Problem 8: How Do I Create and View a Fourier Map?
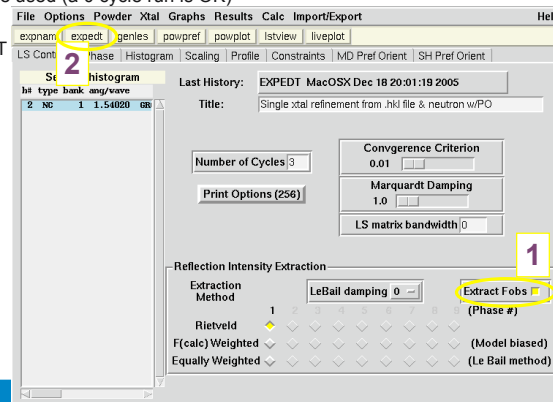
- Bad news: you must use EXPEDT to set up a Fourier map

- Good news -- not too hard

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8.1 Needs Structure Factors from GENLES

1. Note that GENLES must have been run with "Extract Fobs" ON for the histograms to be used (a 0 cycle run is OK)

2. Invoke EXPEDT

8.2A Using EXPEDT to set up DELF map (part 1)

```
The last history record is :
   HSTRY 20 EXPEDT  MacOSX Dec 18 19:56:07 2005        F-EDT
Is this the file you wish to use? (<?>,D,K,Q,R,Y) >Y
Experiment title:
      Single xtal refinement from .hkl file & neutron
The last history record is :
   HSTRY 20 EXPEDT  MacOSX Dec 18 19:56:07 2005        F-EDT
EXPEDT data setup option (<?>,D,F,K,L,P,R,S,X) >F
Enter desired map (<?>,DELF,FCLC,FOBS,NFDF,PTSN,DPTS,EXIT) >DELF
Enter section desired (X,Y,Z - choose Z for DSN6 maps) >Z
Do you wish to specify individual map steps for each axis (Y/<N>)? >N
Current overall map step size is  0.2000  A
Enter new overall map step size in Angstroms >I
The a-axis is  7.277918  A
The new del-x is  0.2022 A
The cell will be divided into   36 points along x
The b-axis is  7.277905  A
The new del-y is  0.2022 A
The cell will be divided into   36 points along y
The c-axis is  16.830175  A
The new del-z is  0.2004 A
The cell will be divided into   84 points along z
```

> Difference Fourier -- probably most useful option for powder diffraction

> X, Y or Z -- does not matter

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8.2B Using EXPEDT to set up DELF map (part 2)

```
Old x limits are  0.0000 to  0.0000
Enter minimum and maximum values of x in fractions of the cell edge >0.5
New x limits are  0.0000 to  0.5000
Old y limits are  0.0000 to  0.0000
Enter minimum and maximum values of y in fractions of the cell edge >0.5
New y limits are  0.0000 to  0.5000
Old z limits are  0.0000 to  0.0000
Enter minimum and maximum values of z in fractions of the cell edge >0.5
New z limits are  0.0000 to  0.5000
At least one asymmetric part of the unit cell is included in the Fourier.
Enter new list of histogram numbers in the order you wish them to be read.
The last occurrence of a reflection will be used.
Include histogram (0 to terminate list) >2 0
Enter FOURIER map option (<?>,A,C,D,E,F,H,I,L,P,R,S,T,W,X) >X
At least one asymmetric part of the unit cell is included in the Fourier.
EXPEDT data setup option (<?>,D,F,K,L,P,R,S,X) >X
STOP EXPEDT terminated successfully statement executed
Press Enter to continue
```

> Important: Make sure that at least one asymmetric volume is enclosed. Repeat the "R" command on "WARNING... Part of the unit cell is not included in the Fourier." expanding the volume, as needed.
>
> If too big, there may be extra peaks in the search (not a problem).
>
> If too small, part of the unit cell will be missed (big problem).

> List histograms with most reliable last (for overlapping segments). Don't combine x-ray & neutron histograms. End with "0".

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8.2C Notes on EXPEDT options

- For map types other than DELF, F_{000} must be included in computation; use "F" option to specify unit cell contents.
- Can change d-space range to eliminate unreliable reflections (option "D"); not usually needed.
- Use the "P" option to set the phase if looking for Fourier density in the 2nd or 3rd… phase.

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## 8.3 Compute the Fourier Map & Search for Fourier Peaks

- Run program FOURIER and then FORSRH

```
A DELF file has been opened
The range of map values is  -0.357 to   0.998
Enter min. Peak value (negative if negative values are desired) >.4
Enter number of peaks to be located (1 to 225) >10
Save the peaks located in the EXP file? (Y,<N>) >y

Min rho =   0.40000  No. of peaks =  10  Peaks saved? Y

The following peaks were found
       Rho      X       Y       Z
   1   0.998  0.1407  0.2819  0.0630
   2   0.451  0.1395  0.2831  0.2084
   3   0.410 -0.0003  0.0002  0.1468

Total CPU time for FORSRH was   0.01 seconds
STOP FORSRH terminated successfully.
```
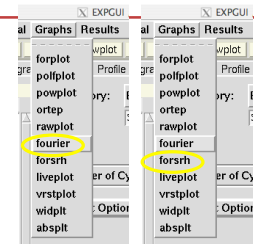
Notes: negative Fourier peaks are expected for neutrons with "negative scattering length elements." (None here) so -0.357 indicates ~ noise level.

Range of 0.0 to 0.0 indicates Fobs were not extracted

Usually only the first few difference Fourier peaks are meaningful in powder diffraction.

Saved peaks are of use in FORPLOT & DISAGL.

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8.4 Viewing a FOURIER Map in DRAWxtl

- GSAS provides FORPLOT & VRSTPLOT
  - I prefer to use DRAWxtl or FOX to view maps.

DRAWXTL Example:
1. Run FORPLOT to export the map

```
Enter graphic screen option (<?>,A,B,Z) >Z
Enter hardcopy option (<?>,A,B,C,D,E) >A
A DELF file has been opened
...
Enter FORPLOT command (<?>,A,C,D,E,G,F,H,I,L,M,N,O,P,Q,R,S,T,V) >E
File FTST_DELF.grd written
Enter FORPLOT command (<?>,A,C,D,E,G,F,H,I,L,M,N,O,P,Q,R,S,T,V) >Q
Press Enter to continue
```
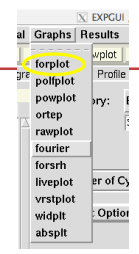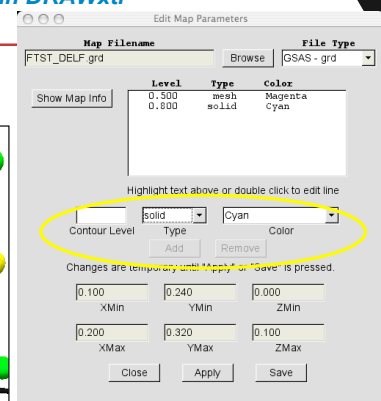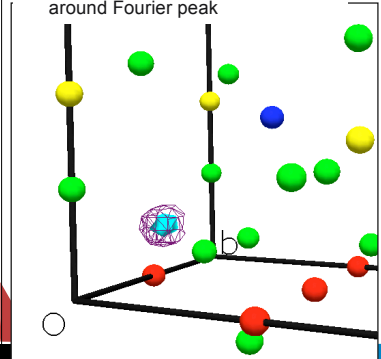
2. Startup DRAWxtl as before (§3.4)

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8.5 Viewing a FOURIER Map in DRAWxtl

3. In DRAWxtl use "Edit Map Parameters" using values as shown to left to see section of map around Fourier peak

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