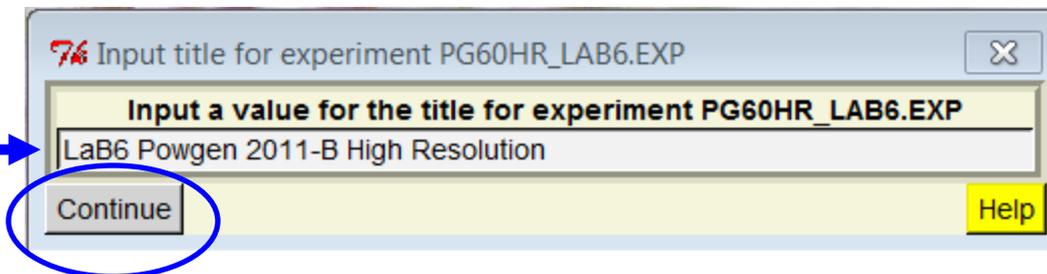
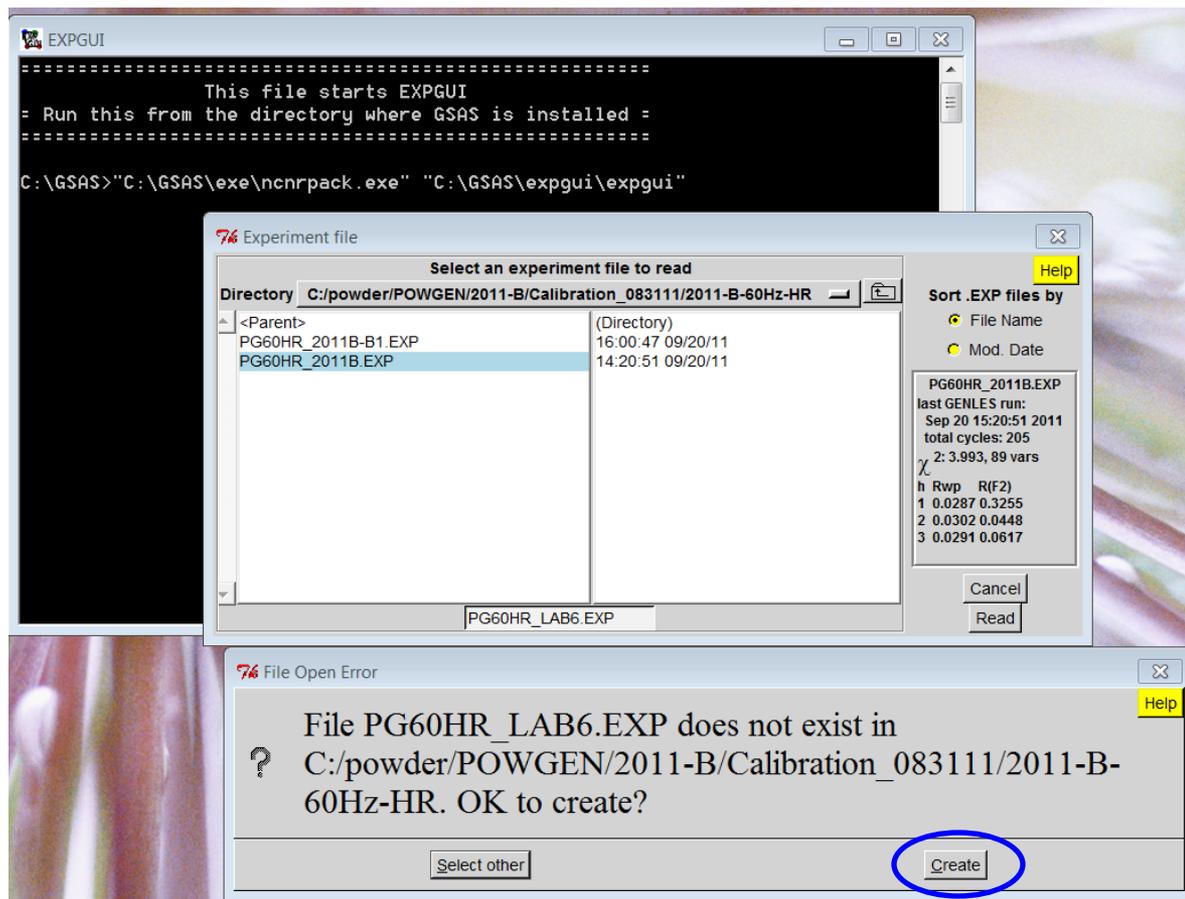


# Brian Toby's EXPGUI: Easy to start a new refinement

Run EXPGUI and go to the required directory and enter a new filename and press "read". When prompted, then press the "Create" icon. Enter title when prompted and continue.

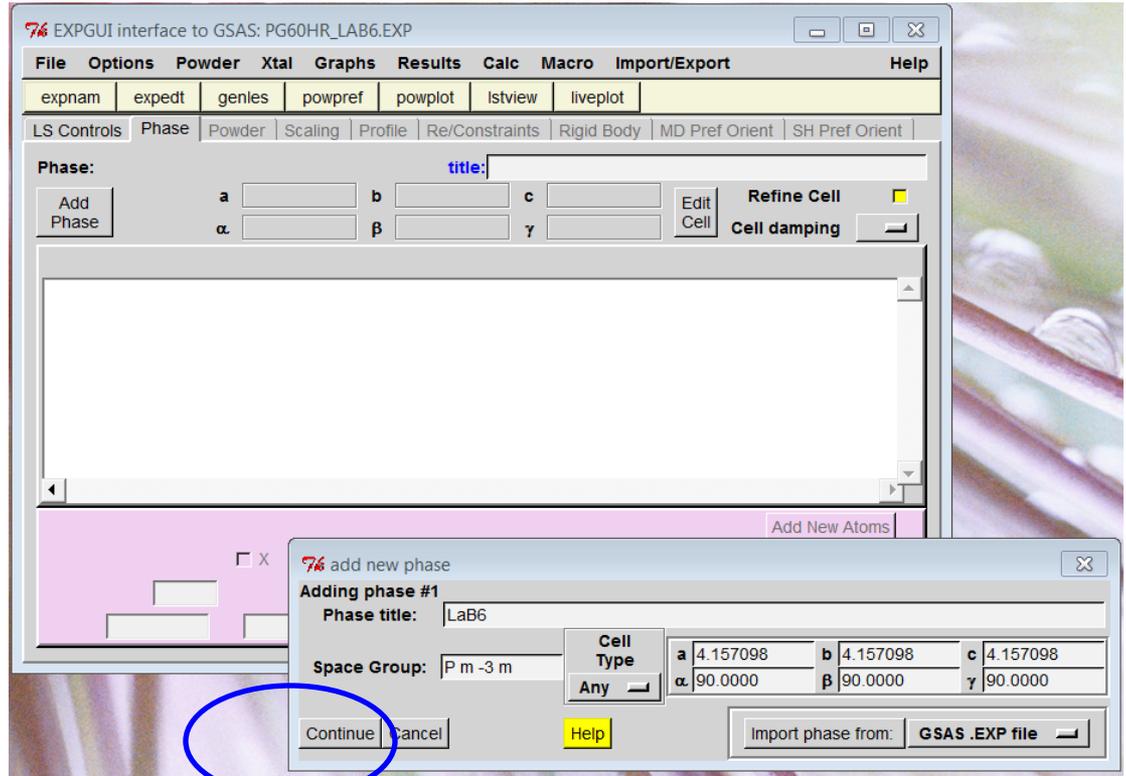


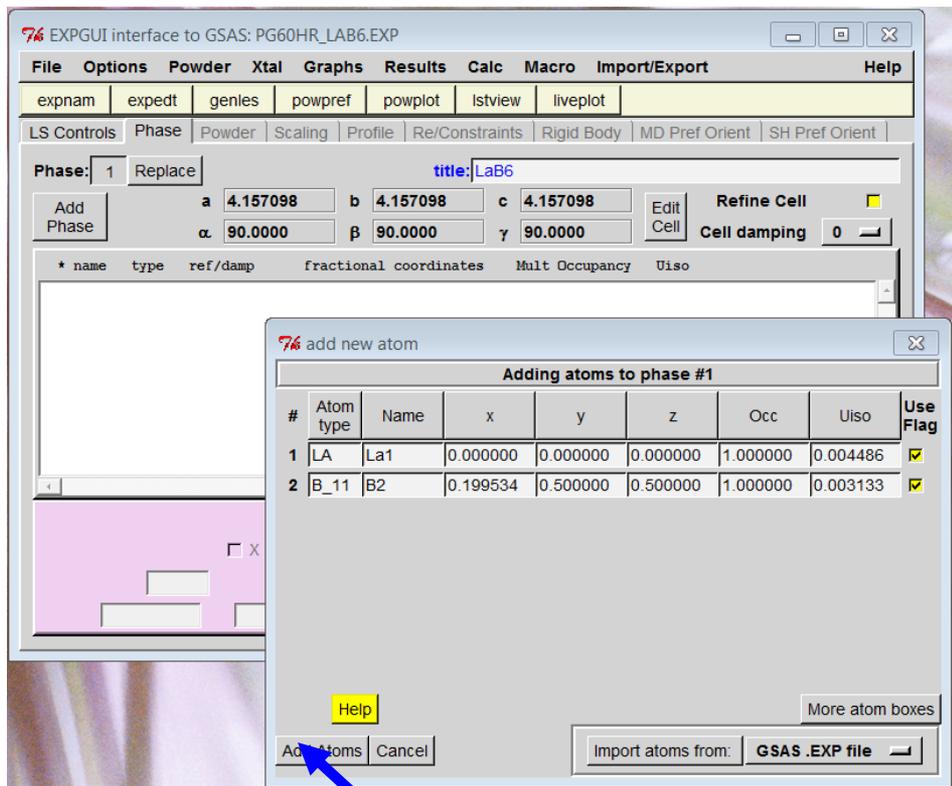
Experiment Title goes here

# Select the Phase Tab

- Click on the Add Phase
- Add Phase Title
- Space Group
- Add Lattice Parameter

• Screen shot shows reading from an existing .exp file. careful about standard notation of Space Groups especially when using cif files for structure.

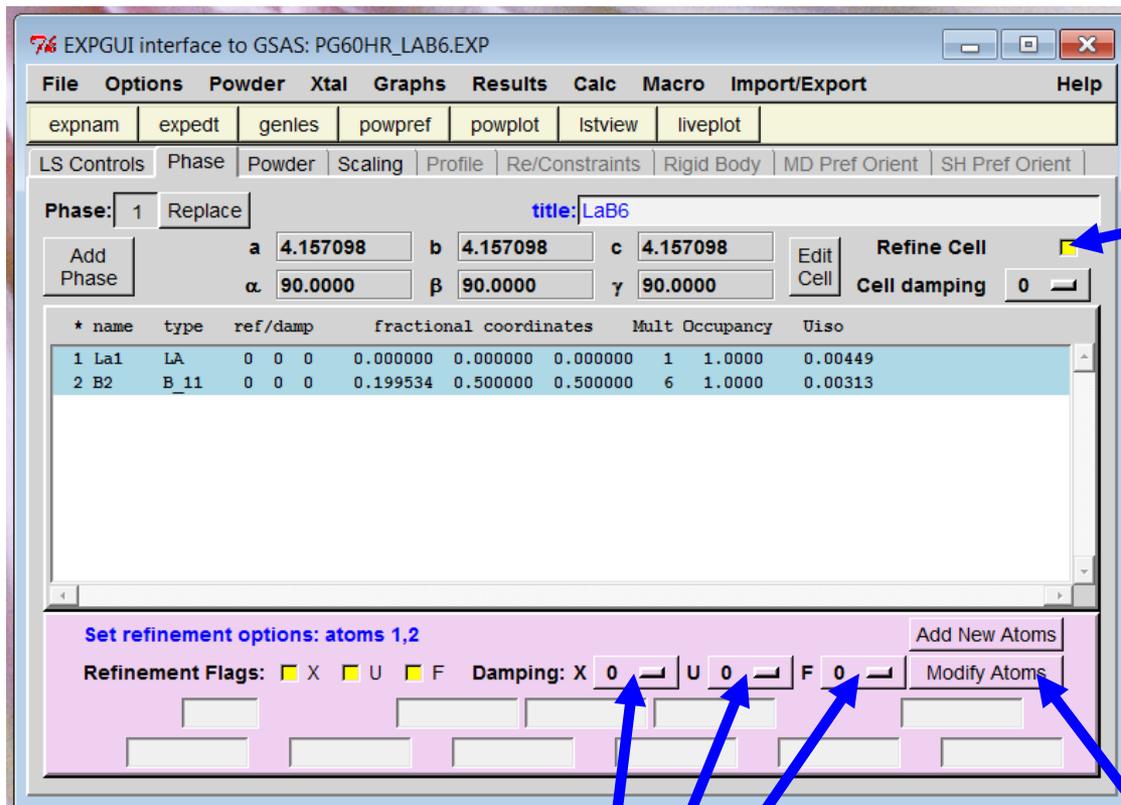




Click on "Add Atoms"

Click "Add New Atoms" and add in the starting model either by hand or importing a .cel, .cif, .exp, .spf or .xlt format file.

Follow similar steps to add multiple phases



Check to refine  
Lattice  
parameter.

Allows you to set damping  
By a pull down menu

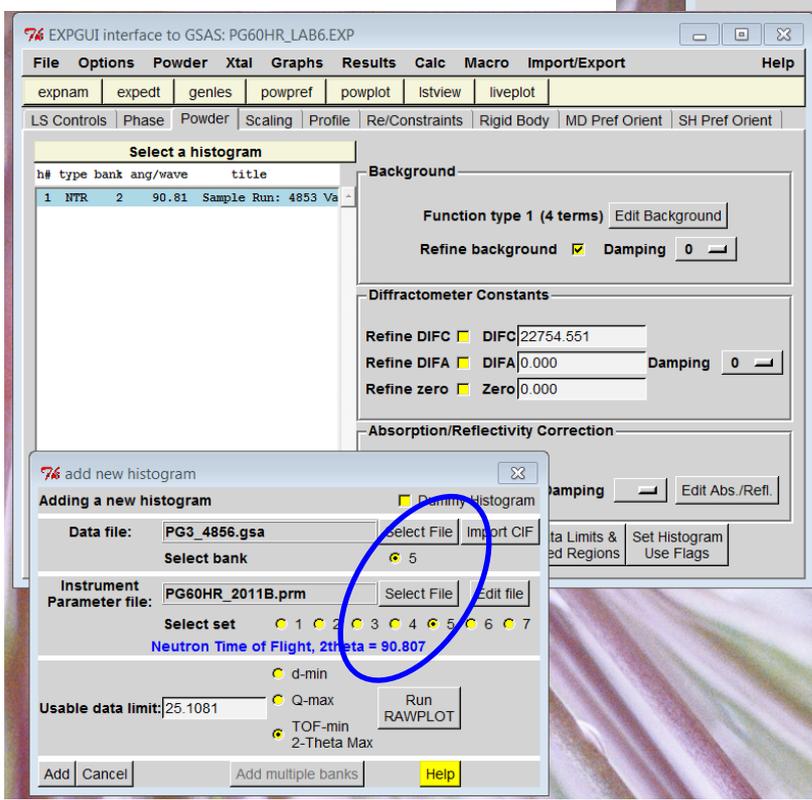
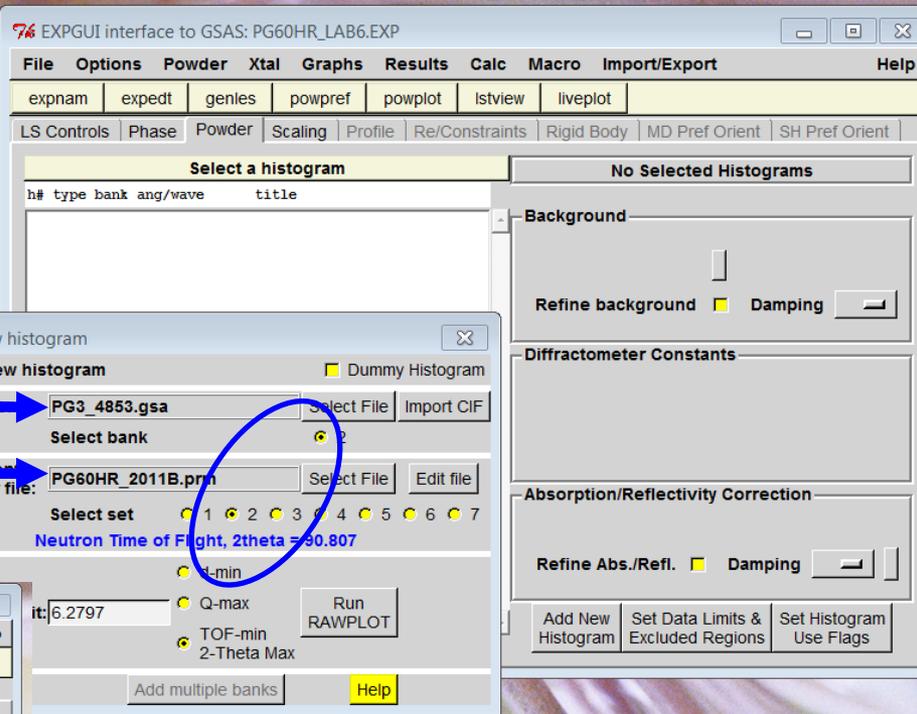
Allows you to set anisotropic  
thermal parameter

# Select the Histogram Tab

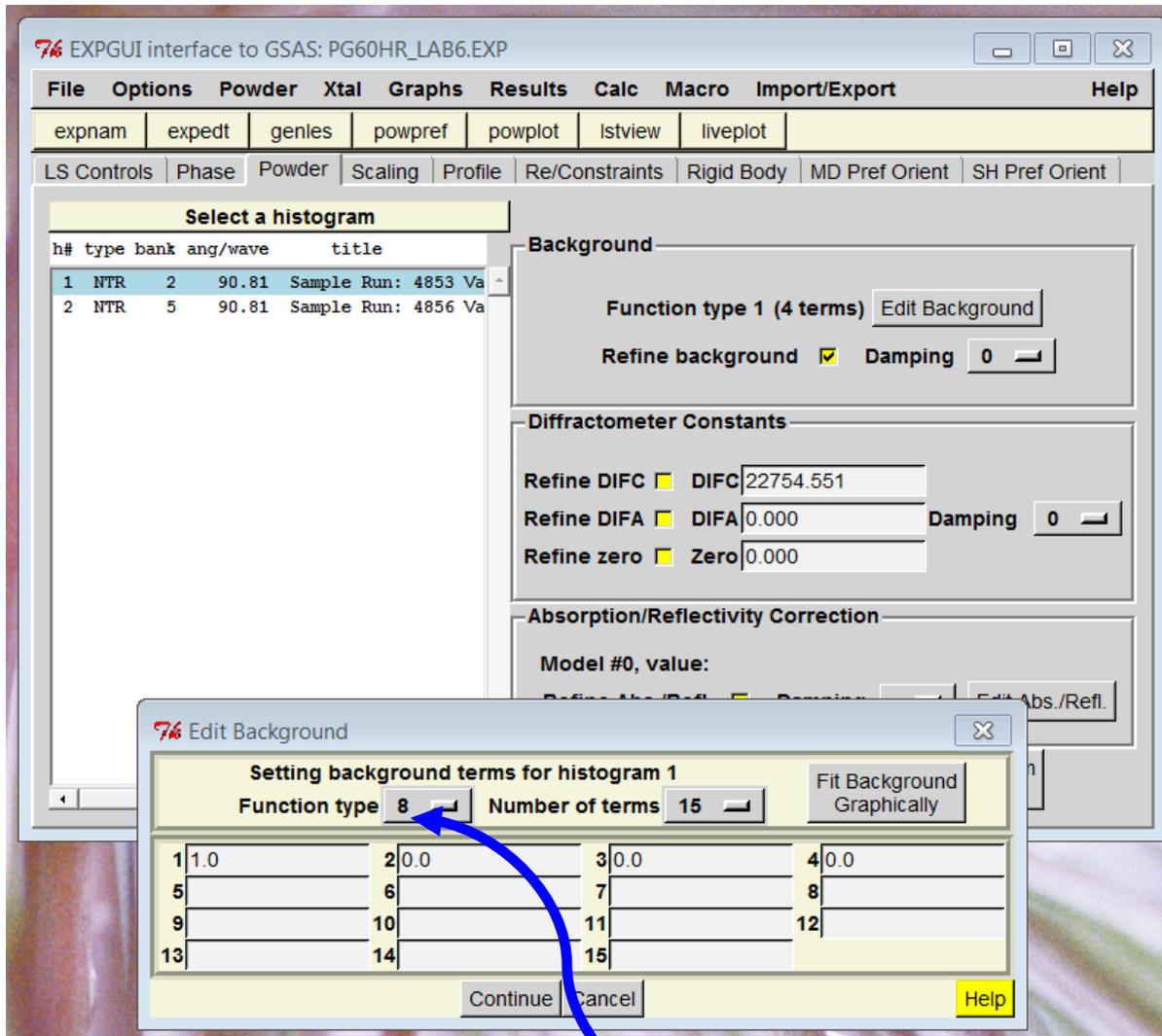
Click on "Add New Histogram"

GSAS data file

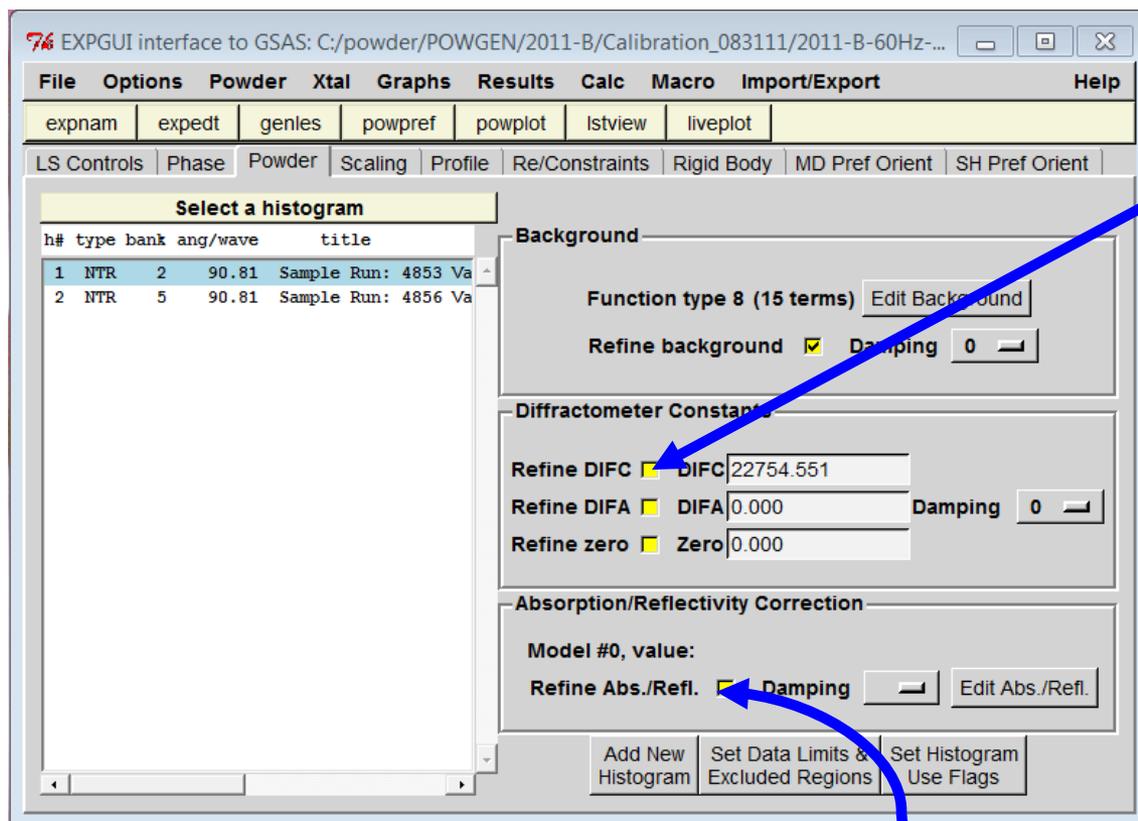
Instrument parameter file



Add second histogram. Powgen histograms are dependent on the center wavelength used for data collection. Multiple histograms can be added for an individual refinement. Make sure the bank # in the parameter file matches up with bank number in data (.gsa) file as shown.



Default background function is set for BG function 1. BG function 8 is often works better for our data.



**Diffractometer Constants set via Calibration. First bank value must be left constant but you may have to refine the DIFA values to correct for sample displacement.**

**Absorption has to be refined often for neutrons. You may have to constrain (using PC version of GSAS) the values to be same for all the banks.**

# Quantitative Phase Analysis/scale factor

The screenshot shows the EXPGUI interface with the following components:

- Menu Bar:** File, Options, Powder, Xtal, Graphs, Results, Calc, Macro, Import/Export, Help
- Sub-Menus:** expnam, expedt, genes, powpref, powplot, lstview, liveplot
- Navigation Bar:** LS Controls, Phase, Powder, Scaling, Profile, Re/Constraints, Rigid Body, MD Pref Orient, SH Pref Orient
- Select a histogram:** A table with columns h#, type, bank, ang/wave, and title.

h#	type	bank	ang/wave	title
1	NTR	2	90.81	Sample Run: 4853
2	NTR	5	90.81	Sample Run: 4856
- Scale Factor:** Scale: 1.000000, Refine , Damping: 0
- Phase Fractions:** Phase 1: 1.0000, Refine , Damping: 0

A blue arrow points from the 'Refine' checkbox in the Scale Factor section to the 'Refine' checkbox in the Phase Fractions section.

Remember to keep one of these fixed.

Refine the remaining scale factors.

# Select Profile Tab

76 EXPGUI interface to GSAS: C:/powder/POWGEN/2011-B/Calibration\_083111/2011-B-60Hz-H...

File Options Powder Xtal Graphs Results Calc Macro Import/Export Help

expnam expdet genes powpref powplot lstview liveplot

LS Controls Phase Powder Scaling Profile Re/Constraints Rigid Body MD Pref Orient SH Pref Orient

Select a histogram

h#	type	bank	ang/wave	
1	NTR	2	90.81	Sa
2	NTR	5	90.81	Sa

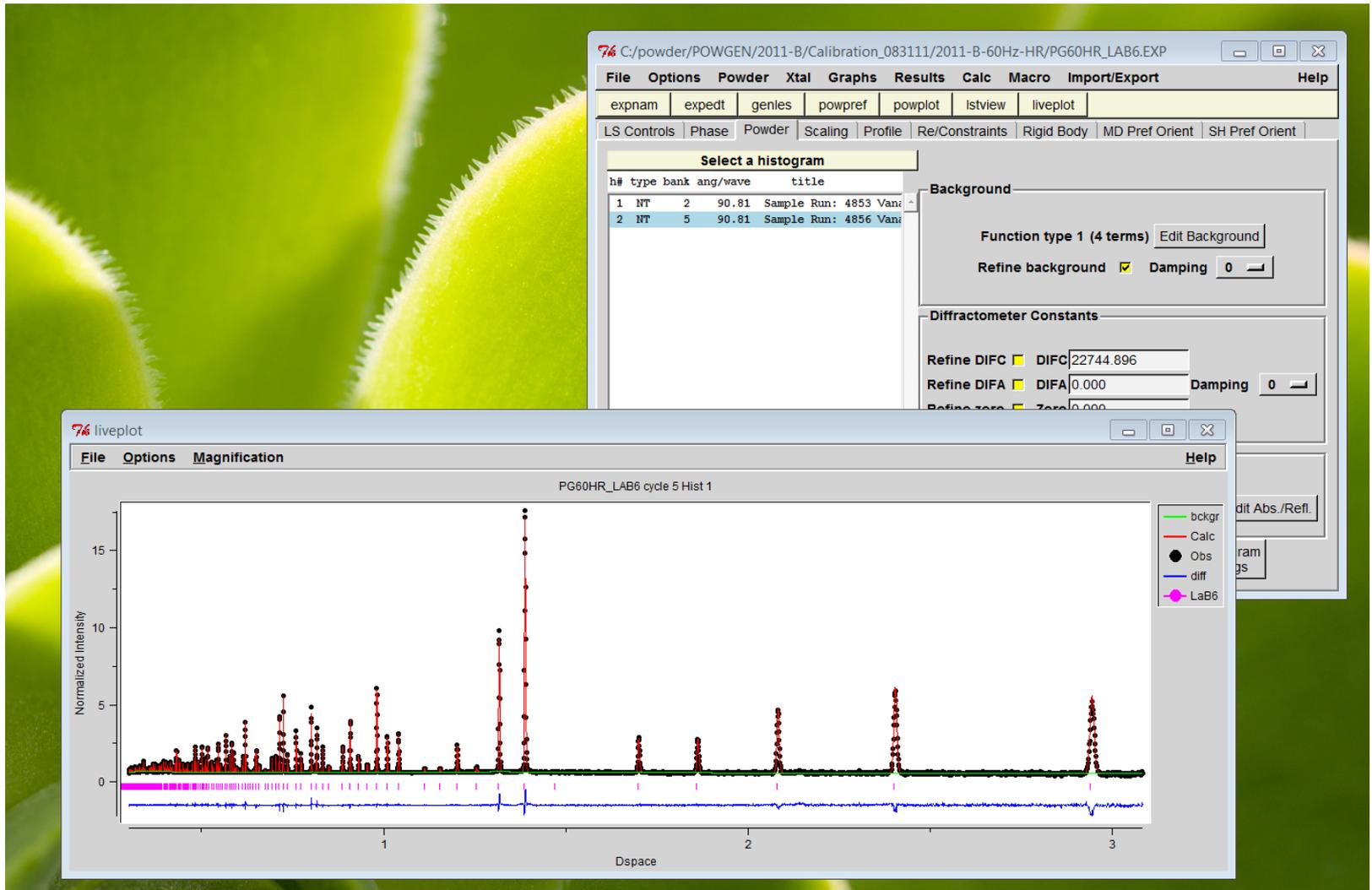
Hist 1 -- Phase 1 (type -3)

Damping 0 Peak cutoff 0.00200 Change Type

alp	<input type="checkbox"/>	0.000000	bet-0	<input type="checkbox"/>	0.000000	bet-1	<input type="checkbox"/>	0.000000
sig-0	<input type="checkbox"/>	0.000000	sig-1	<input type="checkbox"/>	10.000000	sig-2	<input type="checkbox"/>	185.900000
gam-0	<input type="checkbox"/>	0.000000	gam-1	<input type="checkbox"/>	0.000000	gam-2	<input type="checkbox"/>	0.000000
gsf	<input type="checkbox"/>	0.000000	g1ec	<input type="checkbox"/>	0.000000	g2ec	<input type="checkbox"/>	0.000000
rstr	<input type="checkbox"/>	0.000000	rsta	<input type="checkbox"/>	0.000000	rsca	<input type="checkbox"/>	0.000000
L11	<input type="checkbox"/>	0.000000	L22	<input type="checkbox"/>	0.000000	L33	<input type="checkbox"/>	0.000000
L12	<input type="checkbox"/>	0.000000	L13	<input type="checkbox"/>	0.000000	L23	<input type="checkbox"/>	0.000000

Lorentzian widths

Gaussian widths



Always look at the plots while doing refinement to keep track of progress.

GSAS also has a large number of features that cannot be accessed using expgui. In that case you have to go into the command line driven menu. Following three slides show you the structure of that.

# GSAS - General Structure Analysis System

## basic menu list

### SETUP

- Expnam - enter experiment name “\*”
- Expedt - edit \*.exp experiment file
- MS-DOS -
- Cnvfile - convert data file to correct format
- Dlst - delete \*.lst file
- Exit -

### COMPUTE

- Powpref - powder data preparation
- Genles - general least squares

### GRAPHICS

- Powplot - powder pattern plotting

### RESULTS

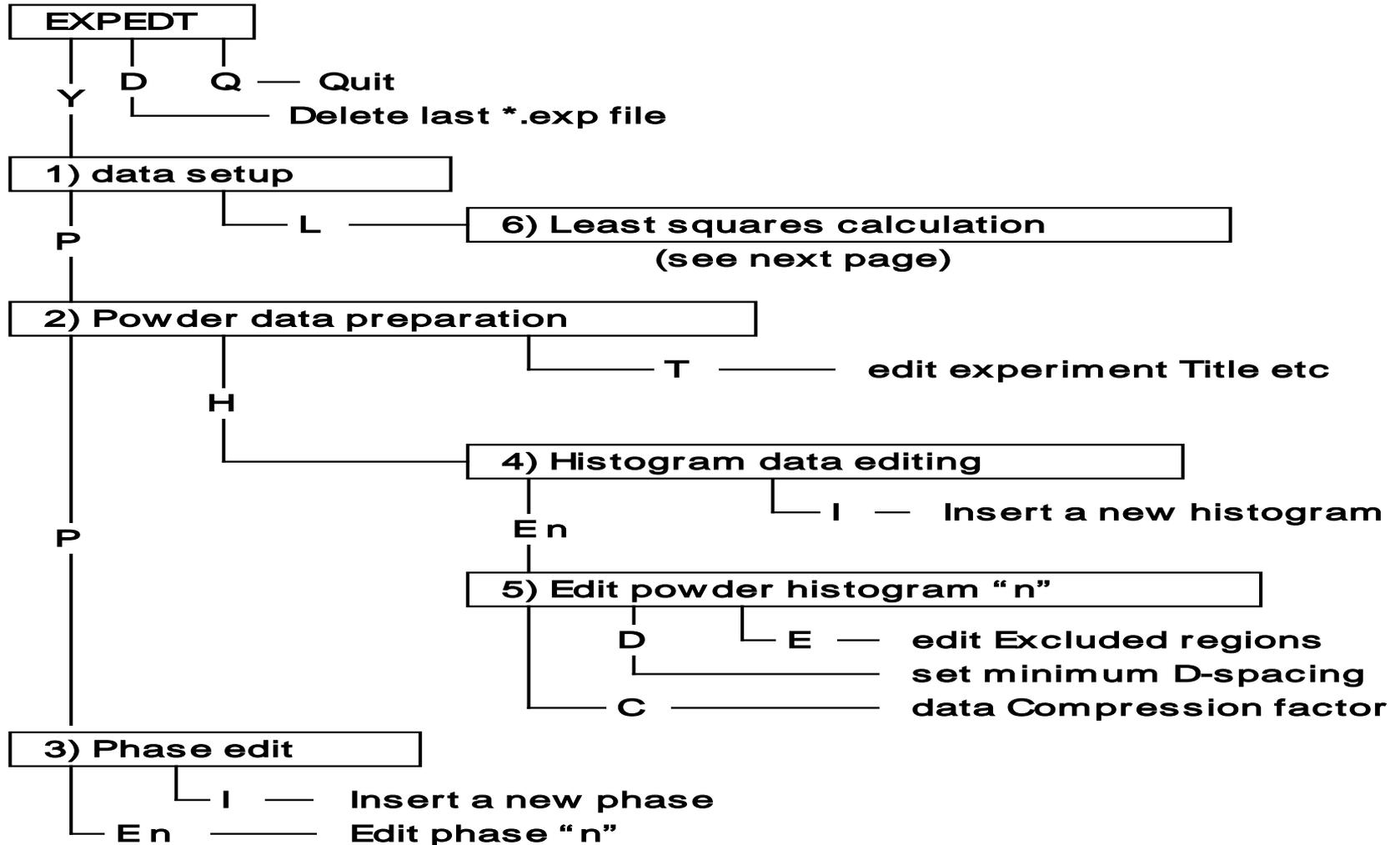
- Disagl - distance and angle calculation
- Gsas2cif - creates .cif file
- Gsas2pdb - creates .pdb file

### UTILITIES

- Rawplot - View Raw data
- Hstdmp - Dumps observed and calculated intensity along with hkl values.
- Reflist - Gives a list of reflections.

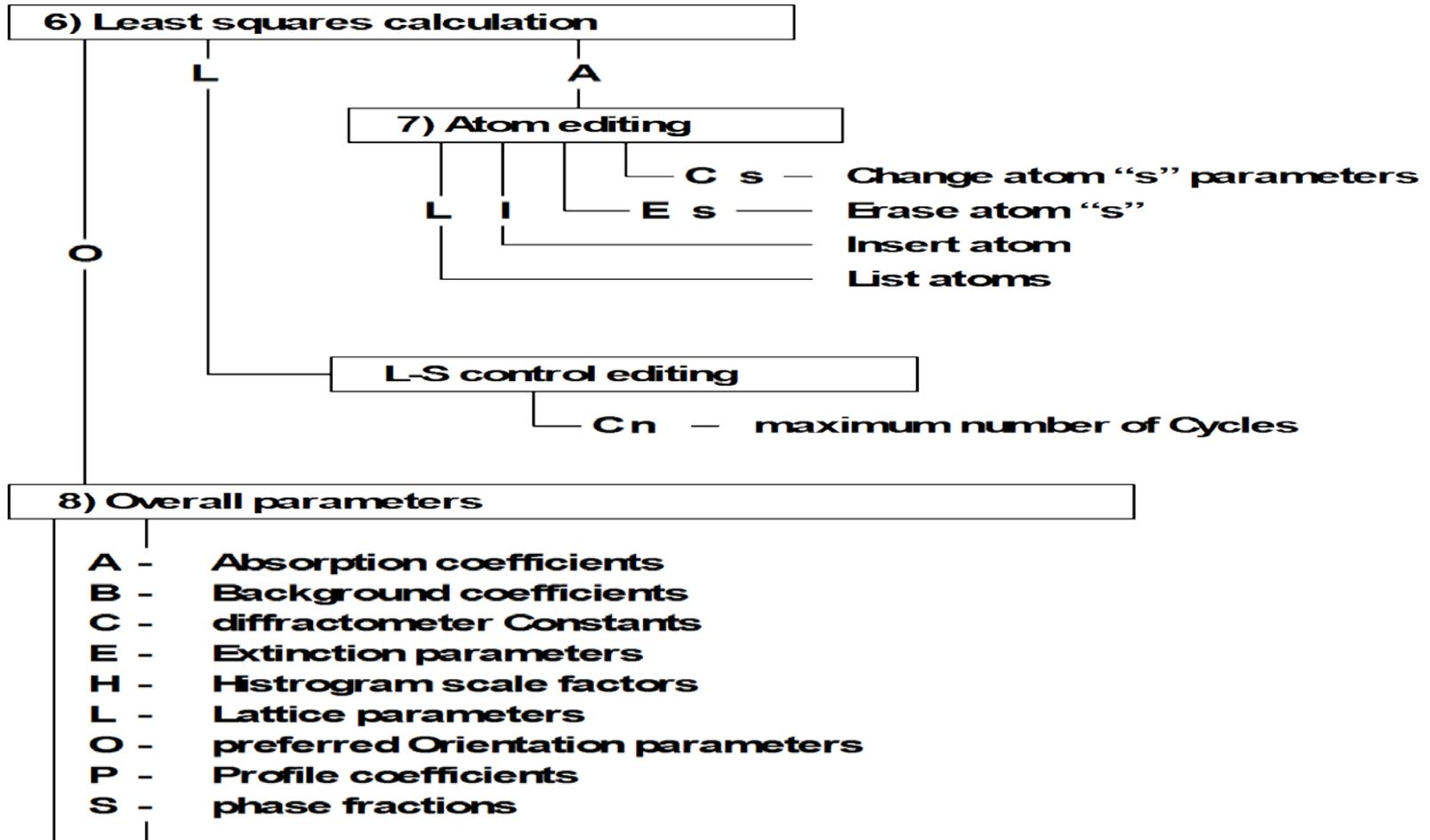
# FLOWCHART for EXPEDT

use X to travel up flowchart



# FLOWCHART for EXPEDT (2)

use X to travel up flowchart



Extra info:

V to turn refinement flags on and off

Dn to damp parameter refinement by  $n \times 10\%$