EMSF.DOC

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A. INTRODUCTION

   EMSF is a multipurpose program for examining and manipulating SF data. Options preceded with a "*" are unavailable at the current time.

DISCLAIMER

   Please note that at the moment EMSF is still under development, so there most assuredly WILL BE BUGS that haven't yet been ironed out. In many cases there are separate programs still available to carry out desired operations. Eventually, most of these programs will be phased out when EMSF is relatively bugless.

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B. PROGRAM OPTIONS

   EMSF provides several options which are selected from a TOUCH-KEY MENU as shown below.

EMSF TOUCH-KEY options:
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-----------------------------------------------------------------
*A  Merge data                     R  R-factor comparisons
 B  BACK-transform SF data to MAP  S  Get STATISTICS
 C  CIRCULAR average (I, LOGI, or A)
 D  DISPLAY data on graphics screen  O  OPEN new SF file
 F  Refine 2,3,4,6-fold origins     W  WRITE data to disk
                                          file
 I  Impose plane group symmetries  E  EXIT program
 K  FIX SF data values             ?  INFO on EMSF program


 PF1  Spawn to VMS DCL commands
 PF2
 PF3  Turns main MENU option list ON/OFF
 PF4  Graphics routines
   *  Option not yet available
```

The first option the user must choose is "O", to OPEN a new file to access SF data. You may perform several operations sequentially before saving the result in a disk file using option "W". Since operations are performed sequentially, the only way to fully recover original SF data is to reuse option "O".

OPTION B: Back-transform SF data to produce 2D MAP

This back-transforms 2D structure factor data to produce a 64x64 or 128x128 or 256x256 2D MAP. The 64x64 MAP is computed the fastest, but a 128x128 or 256x256 MAP gives a more publication quality reconstruction because the MAP is interpolated on a finer sampling grid.

After choosing the desired MAP output size (DEFAULT=64,64), specify the filename for output of the MAP data.

NOTE: information about the reciprocal lattice parameters, etc. that are stored in the header records of the SF file are transferred to real space coordinates and stored with in the MAP file header records so EMMAP displays the MAP with appropriate scaling.

OPTION D: Display SF data on the graphics

OPTION E: Exit program

Use this to EXIT the EMSF program.

OPTION F: Refine 2-, 3-, 4-, or 6-fold phase

Use this option to refine the location of 2-, 3-, 4- or 6-fold phase origins in 2D SF data (the program will not allow 3D data to be processed with this option). By continuing to hit <CR>, the program will automatically refine the location of the phase origin with the lowest residual. At each successive cycle, the step size of the phase search is halved (starting DEFAULT = 0.05 in fractional unit cell coordinates). You may, of course, intervene by changing the step size to a value different from the DEFAULT. Continue the search until the magnitude of the phase residual ceases to change.

Notice that the 2-fold residual search runs much faster than the 3-,4- or 6-fold searches.

OPTION I: Impose 2D plane group symmetry on 2D SF data

This allows one to enforce plane group symmetry on the SF data set. This ONLY works for 2D SF data sets: 3D data sets cannot be be processed with this option. There are a total of 17 different plane groups, one of which, p1, involves no symmetry. Presently, only eight of the 16 non-p1 plane group symmetries can be imposed on 2D SF data as given in the touch-key menu below (those plane groups enclosed in "()" can NOT be applied at present).

OPTION I: EMSF_SYM TOUCH-KEY MENU

A	p2	H	pgg	N	(p3m1)
B	(pm)	I	cmm	O	(p31m)
C	(pg)	J	p4	P	p6
D	(cm)	K	p4mm	Q	p6m
F	(pmm)	L	p4g		
G	(pmg)	M	(p3)		

E EXIT subroutine EMSF_SYM TOUCH-KEY OPTION:_

   NOTE: Please beware that some of the available routines have not been rigorously tested (the FORTRAN code identifies those that aren't).

OPTION K: Fix SF data values

   This option allows one to change the SF data in a number of ways as given in the following touch-key menu list:

OPTION K: EMSF_FIX TOUCH-KEY MENU

A Multiply SF data by a constant
B Invert phases (flip contrast)
C Apply temperature factor to SF data
D Apply phase shift to SF data
E EXIT EMSF_FIX and RETURN to main option menu

   Use "A" to multiply all SF data by a linear scale factor (F FORMAT; DEFAULT=1.0).

   Use "B" to invert all SF data phases. This has the effect of reversing the contrast of a MAP produced when these SF data are back-transformed.

   Use "C" to apply a temperature factor to the SF data. Enter a value for the spatial frequency (inverse pixels, nm, or Angstroms) at which the SF amplitudes will drop to 1/exp of their original values (F FORMAT; DEFAULT=1.0).

The temperature factor for a particular reflection is determined as follows:

TFAC = EXP(-D*D/R*R) where

D is the spatial frequency of a chosen reflection and R is the spatial frequency at which TFAC = 1.0/EXP. Spatial frequencies are given in 1/pixel, 1/nm, or 1/Angstrom units.

The program traps out for SF data that do NOT have values of DSTR (this may be true for OLD SF data files).

Use "D" to shift the phase origin of 2D or 3D SF data. Enter the origin shift in fractional unit cell values (x,y for 2D or x,y,z for 3D SF data) (2F or 3F FORMAT; DEFAULT = 0.0,0.0 or 0.0,0.0,0.0).

OPTION O: OPEN new SF file

Enter the name of the file containing the desired SF data. Any files currently open are closed. After successful opening of the SF data file, a number of parameters stored in the header records of the file are listed at the terminal (see [TSB.DOC]EMPROGS.DOC for a description of these parameters).

OPTION R: Compare two SF data sets

OPTION R: EMSF_COMPARE TOUCH-KEY MENU

A Compute scale factor between two data sets
B Compute R-factor between two data sets
E EXIT EMSF_COMPARE and RETURN to main option menu

OPTION S: Get statistics on SF data

This currently has only one option, to compute and list a Wilson-type plot of the SF data.

OPTION W: WRITE out the current SF data to disk

The current SF data are saved to a new file (name supplied by user). A new header may be entered or the existing one may be kept. You may limit the amount data output by specifying DSTR_MIN, DSTR_MAX limits (DEFAULT = entire data set). You may continue processing the existing SF data using other options or choose to process new data with the "O" option.

OPTION ?: Type HELP file on running the EMSF program

This provides HELP-FILE information on how the EMSF program is used. Note that the KEYPAD keys may be used to skip forward or move backward through the HELP file.