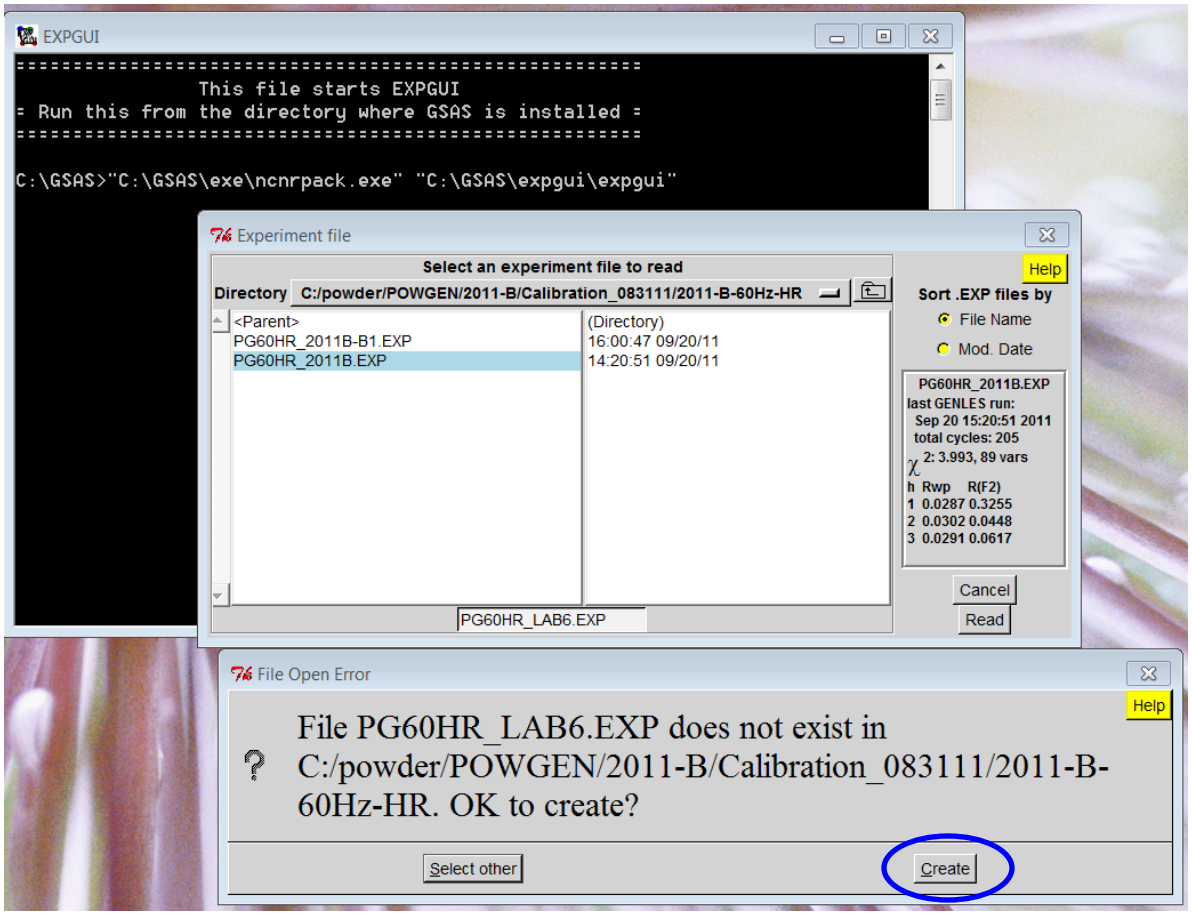
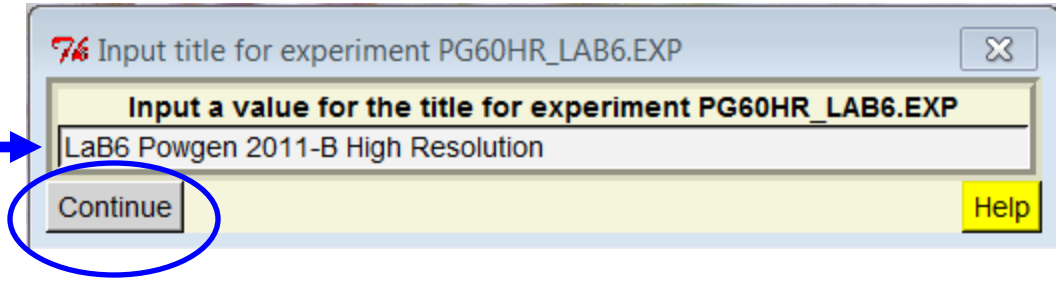
Brian Toby's EXPGUI: Easy to start a new refinement

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.



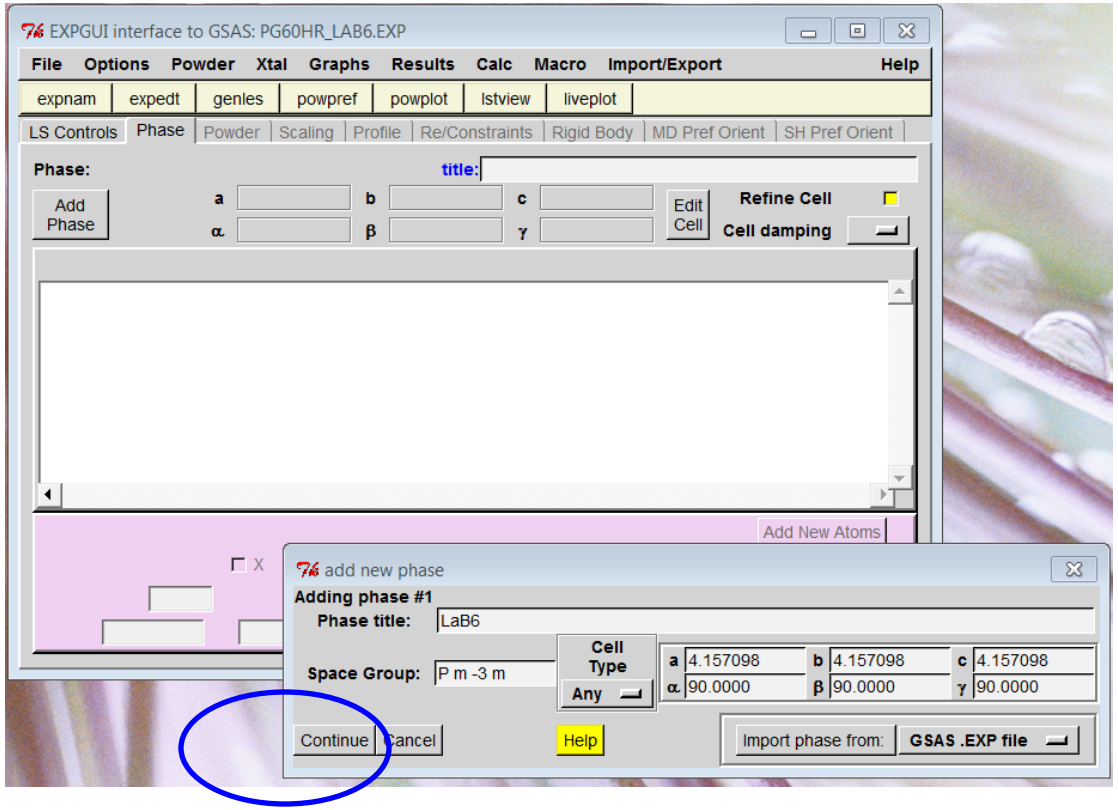
Experiment Title goes here

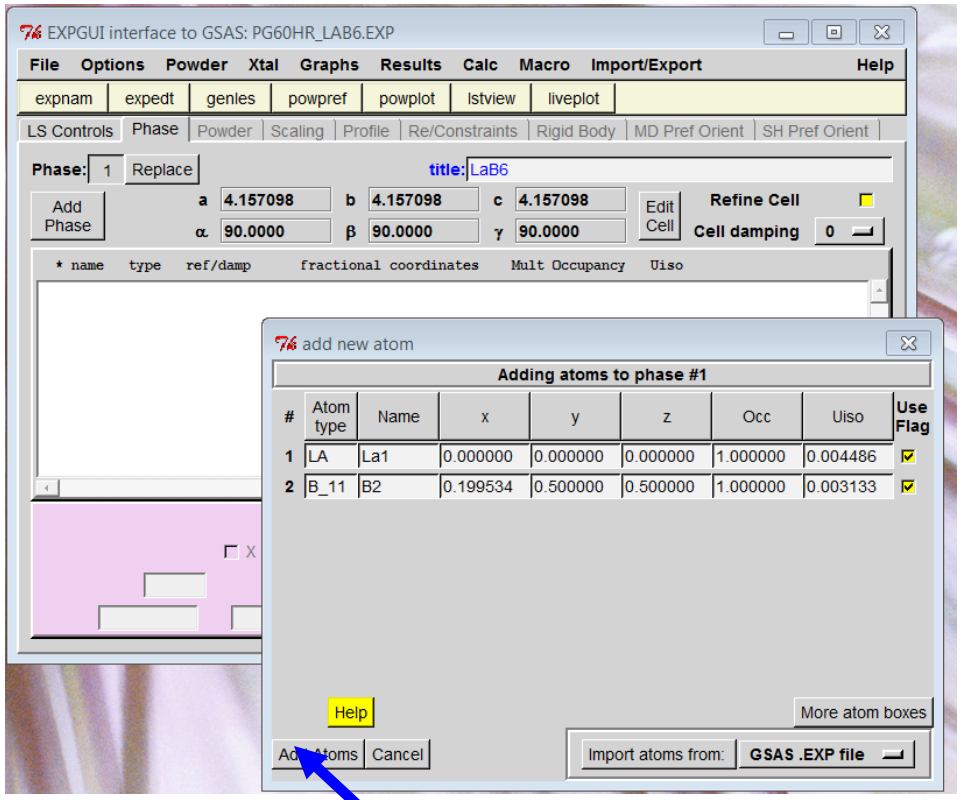


Select the Phase Tab

- 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.

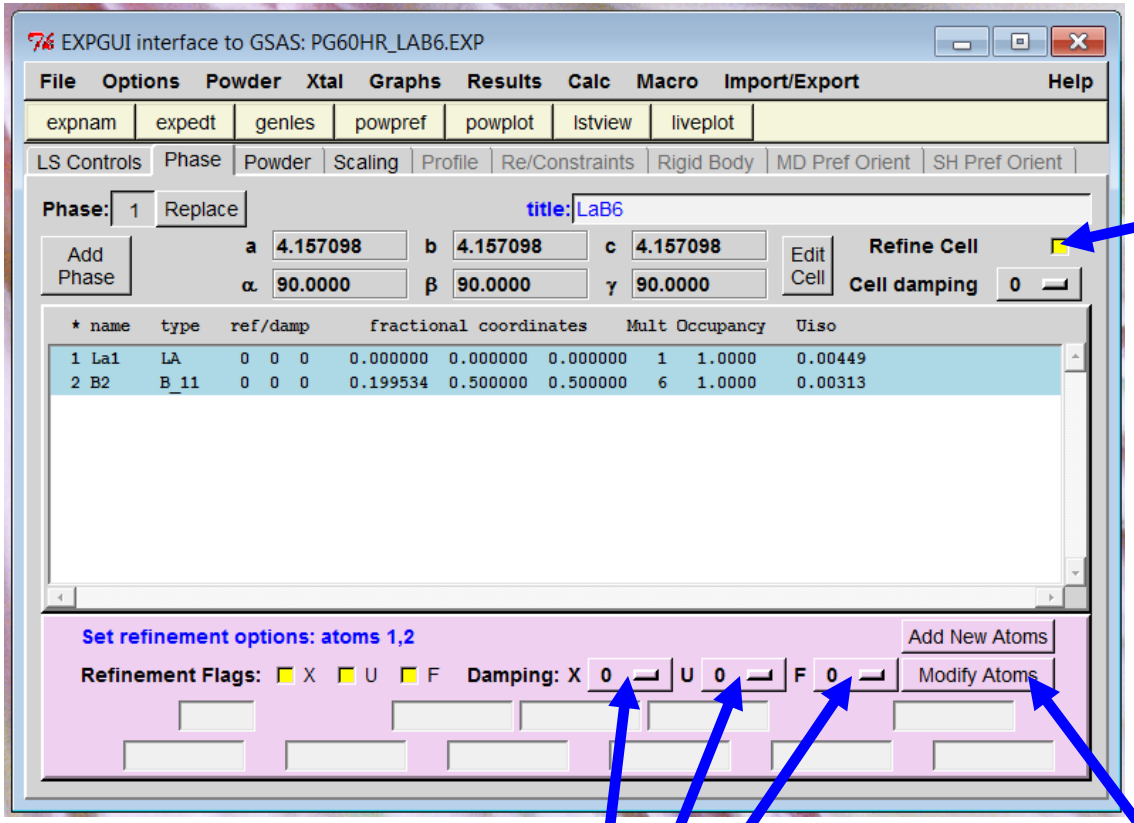




Click on "Add Atoms"

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

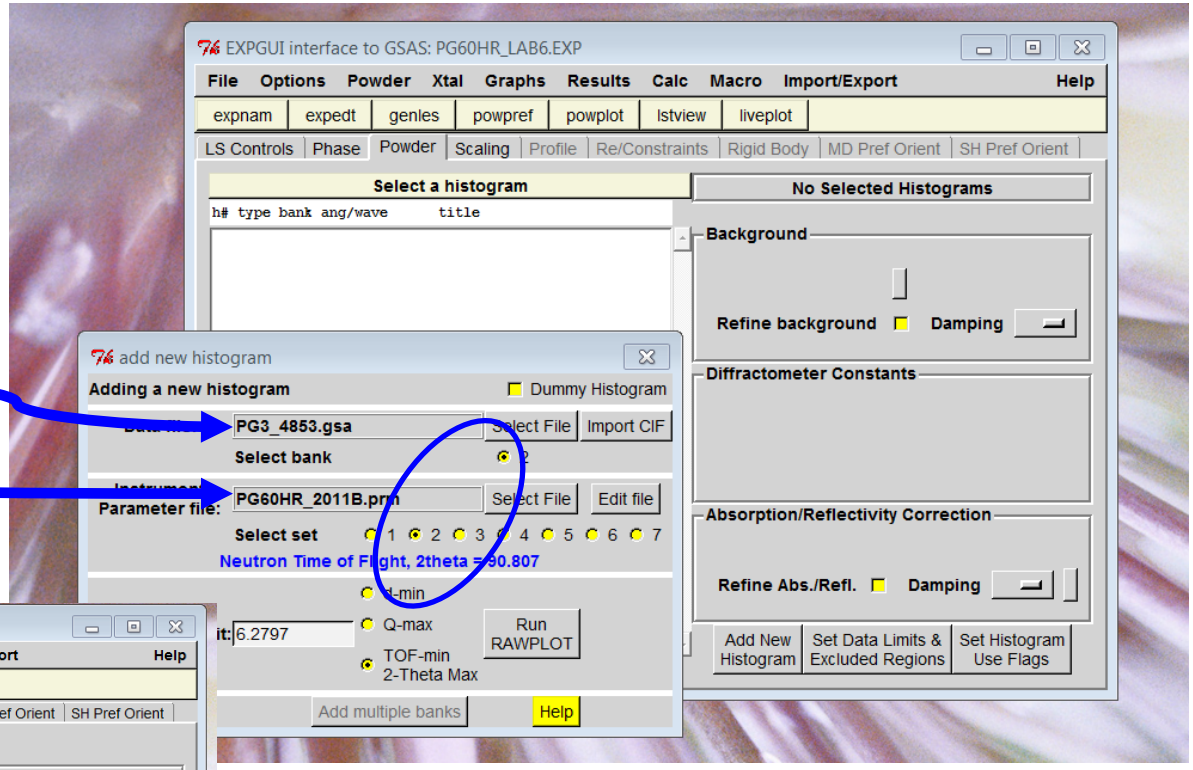
Allows you to set anisotropic thermal parameter

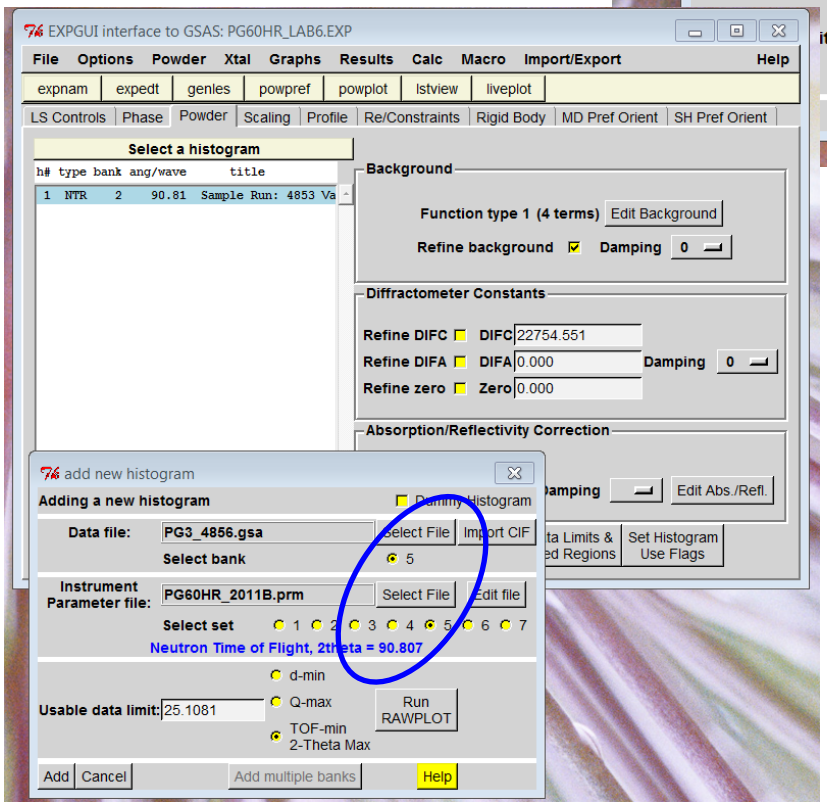
Select the Histogram Tab

Click on "Add New Histogram"

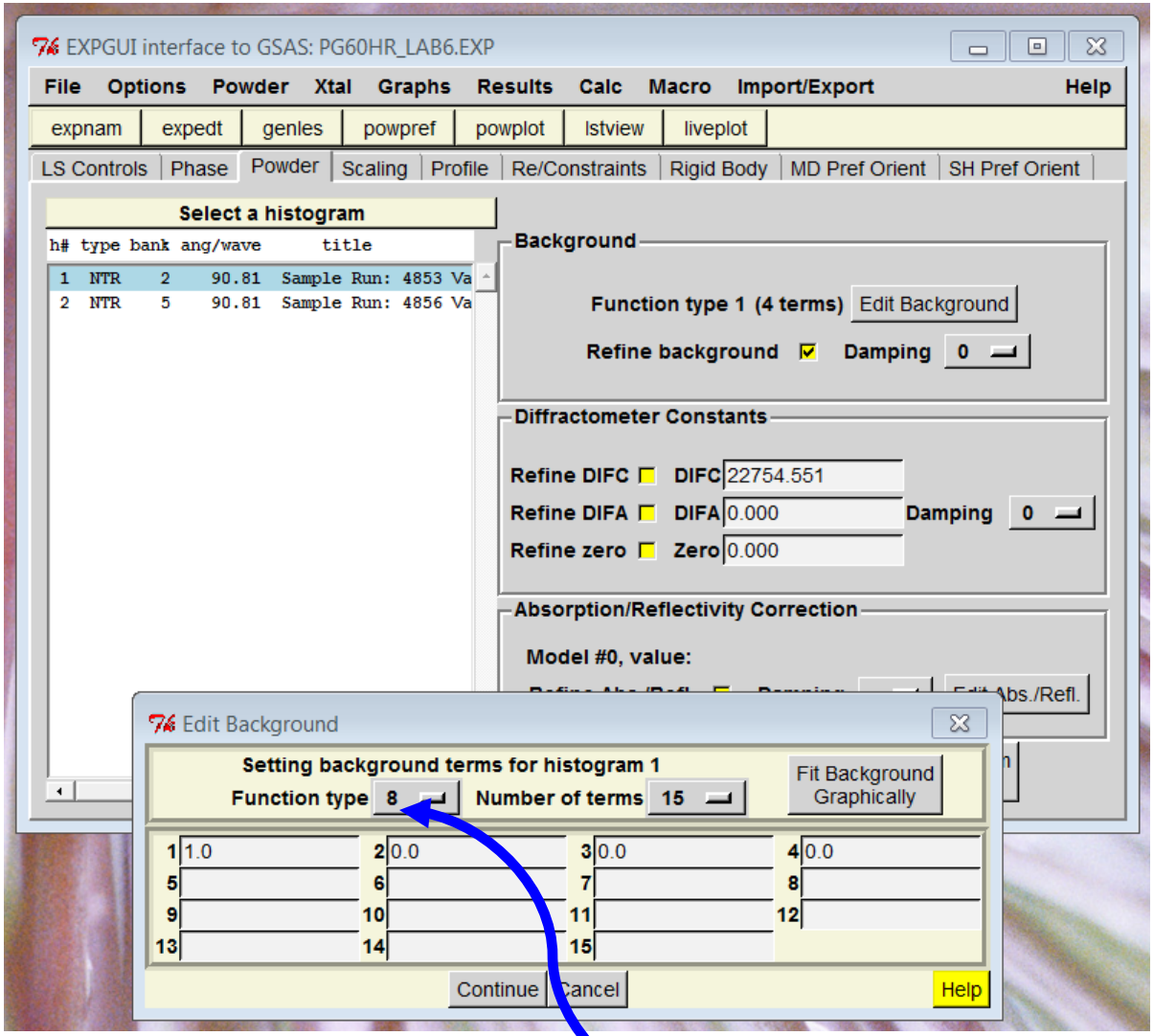
GSAS data file

Instrument parameter file

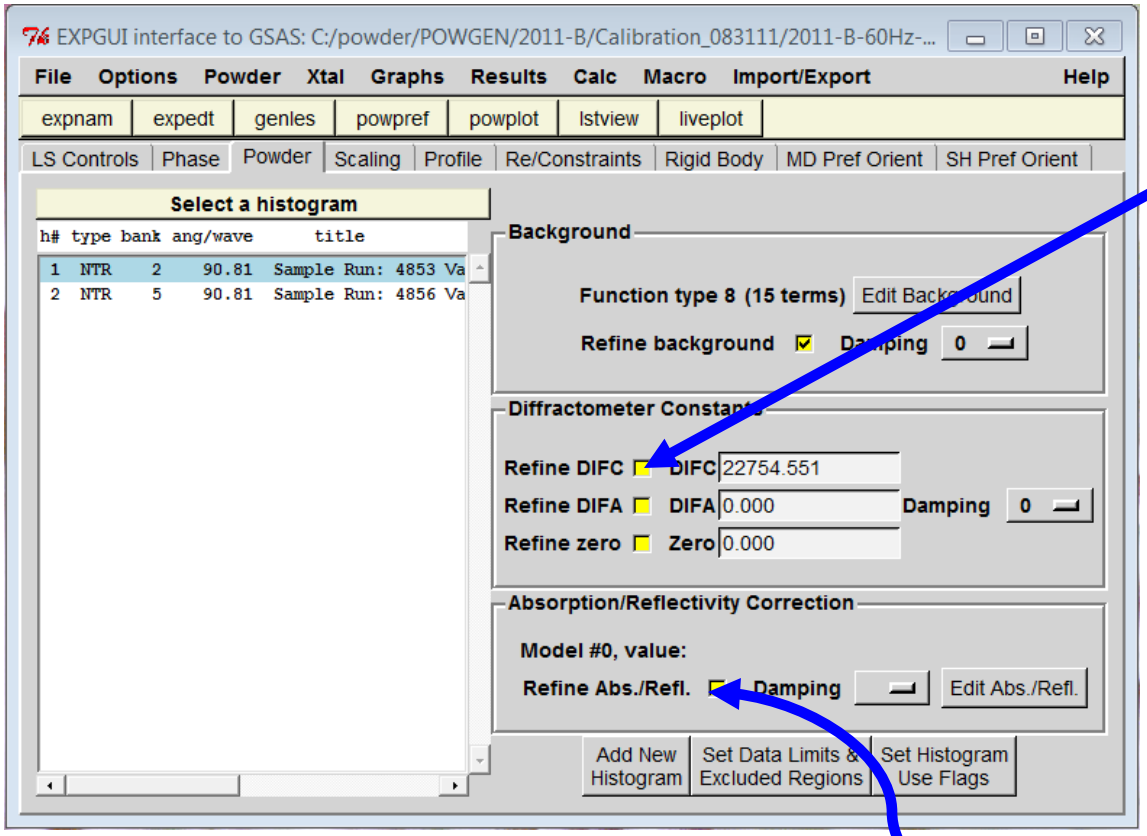




Add second histogram. Powgen histograms are dependent on the center wavelength used for data collection. Multiple histograms can be added for an individual refinement. Make sure the bank # in the parameter file matches up with bank number in data (.gsa) file as shown.



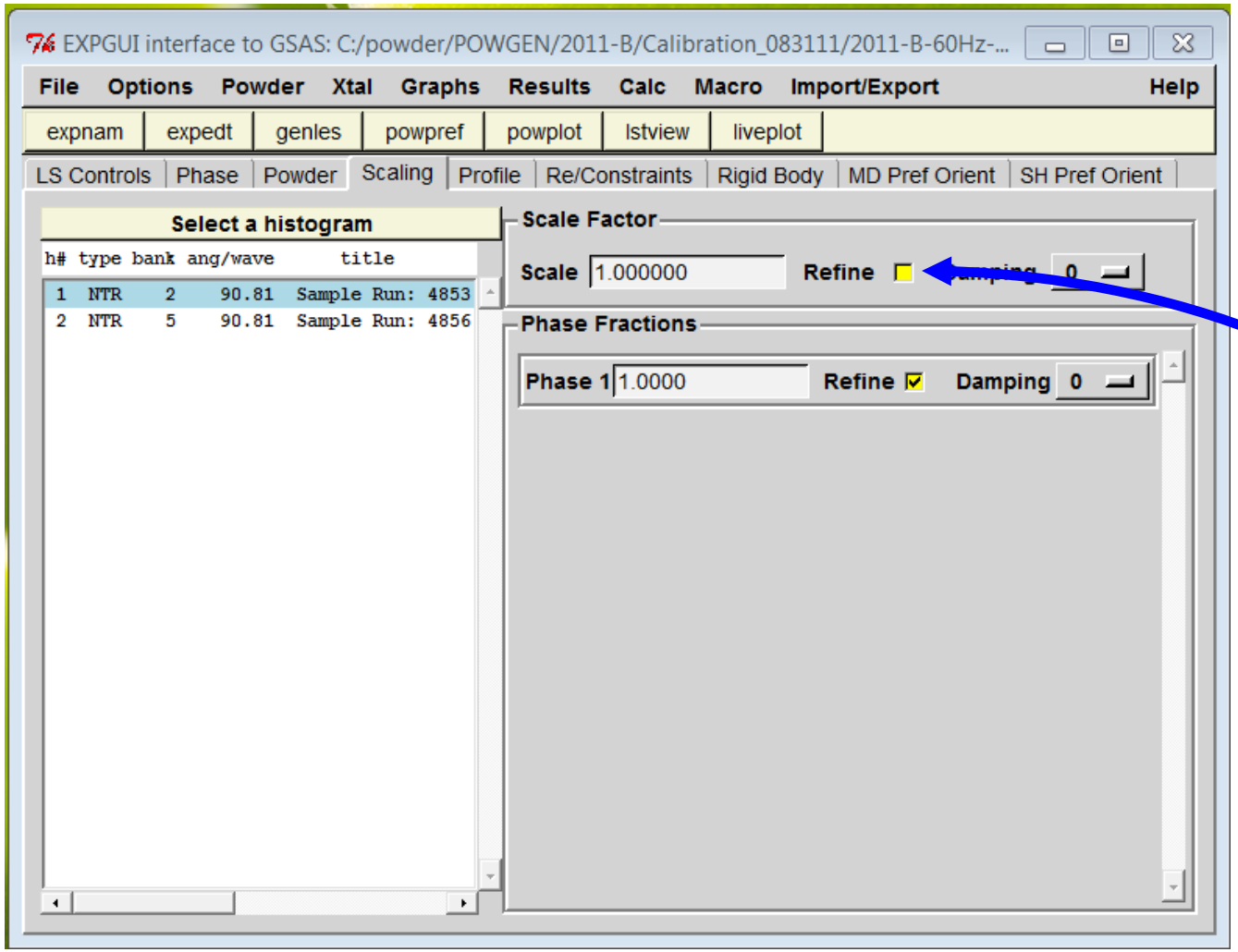
Default background function is set for BG function 1. BG function 8 is often works better for our data.



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.

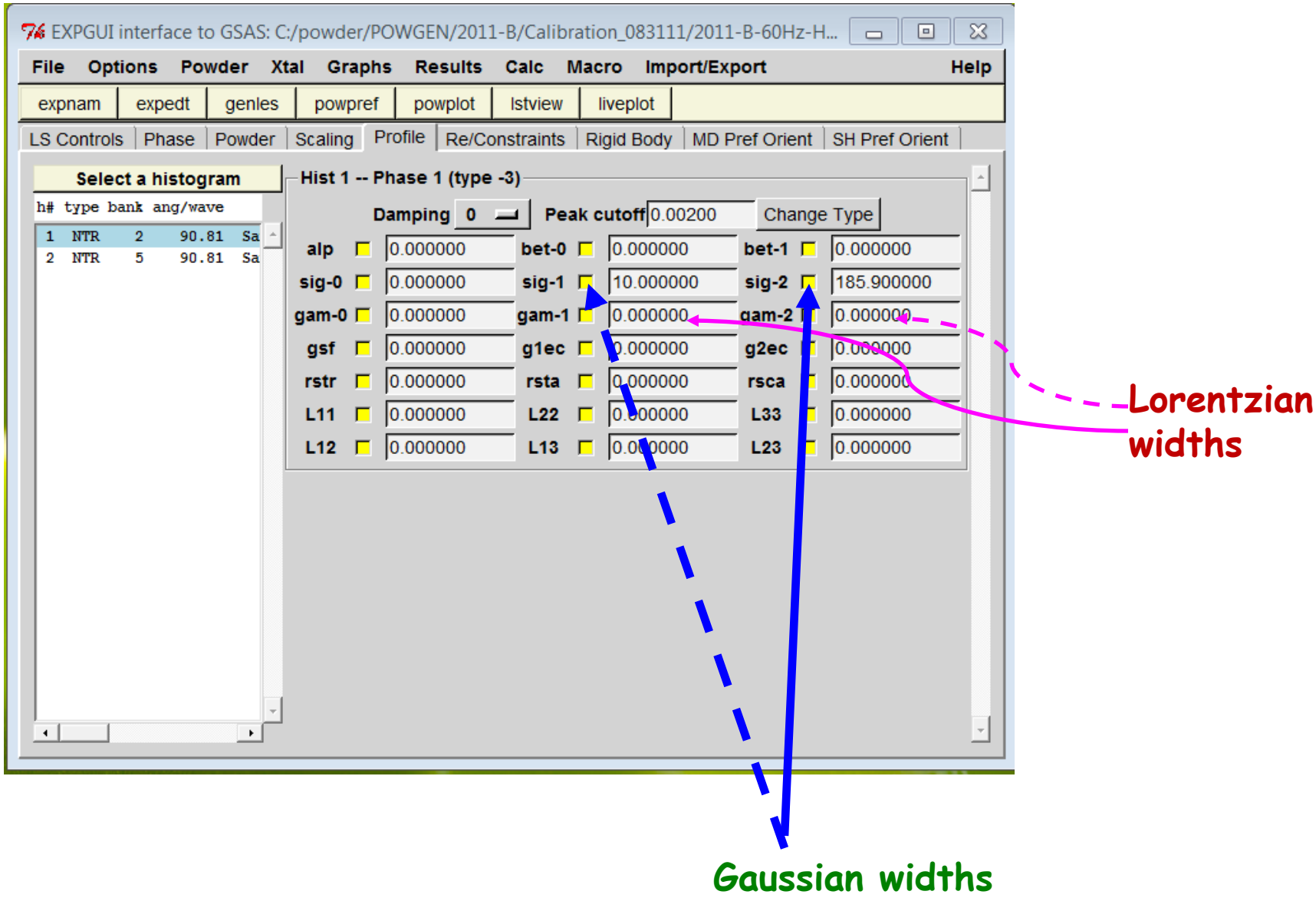
Quantitative Phase Analysis/scale factor

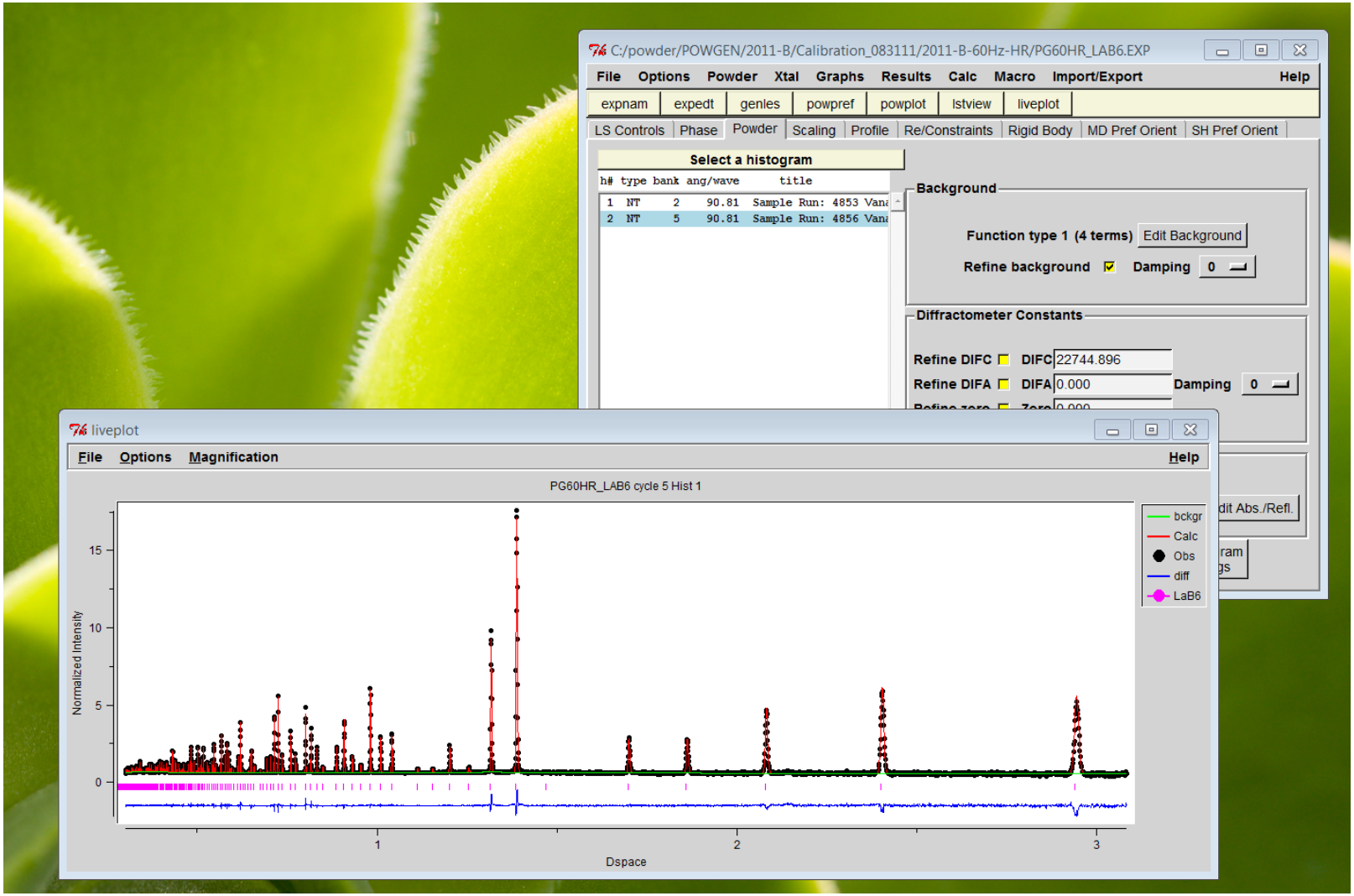


Remember to keep one of these fixed.

Refine the remaining scale factors.

Select Profile Tab





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

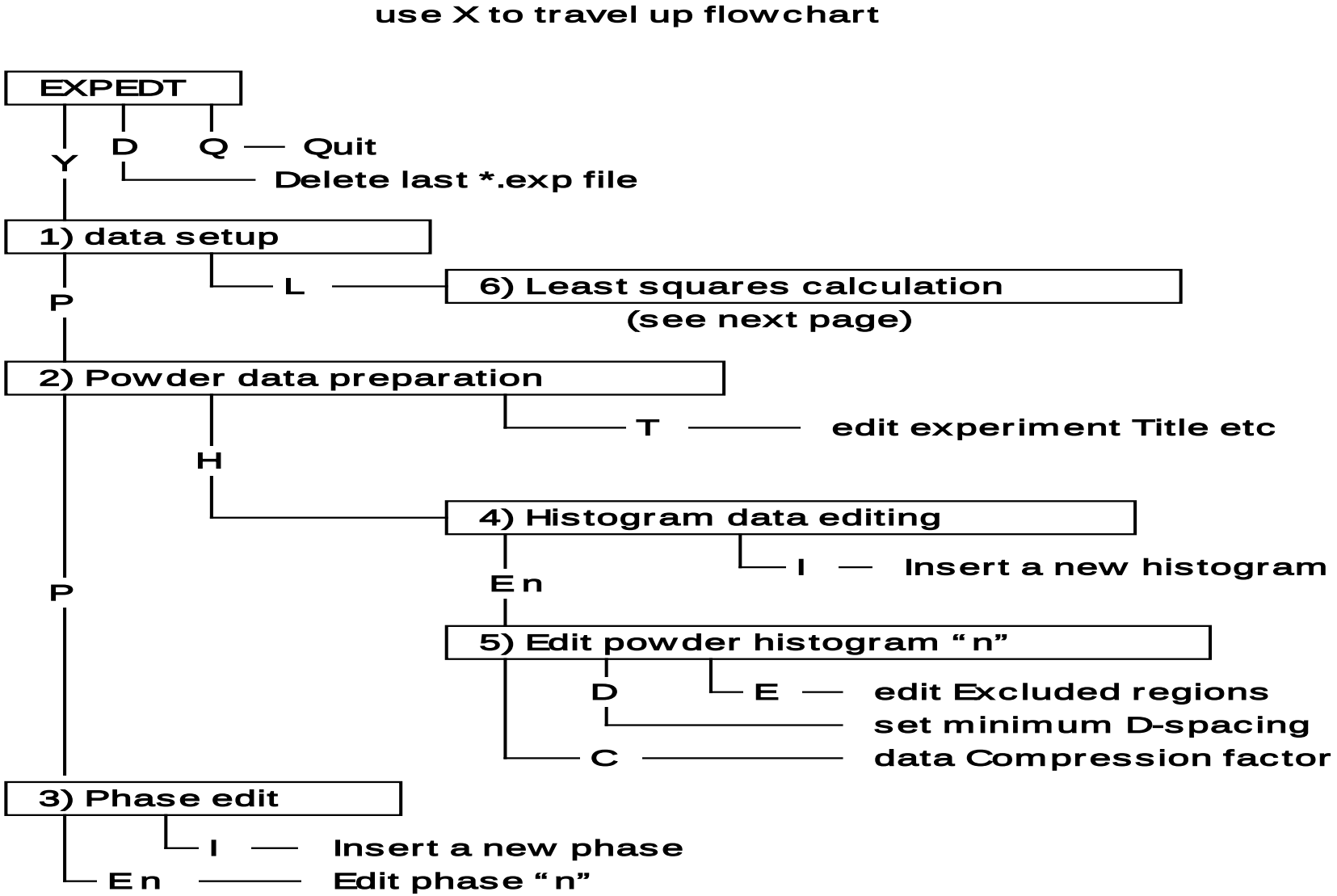
RESULTS

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

UTILITIES

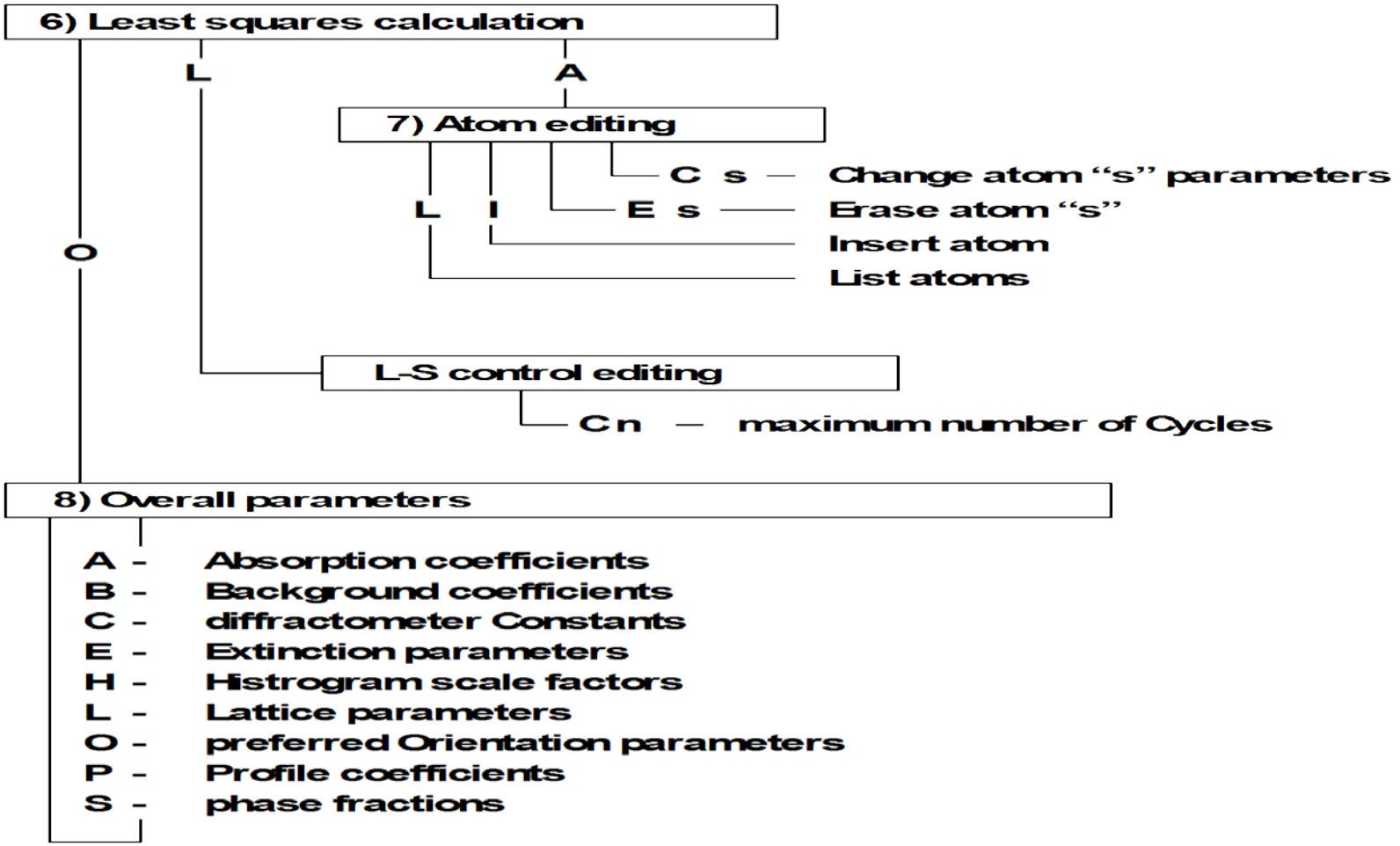
Rawplot - View Raw data
Hstdmp - Dumps observed and calculated intensity along with hkl values.
Reflist - Gives a list of reflections.

FLOWCHART for EXPEDT



FLOWCHART for EXPEDT (2)

use X to travel up flowchart



Extra info:

V to turn refinement flags on and off

D n to damp parameter refinement by n x 10%