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



74 Input title for experiment PG60HR_LAB6.EXP Σ						
Input a value for the title for experiment PG60HR_LAB6.EXP						
LaB6 Powgen 2011-B High Resolution						
Continue	Help					

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.

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Help More atom boxes
Adr Homs Cancel Import atoms from: GSAS .EXP file

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



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

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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

74 EXPGUI interface to GSAS: C:/powder/POWGEN/2011-B/Calibration_083111/2011-B-60Hz 🗖 🔳 🔀	
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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
Dist	-	delete *.lst file
Exit	-	

RESULTS

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

COMPUTE

- Powpref powder data preparation
- Genles general least squares

GRAPHICS

Powplot - powder pattern plotting



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
- D n to damp parameter refinement by $n \ge 10\%$