maximum radius in the transform allowed by the program (which, under all NORMAL conditions, should exceed the best resolution in the image).

Values for NBAND, INCR and NSAMPL (3I format) are entered next (Default values: 10, 4, 4). The Fourier transform is divided into NBAND annular regions, each of width INCR transform steps. NSAMPL specifies the number of radial samples within each

band. Amplitude scaling factors are calculated for each band (NBAND < 21) and are given by:

$$\frac{\text{(Mean amplitude of transform 2)}}{\text{(Mean amplitude of reference transform)}}$$

These scaling factors may be entered into EMICOMAT as they are, or better, after dividing by the mean over all particles for each band.

As an example, in the processing of SV40 virion images where 128x128 Fourier transforms were computed, RMIN, RMAX, NBAND, INCR, NSAMPL were set = 1.0, 36., 6, 6, 6. Thus, all data in the transforms out to a radius of 36 transform pixel steps were used and subdivided into 6 bands 6 transform pixels wide, with each band sampled radially 6 times. The SV40 data is icosahedrally correlated to about a radius of 31 in the transform.

Now enter the filename for the Fourier transform of the second particle and the refined ORIGX2, ORIGY2 as was done for the reference particle. The program now computes and lists out the weighted phase differences (PHFWT1, PHFWT2) and the mean phase differences (PHDIF1, PHDIF2) for each of the radial scale factors tested (RSCALE) at each of the two possible OMEGA values (corresponding to opposite hands).

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The FORTRAN code for EMICOCOR is in [TSB.FOR]EMICOCOR.FOR.
This documentation is in [TSB.DOC]EMICOCOR.DOC 3-Jul-86
