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

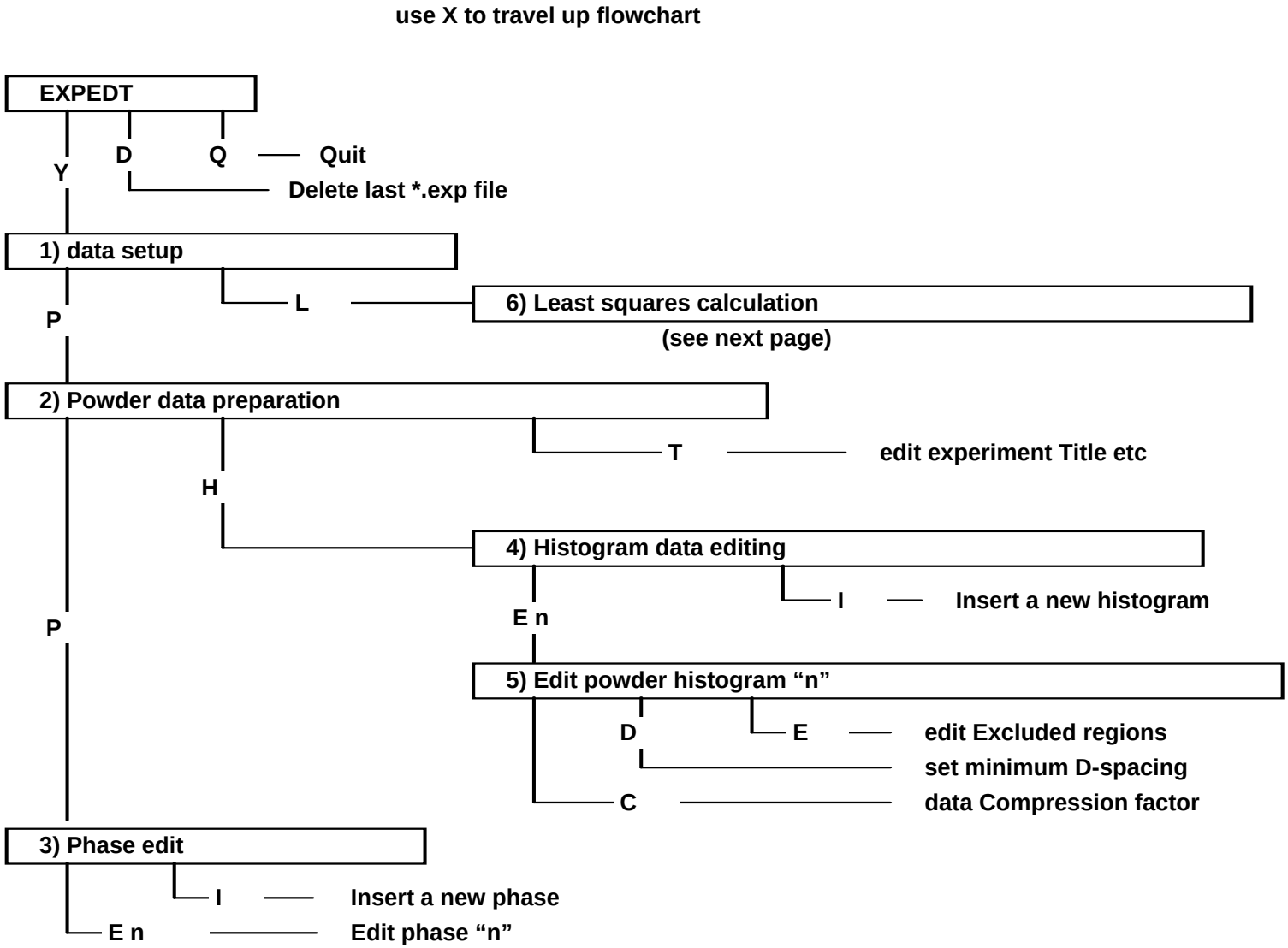
UTILITIES

Rawplot - View Raw data

Hstdmp - Dumps observed and calculated intensity along with hkl values.

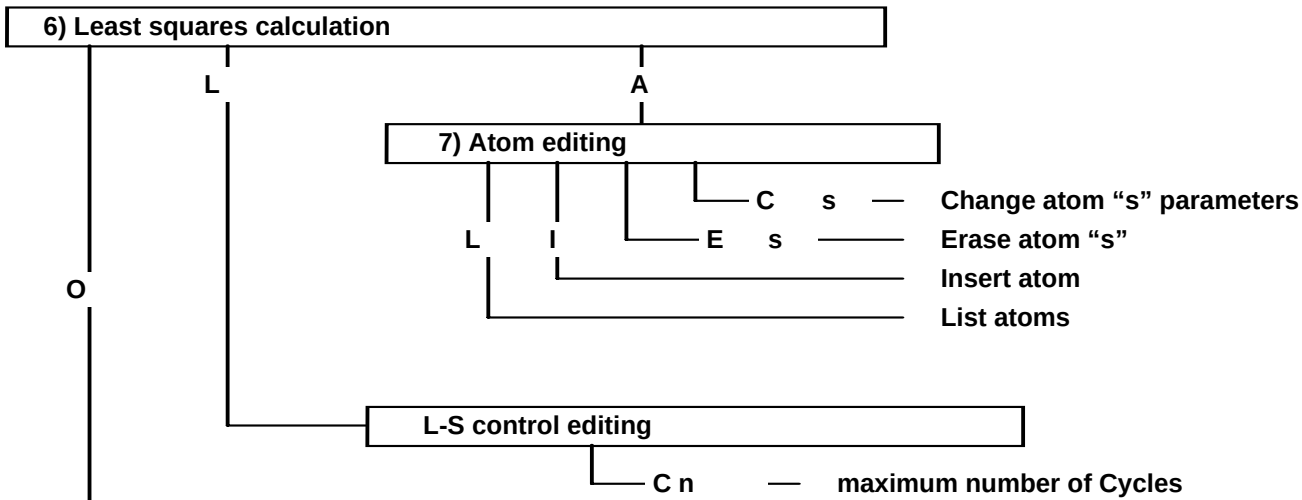
Reflist - Gives a list of reflections.

FLOWCHART for EXPEDT



FLOWCHART for EXPEDT (2)

use X to travel up flowchart



8) Overall parameters

- **A** - Absorption coefficients
- **B** - Background coefficients
- **C** - diffractometer Constants
- **E** - Extinction parameters
- **H** - Histrogram scale factors
- **L** - Lattice parameters
- **O** - preferred Orientation parameters
- **P** - Profile coefficients
- **S** - phase fractions

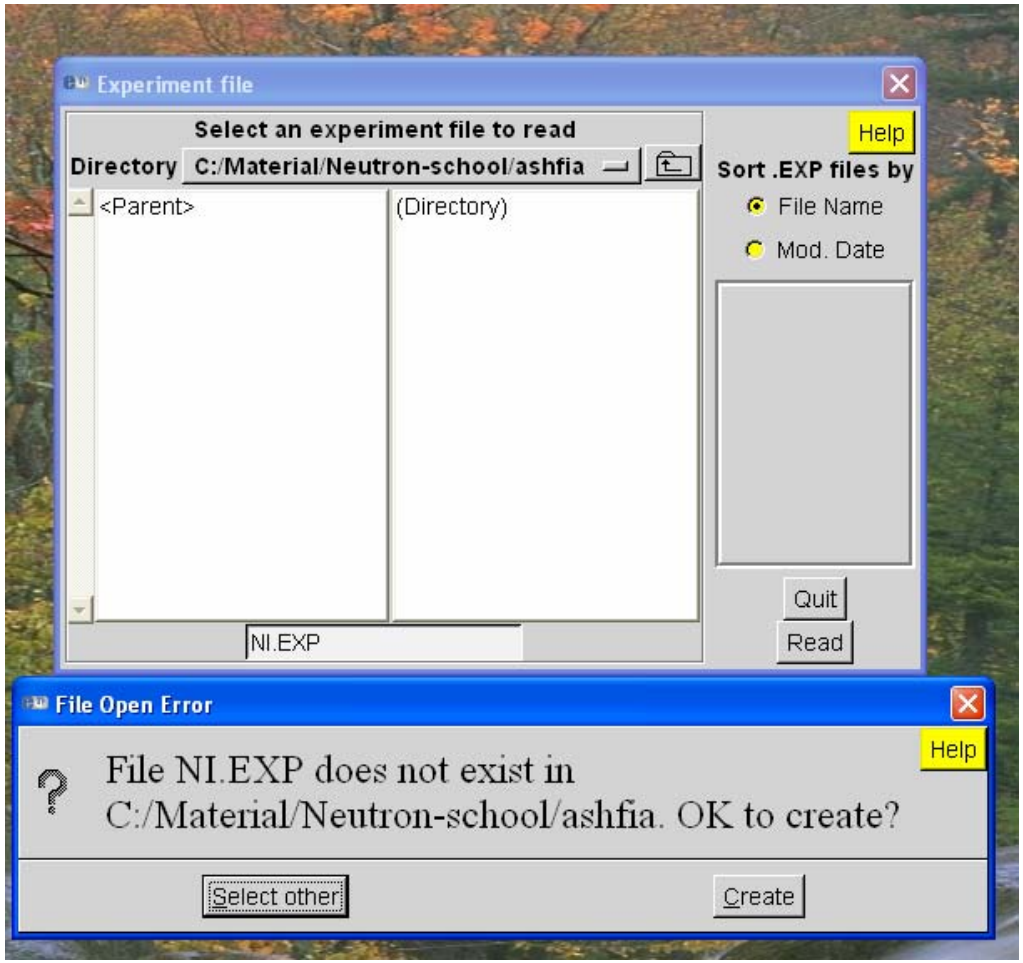
Extra info:

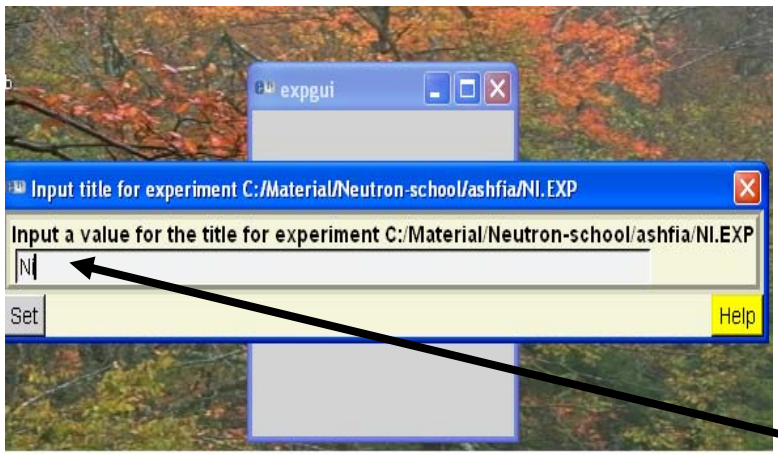
V to turn refinement flags on and off

D n to damp parameter refinement by n x 10%

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

- Run EXPGUI and go to the required directory and enter a new filename (in this case Ni) and press "read". When prompted, then press the "Create" icon.



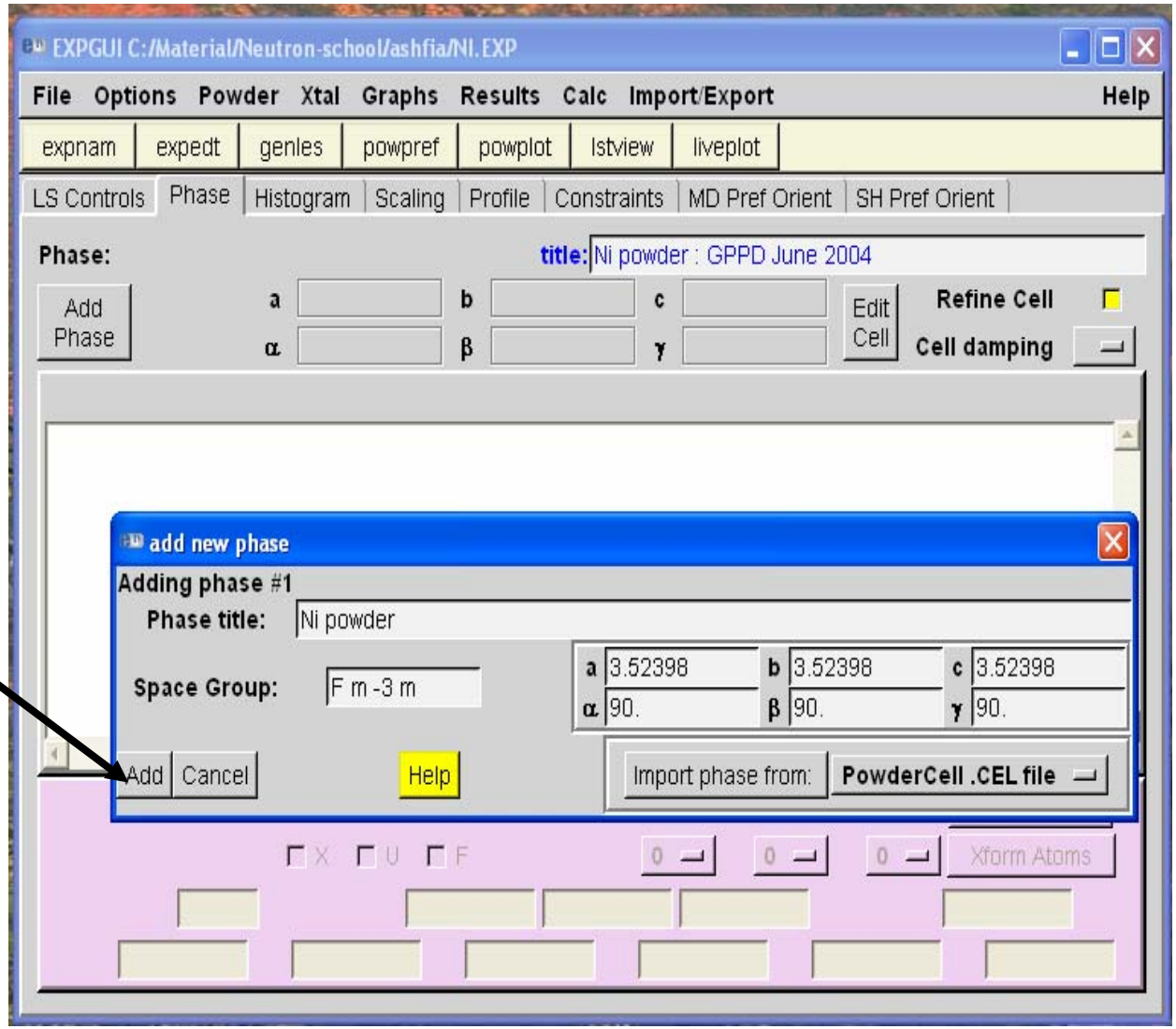


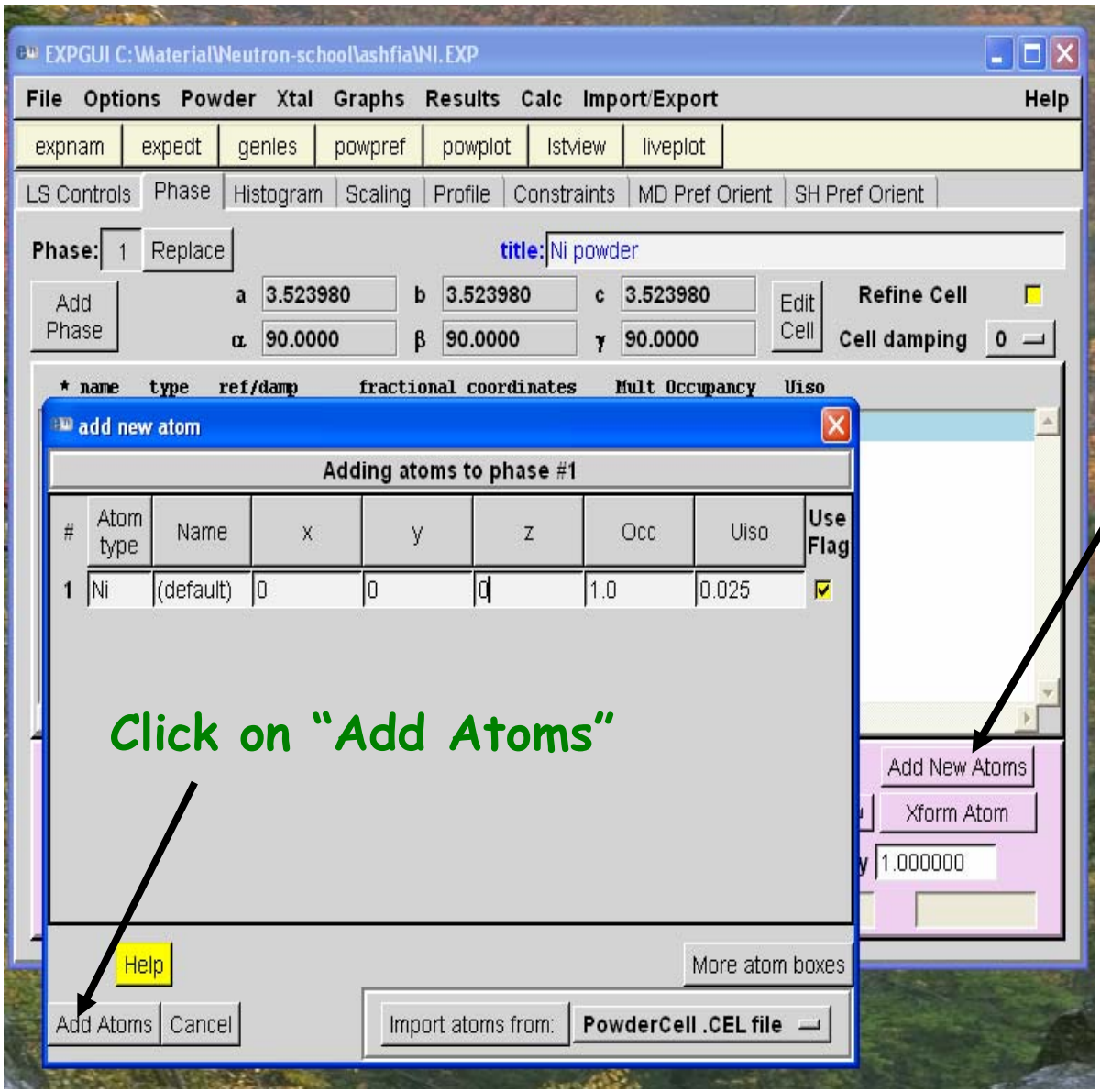
Experiment Title goes here

Select the Phase Tab

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

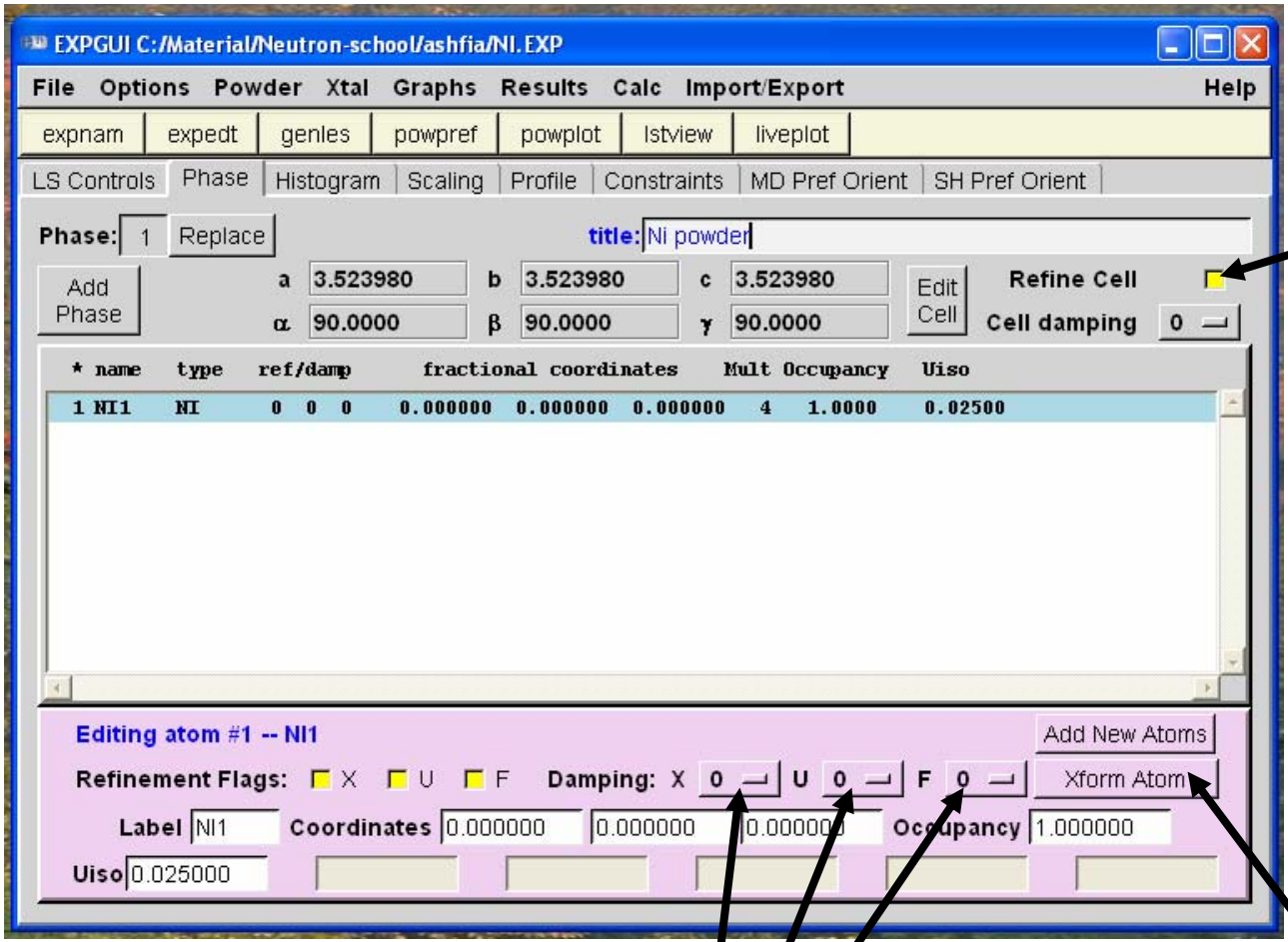
Click on "Add"





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

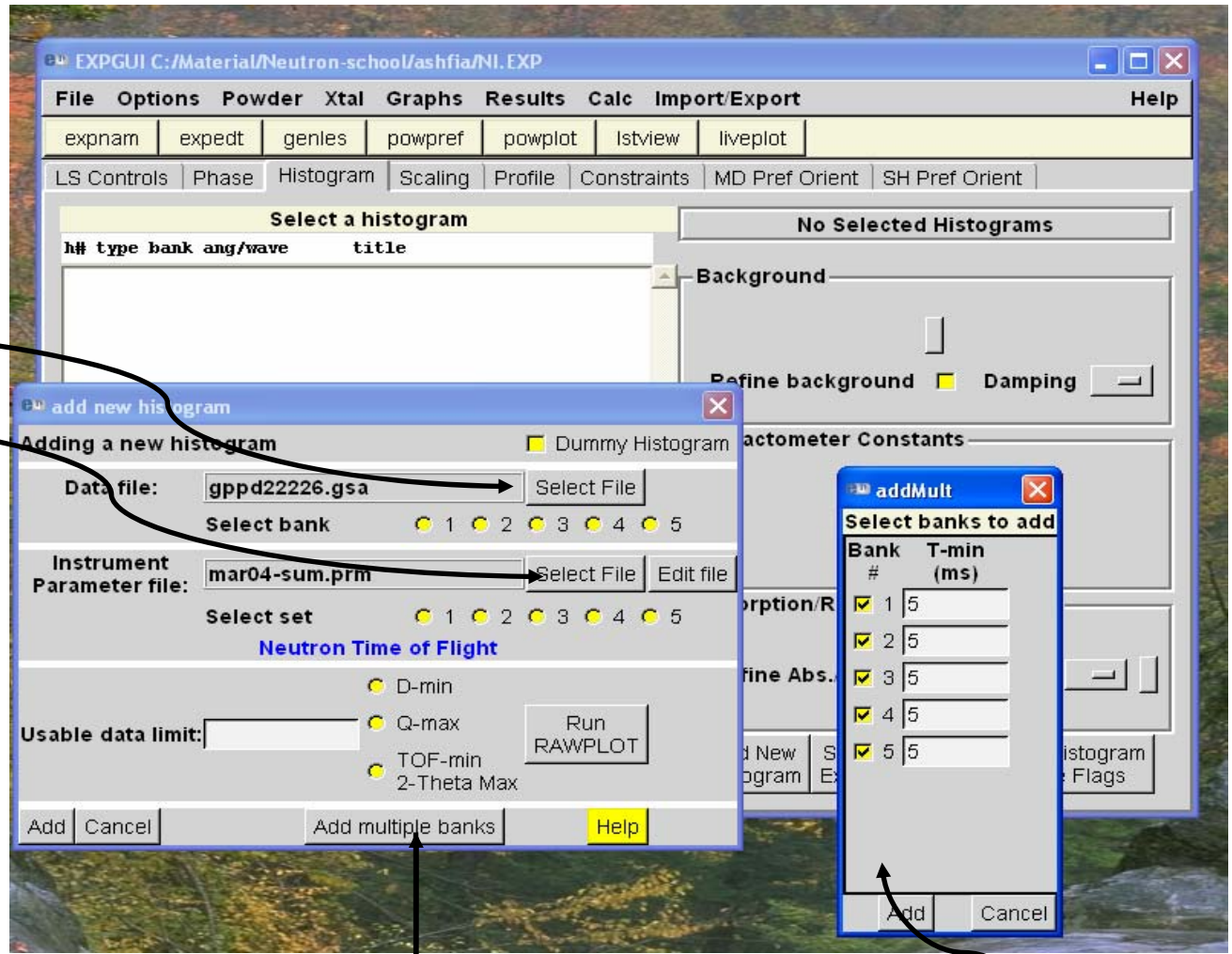
Allows you to set anisotropic
Thermal parameter

Select the Histogram Tab

Click on "Add New Histogram"

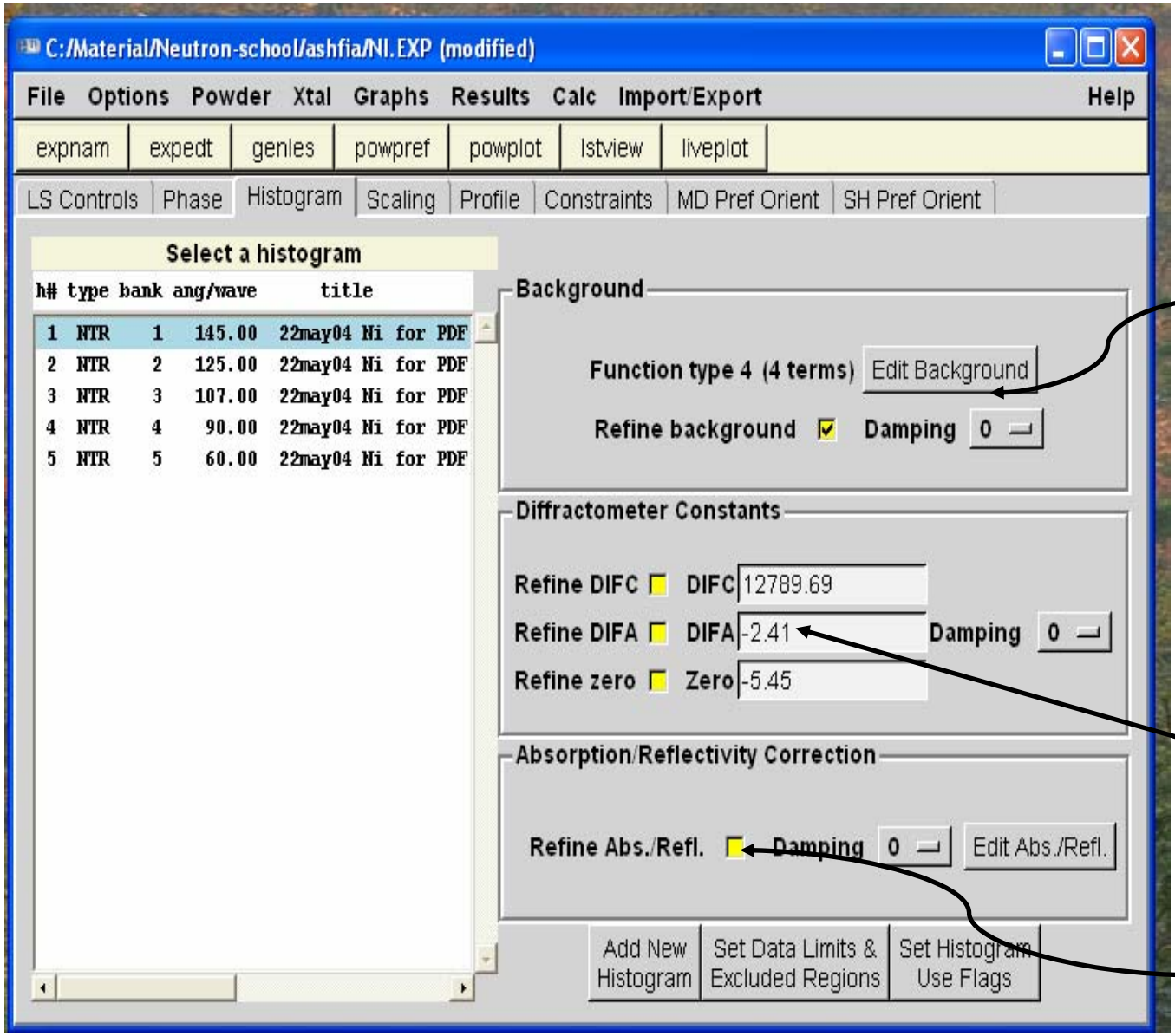
GSAS data file

Instrument parameter file



Use to add multiple banks

TOF min goes here



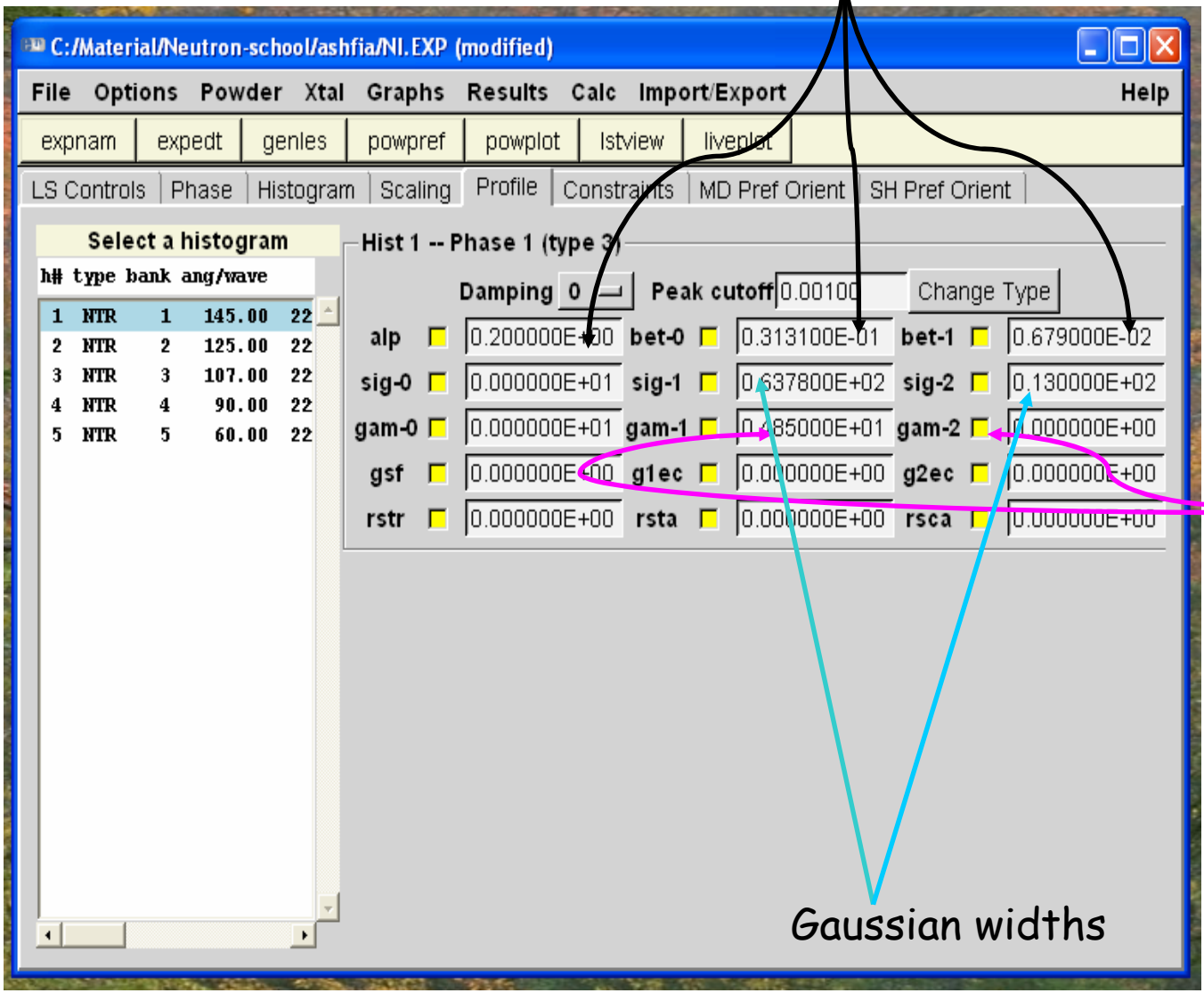
This parameter file is set for BG function 4. BG function 1 and 2 are also commonly used.

Diffractometer Constants set via Calibration.

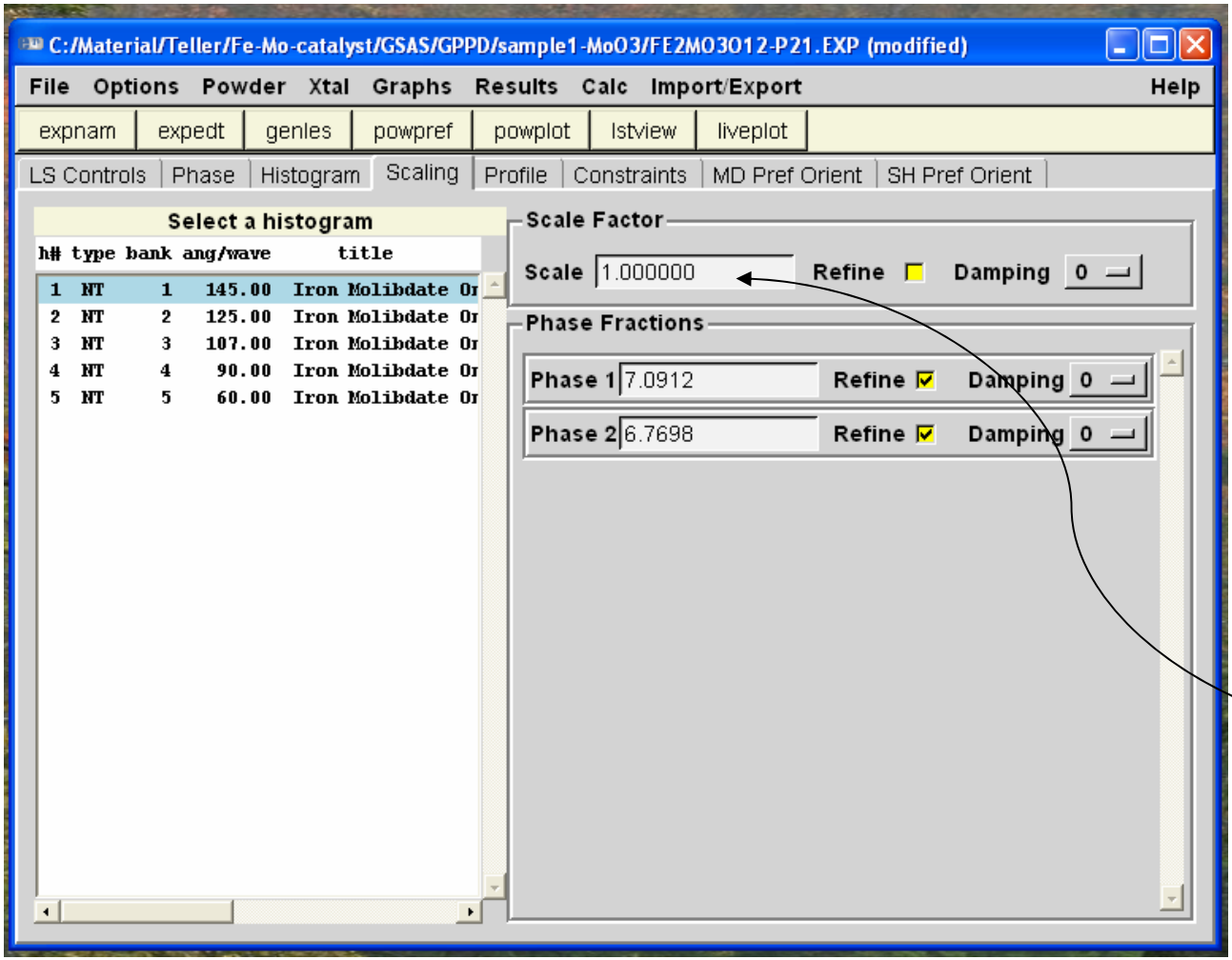
Absorption has to be refined often for TOF neutrons.

Select Profile Tab

You should not refine these

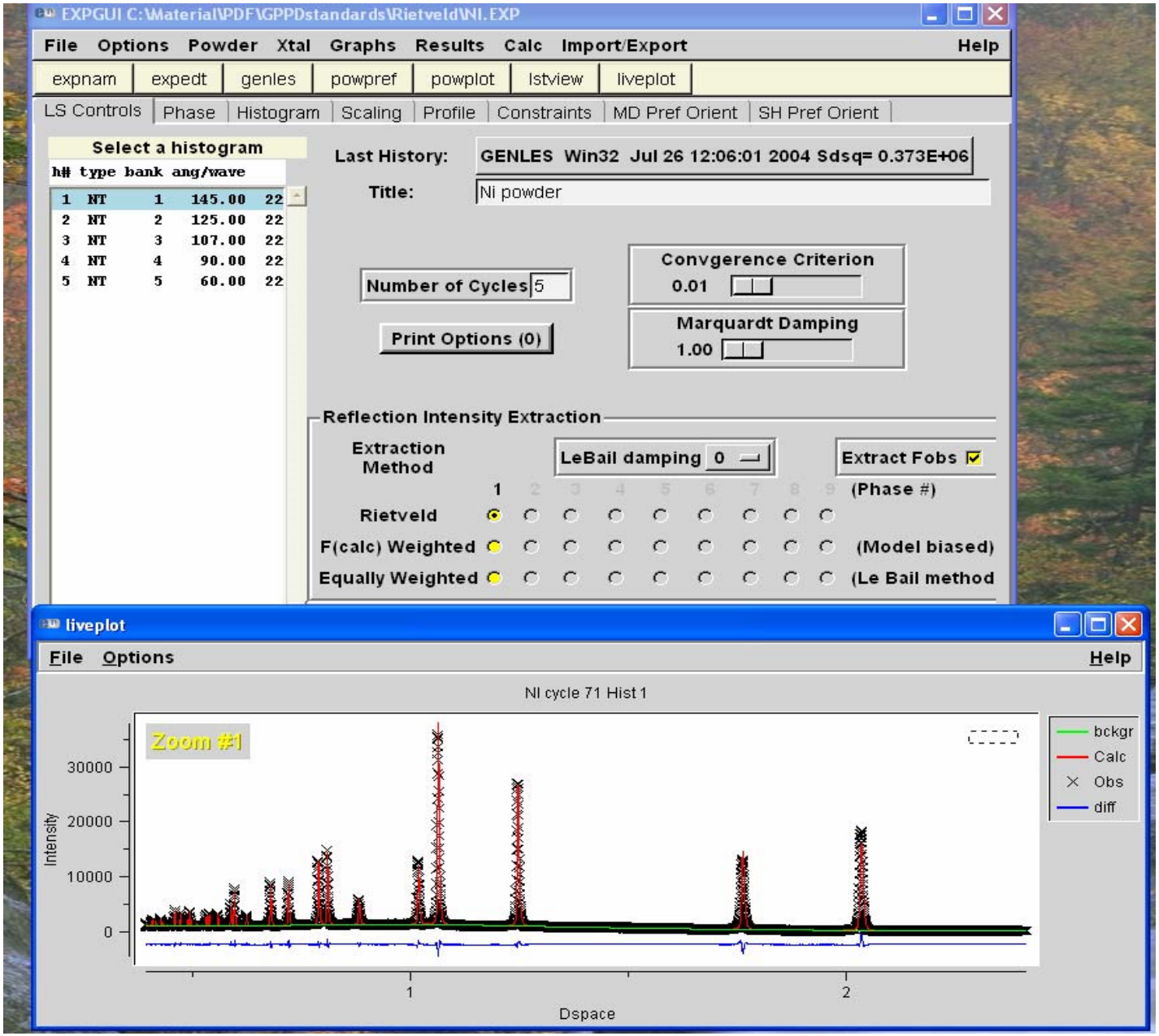


Quantitative Phase Analysis



Remember to keep one of these fixed.

Refine the remaining scale factors.



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

Some Useful Resources:

- Fullprof (packaged with Winplotr)
  http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm

- PC GSAS
  http://www.ccp14.ac.uk/ccp/ccp14/ftp-mirror/gsas/public/gsas/

- EXPGUI
  http://rrdjazz.nist.gov/programs/crystallography/software/expgui/expgui.html
  User friendly interface for Beginners to start using GSAS

- For a more exhaustive list check out
  http://www.ccp14.ac.uk/solution/rietveld_software /

- Rietveld Mailing List
  http://ccp14.sims.nrc.ca/ccp/ccp14/ftp-mirror/howardflack/pub/soft/crystal/stxnews/riet/welcome.htm