Saving Palace CLUTs in *GraphicConverter*

GraphicConverter uses color table files much like Photoshop's. The procedure for creating a Palace CLUT is about the same.

Photoshop users take note — GraphicConverter color table files are not in the same file format as Photoshop's.
If you use both programs, you will need to save a color table file for each program.

First open most any Palace room GIF ("pgate.gif" is prefered, since it's guaranteed to have the complete map). The room pictures *should* all have the same color map, and your avs should use that same set of colors.

Once you've opened the GIF, select "Save As..." under the GraphicConverter "File" menu. A dialog will pop up, showing you the image. Change the Format from "GIF" to "Color Table" (the name will change to "pgate.PAL") and hit the "Save..." button (I saved mine as "Palace.PAL"). Once the color map is saved, you can just close the GIF — you won't be needing it any more.

One extra note of caution — if you've been using GraphicConverter's "split" option (part of the "Save As..." dialog box), make sure you've turned it off before hitting the "Save" button, or you'll get lots of little (and identical) color table files..... you only need one!

Using the Color Map

For any picture you want to use with the Palace, as a room background or a prop, you'll need to make sure it uses that color map. Unless the picture started as a Palace image (like the room GIF, or something pasted *from* the Place prop editor), we'll need to convert it. There are essentially three kinds of pictures we will convert:

- RGB (24-bit or 32-bit) full-color images (such as color JPEGs)
- Grayscale (8-bit) images (such as B&W Photos, JPEG or GIF)
- "Alien" indexed-color images (such as GIFs you might find on the net)

For both grayscale and indexed-color images, you must convert to RGB color via the "Picture->Colors->Change to 16.7 Mill. Colors (32-bit)" menu *first*, before converting to indexed color using the Palace color map. GraphicConverter will always assume that grayscale GIFs should be mapped to exactly 256 grayscales; and it has no good way to directly convert from one color table to another. A short time in RGB mode is the neccesary in-between step.

Remember: *Save Your RGB Image*. You may need it later, for changes or fixes.

To force GraphicConverter to use your stored Palace color map, you select "Colors->Options..." under "Picture." A dialog will pop up. Press "Use Custom Color Table" and the "Open..." button. In the "Dither" check box, press whatever you like — "dither off" will generally give you the smallest file size, while "dither on" will give the nicest tonal gradations. Now press "OK."

Once the color table is ready, we can convert RGB images the Palace map. Select "Colors->Change to 256 Colors (8 bit)" under "Picture." Now look at your image: it's living in the Palace world.
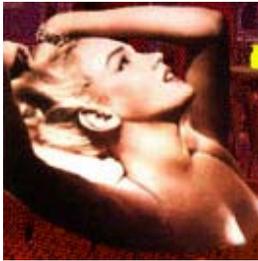
RGB Original

No Dithering
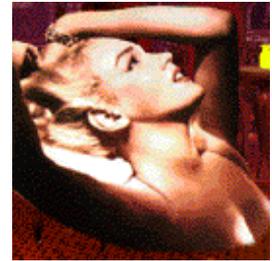
Dithered

Not sure about that "Dither" option? Just hit "Undo" and convert it again in several different ways. Or duplicate the image and convert each copy a different way, to compare side-by-side. Above are three samples, superimposed over a bit of Harry's Bar.

The Palace Ring
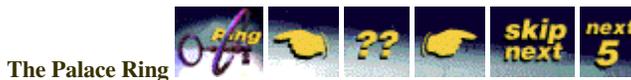
[Feedback/Suggestions/Guess Book](#)

Updated 4 Nov 96

EMFFT.DOC
(last update Mar 5, 1992)

A. INTRODUCTION

EMFFT is used to examine and/or manipulate FFT data. Filtered FFT data may be output to a disk file with the normal FFT format or it may be back-transformed ("B") to produce a filtered IMAGE stored on disk (normal IMAGE file format). Note that use of two or more options may produce additive or multiplicative effects on an FFT.

NOTE ON TERMINOLOGY: the term TSU (transform sample unit) denotes a unit of reciprocal space measure. Each TSU corresponds to a single step in the transform. For example, for a IDIM1 by IDIM2 transform in which IDIM1=IDIM2, each TSU will represent 1.0/(IDIM1*pixel size). Thus, if IDIM1=512 and the pixel size = 0.51nm, then each TSU is (1.0/261 nm). Because the right, left, top, or bottom limits of a 512x512 transform are at 256 TSU, the resolution limit at these extremes is 256*(1.0/261 nm) = (1.0/.981 nm), or 2.0 pixel resolution, consistent with the Whittaker-Shannon sampling restrictions.

B. PROGRAM OPTIONS

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

TOUCH-KEY OPTIONS:

A	Multiply two FFTs (CCF)	M	FFT --> MAP format
B	BACK-transform the FFT	S	Get STATISTICS
C	Compute CIRCULAR average		
D	DISPLAY on graphics device	O	OPEN new FFT file
F	FILTER the FFT	R	READ and transform IMAGE data
G	Extract structure factors	W	WRITE current FFT to disk
K	*FIX values in FFT	E	EXIT program
L	LATTICE refinement	?	INFO on EMFFT 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 either "O", to OPEN a
new FFT file and read in the array of structure factor data, or
"R", to READ in an IMAGE file which is then Fourier transformed.
Whenever option "W" is chosen to WRITE a FFT array to a disk file,
the user must again choose either "O" or "R", or else EXIT the
program ("E"). You may string several operations together before
saving the result in a disk file. Realize that operations are
performed sequentially, thus the only way to fully recover an
"untouched" FFT is to reuse option "O" or "R".

OPTION A: Multiply two FFTS

    This allows one to multiply the current FFT data with another
FFT. The filename for the second FFT is entered by the user.
Note that it is possible, using this option, to produce either an
auto-correlation or cross-correlation FFT which can be back-
transformed using option "F" to produce the corresponding auto- or
cross-correlation image as is accomplished using the program
EMCOR.

OPTION B: BACK transform the current FFT

    This option will take the current FFT, including any filter
masks that have been applied, and back transforms it to produce a
"filtered" IMAGE. If an FFT that has had no mask applied is back
transformed, then an unfiltered IMAGE identical to an original
boxed IMAGE will be the result. The only input required by this
option is a filename for storing the resulting IMAGE and an
optional HEADER. To do anything with the back-transformed IMAGE
you must exit EMFFT ("E" or touch PF1 and run, for example,
EMIMG).

OPTION C: Compute CIRCULAR average

    This option will produce a circular average of the FFT
amplitudes (DEFAULT) or intensities that can be displayed on the
graphics screen and/or dumped to an ASCII file (FFT_1D.TMP). This
option is similar to the "C" option of EMIMG.

    First decide what interpolation factor to use (type a negative
number to exit the routine). If you plan to use the FFT_1D.TMP
data file to produce a plot on one of the personal computers with,
for example, a program like LOTUS FREELANCE, etc., then just use
an interpolation of 1.0. Choose whether you want to display
amplitudes <CR> or intensities (1), whether or not you want to see
a display on the graphics device (DEFAULT=N), and whether or not
you want to create the FFT_1D.TMP file (DEFAULT=N).

If you display the circular average on the graphics screen, you
will then be able to use the data tablet puck to pick points and
get a readout of the radial distance (in TSU) from the origin.
Hit the GREEN button to exit this routine and either start over
with a new interpolation factor, or exit the "C" option by setting
the interpolation value to a negative number.

OPTION D: DISPLAY the current FFT

    "D" is used to display the FFT amplitudes or intensities,
scaled in a variety of ways. The scaled FFT values are displayed
with a black & white Color Look-Up Table, CLUT, using the lowest
6-bit planes of the graphics memory. Several display options are
available as specified in the following touch-key menu.

```
            FFT_DSP TOUCH-KEY MENU                 Values
           ----------------------         ----------------------
        A    AMPS/INTENSITY toggle        amps/INTENSITIES
        C    CLEAR display
        D    DISPLAY the FFT
        M    MAGNIFICATION (FFT size)          512 X 512
       L/R   Portion of FFT displayed         LEFT/RIGHT
       T/B   Portion of FFT displayed         TOP/BOTTOM
        P    POSITION center of display        320   256
        S    SCALING method            LINEAR/log/non-linear
        %    Threshold FRACTIONS             0.000   0.005
        E    EXIT
```

  SUB-OPTION A: AMPS/INTENSITY toggle
    This toggles between a choice of whether amplitude or
intensity FFT data are used.

  SUB-OPTION C: CLEAR the display screen
    "C" erases the entire graphics display screen.

  SUB-OPTION D: DISPLAY the current FFT
    "D" will display the FFT with the current settings given in
the right half of the touch-key menu.

  SUB-OPTIONS L/R/T/B: Select portions of the FFT for display
    These keys select/deselect portions of the FFT for display.
The initial DEFAULT is to have LEFT/RIGHT/TOP/BOTTOM all
selected so the entire FFT is displayed. Certain options are
disallowed (e.g. TOP and BOTTOM or LEFT and RIGHT cannot both
be deselected simultaneously).

SUB-OPTION M: Toggle FFT display MAGNIFICATION

   "M" is used to toggle through different size displays (if
allowed). The initial DEFAULT is to display the FFT at
maximum size allowed by the graphics device (1024x1024 for the
LEXIDATA in B-141 and 640x512 for the LEXIDATA in B-403). The
display can be no SMALLER than the actual dimensions of the
FFT (IDIM1,IDIM2).

SUB-OPTION P: Select center POSITION for display

   Choose "P" to select a new center position (2I FORMAT) for
   the FFT display. The initial DEFAULT (either 640,512 or
   320,256) depends on which graphics display device is being
   used. Anytime you input a new center position, that becomes
   the new DEFAULT. Note that this routine permits FFTs to be
   displayed with a portion outside the graphics screen
   boundary.

   WARNING: EMFFT options such as "L" assume that the FFT is
Displayed EXACTLY centered in the graphics screen, otherwise
they will not work properly.

SUB-OPTION S: Toggle SCALING method

   "S" is a toggle switch that selects how the FFT data are
scaled. Linear scaling is the initial DEFAULT mode, but the
data can also be displayed on logarithmic or non-linear
scales. DEFAULT thresholds (see sub-option "%" below) are
automatically selected each time you switch to a different
mode of scaling. These DEFAULTS can be overridden with the
"%" option. Non-linear scaling produces an asymptotic CLUT
which depends on two parameters, K and S, set using the "%"
option.

SUB-OPTION %: Select threshold FRACTIONS
   The "%" key is used to select threshold FFT values
(FRACT_MIN and FRACT_MAX, given in fractional units of the
maximum, scaled FFT value) so that values below FRACT_MIN*FMIN
are displayed with the lowest CLUT intensity (usually 0) and
values above FRACT_MAX*FMAX are displayed with the highest
CLUT intensity (usually 63). DEFAULT threshold values are
used whenever the linear or logarithmic scale modes are
selected but a different scheme is used if non-linear scaling
is selected (see below).   The DEFAULTS for linear and
logarithmic scaling modes are set as follows:

```
Scale Mode   FRACT_MIN              FRACT_MAX
----------   ---------------------  ----------------
Linear       FAVG/FMAX              (FAVG+FSTD)/FMAX
Log          LOG10(FMAX)*FAVG/FMAX  LOG10(FMAX)*(FAVG+FSTD)/FMAX
```

where FAVG, FMAX, and FSTD are the average, maximum, and
standard deviations of the FFT amplitudes or intensities
(depending on the current choice selected by "A").

   If "%" is chosen when non-linear scaling is chosen, two
parameters, K and S, are specified. K fixes the midpoint of
the CLUT (range = 1.0-255.0) and S effectively sets the slope
(contrast) of the CLUT. The initial DEFAULT values for K and
S are set as follows:

```
   K = 255.0*(FAVG+FSTD)/FMAX
   S = 0.25
```

The value for S is set initially to 0.25 although this may
need to to be changed. Higher values give a steeper curve
(higher contrast) whereas lower values give a flatter curve
(lower contrast). Beware that very small or large values of S
can and probably will lead to overflow or underflow problems
and will crash the program. The value of K will almost
certainly have to be adjusted from the DEFAULT setting. If the
screen appears totally white, K is too small (and S may be too
small). If the screen is totally black, K is probably too
large. Obviously, to get non-linear scaling to work properly
requires much operator intervention and experience. The
linear and logarithmic scaling modes should suffice for most
"normal" circumstances.

   Once K and S are set, the CLUT value for a given FFT
intensity or amplitude is remapped as followings:

```
   CLUT_VALUE = 255.0*(1.0/((10.0**(S*(K-VALUE-1.0)))+1.0))
```

where VALUE = (F*(LUTHI-LUTLO)/FMAX) + 5.5 and LUTLO and LUTHI
are normally set equal to 6 and 63 for the compressed black
and white FFT CLUT.

OPTION F: FILTER the FFT

   "F" is used to generate filter masks to multiply the FFT data
by. There are currently two separate sub-options in the following
touch-key menu:

```
                 EMFFT_FILTER TOUCH-KEY OPTIONS
                 ------------------------------
            A   Apply low and/or hi-pass filter
            B   Apply 2D reciprocal lattice mask
            C   Apply 2D layerline mask
            E   EXIT routine
```

SUB-OPTION A: Apply low and/or high-pass filter (Resolution cutoff)

   Enter values for RES_MIN, RES_MAX, CUT_MIN, and CUT_MAX (4F FORMAT) to identify the inner and outer radii in the Fourier transform (in TSU) for the HI-PASS (RES_MIN) and LOW-PASS (RES_MAX) filters. CUT_MIN and CUT_MAX specify hard (0.0) or soft (>0.0) edges.

   For example, for HI-PASS filtering, the FFT is zeroed out to RES_MIN-CUT_MIN, and rises exponentially up to full weight (1.0) at RES_MIN. A LO-PASS filter has full weight out to RES_MAX and drops exponentially to 1/exp at RES_MAX+CUT_MAX (if CUT_MAX=0.0, the FFT is zeroed beyond RES_MAX). To produce a simple low-pass filter (i.e. with no high-pass filtering), set RES_MIN=0.0. For simple high-pass filtering, set RES_MIN=RES_MAX>0.0. Use CUTMIN or CUT_MAX = 0.0 to apply a sharp cutoffs with no Gaussian falloff.

SUB-OPTION B: Apply 2D reciprocal lattice mask

   This is used to produce a mask with circular "holes" at the positions of an ideal, 2D reciprocal lattice. The vector coordinates of the two principal lattice dimensions (a* and b* given in TSU) may be entered by hand (4F FORMAT) or read in directly from the FFTLAT.DAT file produced after refinement of the reciprocal lattice by use of EMFFT option "L".

   Specify the radius for all circular holes (in TSU). You may create holes with "soft" or "hard" edges. For holes with "hard" edges, points inside the hole are given full weight and points outside are set equal to zero. In "soft" holes, points inside the hole are scaled with a Guassian weighting function with the weight determined by the relative distance of the point from the center of the hole: points at the hole edge are down weighted by 1/exp of their original value. "Soft" holes are generally made using a slightly larger radius than is appropriate for "hard" holes.

SUB-OPTION C: Apply a 2D layerline mask

   This produces a mask consisting of a series of parallel
slits (rectangular holes). Specify values for ANGLE,SPACE and
FALLOFF (3F FORMAT). ANGLE (in degrees) specifies the
orientation of the slits with respect to the horizontal (X)
direction of the FFT (a positive value is measured as a
counterclockwise rotation from the X-axis). SPACE is the
distance between slits in TSU. FALLOFF determines the
"softness" of the slit edges: sample points a distance FALLOFF
from the center line of the slit are downweighted by 1/exp.
There is currently no provision to construct "hard" edge holes
as is allowed in sub-option "B". Also, the parameters ANGLE,
SPACE, and FALLOFF must be entered by hand.

OPTION G: Extract structure factor

   This allows one to extract structure factors from the FFT of
the image of a 2D crystalline specimen. This is usually run after
running option "L" which computes refined parameters for the 2D
reciprocal lattice (AX,AY,BX,BY in TSU), for a* and b*, the two
principal lattice vectors). The lattice coordinates are normally
stored in the file FFTLAT.DAT, which is read back by this routine.
It is thus IMPERATIVE that the correct FFTLAT.DAT file be read in.
You also have the option of entering the reciprocal lattice
coordinates by hand.

   Alternatively, this option can be used after using EMCORAVG
(correlation averaging) if one wants to feed into the Fourier-
based software routines. EMCORAVG.DAT contains the required
reciprocal lattice coordinates. Because EMCORAVG is often run in
the mode which forces the reciprocal space lattice coordinates
to occur at integer transform sample unit positions, (enabling
peaks of the reflections to be exactly sampled in the FFT), this
routine uses the ORIGINAL refined lattice coordinates for
determining a*, b*, c*, alpha*, beta*, gamma*, d*, etc., but uses
the "enforced" coordinates to extract the structure factor
measurements. The ORIGINAL lattice dimensions are retained in the
header records of the structure factor file in order to override
the distortions imposed when forcing the reciprocal lattice to
exact TSU positions.

   Begin by specifying a filename and header text for the SF
output file.

Structure factors are computed in one of two ways:

   1) Transform intensity data, obtained within a circular or

elliptical window, which is centered about the ideal
reciprocal lattice position for each reflection, are
INTEGRATED with each transform sample point weighted by a
Gaussian function whose magnitude is proportional to the
distance from the calculated lattice position
to the sample point as given below:

The intensity at each sample point is weighted by W**2, where

$$W = \exp \left(\frac{-d*d}{2.0*r*r} \right)$$

    with   d = distance (in TSU) of the sample point from the
                   ideal lattice position.
              r = radius of the window (in TSU).

   For example, with r = 1.00

              d   = 0.00   0.50   1.00   1.50   2.00
              W   = 1.00   0.88   0.61   0.32   0.14
              W**2 = 1.00   0.78   0.37   0.11   0.02

   Choose the window shape (DEFAULT=circular) and RADIUS
(DEFAULT=1.0 TSU: this must be large enough to include the entire
spot) and set the cutoff variable, CUT (DEFAULT=2.0). CUT
determines the actual dimensions of the window used for
integration and background calculations. Intensities are
integrated inside a window with a radius = RADIUS*CUT and
background measurements are determined from within an annulus
whose inner and outer radii are RADIUS*CUT and 2*RADIUS*CUT,
respectively. If you choose not to subtract backgrounds, CUT is
set automatically = 2.0. Applying the background correction to
the structure factor measurements helps to reduce the noise,
especially for the higher resolution data. The background value
at each lattice point is estimated from the average intensity in
an annular region outside the integration window. **WARNING:** Choose
RADIUS and CUT with care to avoid artifacts produced when peaks of
neighboring spots are erroneously included in the background area.

   The structure factor amplitude is computed as the square root
of the (weighted) integrated intensity. Measurements are then
scaled down by an arbitrary factor of 1000.0 to help avoid
overflows in the formatted output file.

   The structure factor phase for each reflection is obtained by
interpolation of the four sample points adjacent to the calculated

lattice position. Phase measurements cannot be computed by
integration of all the sample points inside the reflection window
mainly because the phase term shows large fluctuations across and
just outside the the reflection peak due to the SIN(X)/(X)
influence from the edges of the boxed (and floated), digitized
micrograph.

   2) Structure factor amplitudes may be computed by interpolation
      as is done to obtain phases. If this option is used, there
      is no need to set a window shape or size, and the option to
      subtract backgrounds is not available. This option is
      mainly useful for extracting structure factor data from
      models or from the Fourier transforms of image averages
      after running the correlation analysis procedures (where
      there should be little or no noise surrounding the
      reflections).

   Specify the Miller indices of the two principal lattice vectors
(DEFAULTS = 1,0,0 and 0,1,0). This option is really only
important for correctly identifying the spot indices for a three-
dimensional data set such as from several tilt series from
orthogonal sections of a Three-dimensional crystal. The [hkl]
indices for the two principal lattice vectors in the two-
dimensional projection data provides a transformation matrix which
is used in subsequent programs (eg. EMSF2DBT) to identify the
orientation of the data when processed. For example, assume we
had an [h0l] projection such that the c* direction was horizontal
and a* was vertical in the FFT. Since the lattice refinement
routines ("L" option) use the convention a* = near horizontal
vector and b* = near vertical vector, then the two principal
lattice directions would be identified as [hkl] = 0,0,1 for a* and
[hkl] = 1,0,0 for b*. Thus, to transform from the 2D h'k' indices
used in option "L" to 3D [hkl] indices output by this routine, the
following transformation matrix algebra is performed:

$$\text{hkl} \quad = \quad \text{h'k'} * T \quad \text{where} \quad T = \begin{vmatrix} a11 & a12 & a13 \\ a21 & a22 & a23 \end{vmatrix}$$

   Thus, h = h'*a11 + k'*a21
          k = h'*a12 + k'*a22
          l = h'*a13 + k'*a23

```
     Example for T = |0 0 1| :      h' k'      h  k  l
                      |1 0 0|       ------     ---------
                                     1  0        0  0  1
                                     0  1        1  0  0
                                     1  1        1  0  1
                                     2  3        3  0  2
                                    -5  9        9  0 -5    etc.
```

    The SF output file contains information on the unit cell
parameters, the transformation matrix, and the structure factor
data (amplitudes and phases) in the format given in
[TSB.FOR]EMPROGS.DOC. The SF data can be refined using EMSFREF
and back transformed using EMSF2DBT (or EMSF3DBT) to produce MAP
files which can be displayed with EMMAP.

    This routine also generates a temporary file (FFTSPT.TMP) which
contains a listing of several of the parameters used to compute
the structure factors as well as the structure factor data.

    You also have the option (DEFAULT=N) to create a file
(FFTBOXES.TMP) that lists the 9 by 9 arrays of amplitudes and
phases for each spot, in a format similar to that used in the
EMFFT option "L" (sub-option "B"). Be sure to print out the file
on the line or laserprinter in LANDSCAPE (NOT PORTRAIT) mode,
otherwise much of the file will not print out on the page. The
data as printed out in the FFTBOXES.TMP file may differ slightly
from the data output in the structure factor and FFTSPT.TMP files
because some parameters (e.g. RADIUS=1.0; CUT=2.0) are fixed.

OPTION K: Fix values in FFT

Option not yet available.
Documentation needs to be written.

OPTION L: LATTICE refinement

    "L" allows you to refine two-dimensional crystalline lattice
parameters. Before running this option, you must be sure that you
have displayed the FFT to maximum size on the graphics device.
You are given one of the two following warning messages depending
on which graphics device you are using:

    WARNING: FFT must be displayed at 1024x1024 size and centered
              at 640,512
    WARNING: FFT must be displayed at 512x512 size and centered
              at 320,256

"L" currently has provides two separate sub-options in the
following touch-key menu:

                    EMFFT_LATREF TOUCH-KEY OPTIONS

                    A   Use overlay grid to refine lattice
                    B   Least squares fit of individual spots
                    E   EXIT routine

    SUB-OPTION A: Use overlay grid to refine lattice

    This allows you to select two spots of known indices with the
data tablet puck and the program then draws a reciprocal lattice
net over the displayed FFT. You can then reenter either or both
spots and keep redrawing the lattice net until you are satisfied
that the net accurately fits the lattice reflections. This method
is somewhat more subject to error than sub-option "B" (below)
which does a least squares fit on the basis of as many input spots
as you care to identify.

    First enter the densitometer pixel size in nanometers
(DEFAULT=0.51nm which corresponds to 25 micron sampling of a
micrograph at 49,000 magnification). This is only used for giving
real-space lattice statistics while you are fitting the net.
Thus, if you aren't interested in accurate real-space parameters,
you can just ignore this by hitting the <CR> key. Next enter the
Miller indices for the two spots, [H1,K1] and [H2,K2], you plan to
select with the tablet puck (4I FORMAT). If you misindex these
spots, the reciprocal lattice net and lattice parameters will be
incorrect and you will be unable to build a proper filter mask
with option "F", for example. Choose the R,G,B color of the
overlay grid (3I FORMAT: DEFAULT=150,150,150=light grey). At this
point control is transferred to the data tablet puck and the
following menu appears on the terminal screen:

Mark two spots with tablet cursor:
YELLOW = enter new position
WHITE = keep old position
BLUE   = turn grid on/off
GREEN = EXIT

ASTAR   BSTAR   GAMSTR   ADIM   BDIM   GAMMA

    Carefully select the positions of the [H1,K1] and [H2,K2] spots
(in that order) with the YELLOW puck button. After entering these
two positions, the overlay reciprocal lattice net is drawn. Use
the BLUE puck button to toggle the net off and on. To change the
lattice, you must always enter two spots. Use WHITE to accept the

previous position and YELLOW to select a new position. Hit GREEN
to exit from the selection process after which you are allowed to
restart or finish the session. If you choose to restart, the
routine will again prompt you for the pixel size, grid overlay
color, etc. as before.

   If you want to exit the routine completely, you have the option
to save the reciprocal lattice parameters in the file FFTLAT.DAT
(DEFAULT=N). This file stores the X and Y coordinates (in TSU)
for the [1,0] and [0,1] lattice vectors. These two vectors can
then be used in subsequent EMFFT routines such as "F" to build
filter masks with holes positioned at the points of an ideal
lattice defined by these principal vectors.

   SUB-OPTION B: Least squares fit of individual spots
      This option helps determine the lattice parameters of
   diffraction patterns. The LEXIDATA TABLET cursor is used
   to pick out spots for a least-squares determination of a
   crystalline lattice. The optional end product of the routine
   is a file (FFTLAT.DAT) containing the coordinates (in transform
   sample point units) of the [10] and [01] lattice vectors.

CRYSTAL LATTICE REFINEMENT STEPS

1. Choose a cursor type and color.

2. Mark two reference spots with the Lexidata tablet cursor and
    enter the H,K index for each. Be certain that the two spots
    do not both lie on a line which intersects the origin of the
    diffraction pattern. WARNING: the indexing must conform to
    usual crystallographic conventions in order for certain
    options in the refinement program "EMSFREF" to work correctly.
    Also, it is highly recommended that you choose two reference
    spots which have reasonably high indices (i.e. don't just mark
    the [10] and [01] spots) since this will give a better initial
    estimate of the reciprocal lattice parameters. If you are
    somewhat sloppy at this step, the indexing of high resolution
    spots may be wrong due to the magnification of small errors
    made when low resolution spots are used as reference.

3. Choose the maximum number of contour intervals (default
    NC = 25; range = 5-25) and the maximum contour value (default
    CLIM = 999.0; range = 0.0-999.0) to scale the contoured
    amplitude displays. If the amplitudes cover a large dynamic
    range, it is best to set NC = 25 and CLIM < 999., otherwise
    some of the weaker, high resolution spots that are important
    for accurate lattice refinement may not show up in the display
    because they won't be contoured at the lowest level.

4. Pick spots using the YELLOW puck button. 9x9 amplitude and
    phase arrays will be displayed at the terminal and a contour
    display of the amplitude array will be appear on the LEXIDATA
    (the diffraction pattern will disappear from the graphics
    screen at this point).

5. Place the tablet cursor over the spot center and hit the
    YELLOW button to accept the position. WARNING: Try not to be
    overinfluenced by sharp peaks; mark the center of gravity of
    the WHOLE spot. DX,DY, listed at the terminal, identifies the
    position you have chosen, measured in coordinates relative to
    the center of the 9x9 array (+X to the RIGHT and +Y UP).
    If you wish to bypass the spot, hit either the WHITE, BLUE or
    GREEN buttons.

6. After a minimum of two spots have been successfully entered,
    the current values for the lattice parameters can be obtained
    by hitting either the WHITE, BLUE or GREEN button. After the
    lattice parameters are listed, you have the option (Y,W or B)
    to delete measurements by hand, or to continue (G). To delete
    spots, type the H,K index (2I format) for each spot followed
    by a <CR>. A second <CR> will return you to the program where
    you may then EXIT the routine or start entering additional
    spots. Please note that, depending on which option you choose
    at this part of the routine, you may be required to enter
    subsequent options either from the data tablet puck or from
    the terminal keyboard. Thus, if you hit the GREEN button to
    bypass deleting spots by hand, then your next option is
    answered through the puck, NOT at the terminal keyboard. This
    helps insure that you don't have to needlessly keep moving
    your hand from the tablet puck to the terminal and vice versa.
    Likewise, if you hit Y,W or B to delete spots, then your next
    option will be answered from the terminal keyboard unless you
    resume picking out new spots for refinement.

7. When the routine is exited, you are given the option to store
    The x,y coordinates (in transform sample point units) of the
    [10] and [01] lattice vectors in the ASCII file FFTLAT.DAT.
    This is then used by EMFFT option "G".

ADDITIONAL NOTES: Experience with samples such as catalase
crystals and gap junction membranes indicates that the lattice
parameters should be considered valid if at least 10 or more well
resolved spots can be refined so that none deviate more than .75-
1.0 transform sample point from the ideal lattice. Treat with
caution any spots that deviate more
than 1 sample point.

OPTION O: OPEN an existing FFT stored on disk

   "O" allows you to read in an FFT stored on disk.

OPTION R: READ and transform IMAGE data

   "R" allows you to read in an IMAGE and Fourier transform it for
use by the remaining EMFFT options. The DEFAULT size of the FFT
will be the smallest power of two in each dimension with a minimum
size limit of 128 by 128. Thus, if your IMAGE is 63 by 513 pixels
(NCOL,NROW), then the DEFAULT FFT size is 128 by 1024. You may
INCREASE either FFT dimension up to a maximum of 1024 TSU.

OPTION S: Get FFT STATISTICS

   "S" is used to obtain the current values of FFT_AVG, FFT_STD,
   and FFT_MAX.

OPTION W: WRITE the current FFT to disk or line printer

   "W" allows you to save the current FFT (including any changes
that have been applied) to a disk file with the standard FFT file
format (DEFAULT) or a file that is ASCII formatted for dumping to
the lineprinter ("1").

   The lineprinter-type output file contains the FFT amplitudes
and/or phases in a format suitable for dumping to a lineprinter or
laserprinter. Currently, the output is restricted to the central
128 TSU, centered about the Y-axis (meridian) of the FFT. This is
completely adequate for displaying 128x128 up to 256x1024 FFT
files, but may leave out significant data from FFT data with
IDIM1>256. With this option you can output amplitudes and/or
phases. If you output phases, you may change the FFT origin
(FFT_ORIGX,FFT_ORIGY) if you wish. The amplitudes are normalized
to a LOG2 scale with a maximum value of 9. Phases are coded using
the characters 0-9,A-Z to represent 0-360 degrees in 10 degree
steps.

   After using "W", you MUST select "O" or "R" to continue.
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The FORTRAN code for EMFFT is in
   JUSTEM$DKA0:[TSB.FOR]EMFFT.FOR,.SUBS.

This documentation is in JUSTEM$DKA0:[TSB.DOC]EMFFT.DOC 5-Mar-92
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