EMMAP.DOC
(last update May 16, 1988)

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A. INTRODUCTION

EMMAP is a multipurpose program for examining and/or manipulating 2D or 3D MAP data. Options preceded with a '-' are unavailable at the current time.

DISCLAIMER

Please note that at the moment EMMAP 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. For example, option "X" exists as a program called EMMAPPRJ which can be invoked using the EM master program. Eventually, most of these programs will be phased out when EMMAP works. To check which programs exist separate from EMMAP, type ?MAP<CR> in the EM program to get a list of the available EMMAP* type programs.

B. EMMAP OPTIONS

-A   ADD/SUBTRACT two MAPs   T   TRUNCATE/ADD cols, rows, secs
B   Compute depth-cue and shaded   U   REVERSE order of sections
     MAPs
D   DISPLAY MAP on graphics screen V   AREA/VOLUME calculation
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L   Check/change HEADER parameters O   OPEN new MAP file
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P   Cartesian --> POLAR   ?   INFO on running EMMAP
S   Get STATISTICS

PF4 = EXIT program
PF3 = switch for menu option list
*** = documentation not checked/finished yet

The first option the user must choose is "O", to OPEN a new
file to access MAP 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 MAP data is to reuse option "O". Also,
some operations, such as INTERPOLATION ("I") or ROTATE ("R")
create new MAP data with dimensions (NCOL x NROW) different from
the original data read in using the "O" option.

OPTION A: ADD two 2D MAPS together

Use this option to add or subtract two two-dimensional MAPs.
A MAP file with the array MAP1 must already be open (with option
"O"). If NSEC is not 1, a warning is printed, and the user must
re-enter the option. The subroutine MAPMOD_MAPADD is called, and
within this subroutine the user enters the name of the MAP file
containing the second array MAP2. The result is stored in the
scratch file, and the user can save the results by choosing option
"W" to write out the scratch file to disk.

OPTION B: Compute depth-cue and shaded MAPS
This routine is similar to the separate program named
SURFACE. It is used to compute depth-cued and surface-shaded
representations of three-dimensional density maps.

There are two separate options to this routine. The first
computes depth-cue maps from the input 3D map and the second
applies shading to the depth-cue maps. Please be aware that the
shading algorithm is NOT STRICTLY CORRECT when the light-source is
not coincident with the view direction. Chris Ho has written a
routine (PLOT3D) which computes a mathematically correct shading
(allowing for multiple light sources as well), but this routine is
many times slower the one described here. Consequently, this
option is still useful for quickly getting an idea of
what the 3D structure looks like when shaded.

TOUCH-KEY SUB-OPTION A: Produce depth-cue MAP(S)

Enter the sections you wish to use to compute the depth-
cue map (DEFAULT = 1,NSEC). For example, if NSEC = 35 and
you want to scan the top half of the map, enter 17,35.
Currently you do not have the ability in EMMAP to specify
PHI, the projection (or viewing) angle. Thus, PHI = 0.0
(i.e. view down the Z-axis). If you wish to compute a depth-
cue MAP with a view other than at PHI = 0.0, use the SURFACE
program.

Enter values for SURF_DENS, SURF_DENS_DELTA and SURF_DENS_NUM. SURF_DENS, which specifies the surface contour level, must be between MAP_MIN and MAP_MAX. SURF_DENS_DELTA and SURF_DENS_NUM are used only in the initial stages of computing surface shaded views of 3D data. They allow the user to produce a series of depth cue MAPs, stored as a 3D MAP such that each "section" of the output MAP contains a depth cue MAP computed using a different value of SURF_DENS. SURF_DENS_NUM specifies the number of depth cue MAPs to calculate and SURF_DENS_DELTA specifies the difference in the value of SURF_DENS used to calculate each of the depth cue MAPs. If SURF_DENS_DELTA and SURF_DENS_NUM are ignored (i.e. set = 0.0, 0), then a regular 2D depth cue MAP file is produced.

Enter a filename for output of the depth-cue MAP. The depth cueing can be performed on the 3D MAP as is or after the contrast is reversed (i.e. all MAP values are multiplied by -1). Choose whether or not to reverse the MAP contrast when computing the depth-cueing. This option accommodates the
handling of 3D MAPs of frozen-hydrated specimens where the MAP has negative values for specimen (e.g. protein) and positive values for the ice   background. The value entered for SURF_DENS refers to the density contour level AFTER reversing the MAP contrast.

TOUCH-KEY SUB-OPTION B: Compute shaded surface from depth-cue MAP

This option will take ANY 2D or 3D MAP file and create a Shaded representation. It is usually used with 2D depth-cue files produced using OPTION "A". Set the ILLUMINATION ANGLES with respect to the viewing direction (i.e. +X illuminates from the "EAST", -Y from the "SOUTH", etc.).

WARNING: Currently this option only produces a "correctly" shaded image for X,Y = 0.0,0.0, i.e. "FRONTLIGHTING". Shading from the side may look great, but it is NOT mathematically correct. Next set the MIX factor to change the emphasis of SHADE lighting verses DEPTH-CUE lighting. Usually 0.5 < MIX < 1.0. A certain amount of trial-and-error is required for success.

A new option (Feb 87) has been added to allow for splitting up the shading into two intensity ranges (0-127 and 128-255) according to a specified radius. All values within the specified radius (measured from a specified x,y,z

position) are assigned intensities in the range 0-127 and those outside the radius are assigned intensities between 128 and 255. Answer "1" to the user prompt to then enter values for CENX,CENY,CENZ and RADIUS. CENX,CENY and CENZ refer to the x,y,z position from which the radius is checked. CENX and CENY are measured in the plane of the depth-cue MAP and CENZ refers to the height above the base plane of the depth-cue MAP. This option proved extremely useful for separately identifying, using different color-tables, the capsid and chromatin core regions of the frozen-hydrated SV40 three-dimensional reconstruction.

Lastly, enter the name of the output file for storing the SHADED surface map.

Use EMMAPDSP to display both the depth-cue and shaded MAP files produced by this option.

OPTION C: COMPUTE circular or spherical average

In option C, the 1D circular average of a 2D map or the 1D spherical average of a 3D map is computed. The user is prompted first for the center about which averaging occurs. (For an odd-sized, 3D image reconstruction the center of the map coincides with the center of the particle.) Next, the interpolation factor (INTEGER) is entered. This factor determines the sampling interval. Generally, the smaller the interpolation factor the smoother the 1D curve will appear. To exit the routine, a factor < 0 must be entered. Finally, the user is given the choice of displaying the 1D curve on the LEXIDATA graphics device. The routine then computes the average and writes it out to an ASCII file, named by the user.

CAUTION: The spherical average computed from a half map gives slightly different results than those computed from a full map (unfixed bug!).

OPTION D: Display 2D or 3D MAP data on the graphics screen

This operates essentially the same as the program EMMAPDSP except that currently there is no provision for producing contour-type displays.

OPTION E: EXIT program

This terminates the EMMAP program.

OPTION G: Rescale values in 2D or 3D MAPS

     Select a range of MAP values (MIN_OLD,MAX_OLD) that fall within the bounds MAP_MIN to MAP_MAX, and specify the new range (MIN_NEW,MAX_NEW).

     The formula for converting an existing MAP value (OLD) into a rescaled value (NEW) is given by:

$$NEW = MIN\_NEW + \left((OLD-MIN\_OLD) * \frac{(MAX\_NEW-MIN\_NEW)}{(MAX\_OLD-MIN\_OLD)} \right)$$

     Note that contrast in a MAP can be inverted by specifying a value for MAX_NEW which is < MIN_NEW. For example, in the simplest case one might set MIN_NEW = MAP_MAX and MAX_NEW = MAP_MIN.

OPTION K: Fix values inside 2D or 3D MAPS

     Two types of manipulations are currently available:

     (A) Replace values inside/outside sphere(circle) or octant.
     (B) Replace values inside/outside the range LO-HIGH with DENS.
     (C) Reweight 3D MAP sections.

     In sub-option (A), for a 2D MAP, only the values inside or outside a circular boundary can be set reset. The user specifies the x,y coordinates of the center of a circular boundary of radius r, and a density DENS to reset all MAP values either inside or outside the defined boundary. x,y = 1.0,1.0 for the lower left corner of the MAP and FLOAT(NCOL),FLOAT(NROW) for the upper right corner. For example, for a 67x72 pixel MAP, to specify a circle of radius r at the center,x,y = 34.0,36.5.

     For a 3D MAP, the user has the option of resetting values either inside/outside a sphere or inside an octant volume. Specify the x,y,z coordinates for the center of the sphere or octant, and the radius, r, if a sphere is chosen, and the new density value (DENS).

     In sub-option (B), all values inside or outside the user specified range LO-HIGH are reset to the density specified by the user (DEFAULT = MAP_AVG).

In sub-option (C), different weights can be applied to separate sections in a 3D MAP. Specify numbers identifying the first and last sections to reweigh (SEC1, SEC2), as well as beginning and ending weights for the range of sections (WT1, WT2). If SEC2 > SEC1, intermediate sections are weighted according to a simple linear scale between WT1 and WT2.

OPTION L: Check/change header parameters

This option calls the subroutine MAPMOD_HEADER. This routine displays the values of each of the header parameters, and allows the user to change the parameter values. The new values are written to the output file when the user enters "W".

OPTION M: Convert MAP data to IMAGE data

The user may convert a 2D MAP data file or a section from a 3D MAP to IMAGE format. This can be used to allow MAP type data to be displayed using EMIMGDSP, or for that matter, to be processed using any EMIMG* program.

Please be aware that, if the MAP is non-orthogonal (i.e. the two cell axes are not perpendicular, MAP_ABANG not = 90) then the IMAGE will appear distorted when displayed using EMIMGDSP. Recall that EMMAPDSP has built in provisions for computing data interpolations and skewing to display MAP data with correct geometry, but EMIMGDSP just displays the IMAGE as is. Also, if the ratio of the two cell axes (AOVERB) in the MAP is not = NCOL/NROW (normally it will be), then the IMAGE data will be distorted. This will only happen if the MAP data are not sampled equally in the two directions.

For conversion of 2D MAP data to IMAGE format the user merely has to specify an output file name for the IMAGE data. For 3D MAP data the user must identify which section is to be converted before the IMAGE is written to a disk file.

OPTION N: Add random noise to the MAP data

This option allows the user to add a specified amount of random noise to 2D or 3D MAP data. The user enters a value for the parameter NOISE (DEFAULT = MAP_STD) which limits the range of noise added. The amount of noise added to each MAP data point is a random number in the range –NOISE to +NOISE. New values for MAP_MIN, MAP_MAX, MAP_AVG and MAP_STD are determined. The user may use option "G" to rescale the MAP data values after the noise is added.

OPTION O: OPEN new MAP file

Enter the name of the file containing the desired MAP data. Any files currently open are closed. If the MAP data are 2D, the array of data values are read into an NCOL by NROW REAL*4 array. If the MAP data are 3D then the data values are handled differently depending on subsequent options selected. If NCOL or NROW are greater than LIM (at Purdue LIM = 1024), the user receives a warning that the size of the MAP exceeds program limits, and the user must use a different data file or exit the program entirely.

OPTION P: Convert 2D MAP from CARTESIAN --> POLAR

This option converts 2D MAP data from Cartesian to polar. Cartesian MAP is subdivided into a number of annuli (NRADII), where each annulus is sampled an equal number of times (NROT). Enter the number of points/annulus (DEFAULT = 128) and the number of annuli (DEFAULT = the smaller of (NCOL/2)-1 and (NROW/2)-1, where NCOL and NROW are the number of columns and rows in the MAP). Specify the radius limit (DEFAULT = NANNULI), and the x,y position (DEFAULT XCEN,YCEN = (NCOL-1)/2,(NROW-1)/2)) defining the center (in the Cartesian system) for computing the polar MAP. The user must specify values for NROT and NRADII within defined limits (NROT 1-1024; NRADII 1-256). The default for NRADII is the minimum between (NCOL/2)-1 and (NROW/2)-1.

For example, if you start with a 100 x 50 pixel MAP, then, if default values are used for NRADII, NROT, RADIUS, XCEN and YCEN, then the polar MAP will contain 24 annuli, each sampled 128 times. This polar MAP will be computed from the center (49.5,24.5) of the Cartesian MAP out to a radius of 24. You may, of course, change any or all of these parameters within defined limits. It's up to the user to be sure not to compute something ridiculous.

Option S: Get statistics on 2D or 3D MAP

This determines the minimum (MAP_MIN), maximum (MAP_MAX), average (MAP_AVG) and standard deviation (MAP_STD) of the data values in the 2D or 3D MAP and lists them at the terminal.

Option T: Truncate/add sections/rows/columns from/to a 2D or 3D MAP

This option may be used to cut out part of a MAP or to add density values outside the existing boundary. If, for example,

you have a 99x99x99 3D MAP and wish to save only the top 50 sections, then enter values for SEC1,SEC2 = 50,99 and use the default values (99,99) for COL1,COL2 and ROW1,ROW2. If you wish to add a 2 pixel border to each section, then enter COL1,COL2 = -1,101 and ROW1,ROW2 = -1,101.

IMPORTANT NOTE: Currently this option ONLY WORKS IMMEDIATELY after opening a file with option "O". Thus, you cannot open a 3D MAP and use another EMMAP option before running option "T" or serious problems will ensue. Also, the option won't work yet for 2D MAP files.

Option U: REVERSE the order of 3D sections

This option is used to reverse the order of sections in a 3D MAP and may be used, for example, to reverse the hand of the 3D data.

Option V: Compute AREA/VOLUME at defined density levels in MAP

This determines the fraction (area/volume) of MAP data values above various equally-spaced cutoff values. The complete range of data values (MAP_MIN - MAP_MAX) are sub-divided into NBIN equal-sized levels. The user specifies a value for NBIN in the range 2-1000 (DEFAULT = 100). At each level, starting with the lowest level (i.e. density values in the range from MAP_MIN to MAP_MIN+((MAP_MAX-MAP_MIN)/NBIN)), the TOTAL FRACTION of density values in the MAP which are HIGHER than the value representing the current level is listed at the terminal. Thus, the first level will have 100% of the data with values which are higher and the last level will have 0% higher.

This routine is useful for establishing the surface density value used by option "B" or the program SURFACE to compute shaded representations of 3D MAP data.

Option W: WRITE out the current MAP to disk

The current MAP data are stored in a new disk file (name supplied by the user). A new header may be entered or the existing one may be kept. You may continue processing the existing data using other options or choose to process new data with the "O" option.

Option Y: Multiply MAP with envelope

This option is used to multiply a MAP array with an envelope array. The user enters the name of the envelope file, and if the

MAP file and the envelope file are not the same size, a warning is printed and the subroutine ends. Otherwise, the MAP file data is multiplied by the envelope file data, and the new values are written to the scratch file.

Option ?: Type HELP file on running the EMMAP program

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