



**An Overview of GSAS and EXPGUI**

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**Outline**

- What are GSAS & EXPGUI
- Why use them?
- What does GSAS do?
- History & contents of GSAS
- What does EXPGUI do?
- An overview of EXPGUI windows
- EXPGUI utilities & other features



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**What is GSAS?**

**GSAS** (General Structure and Analysis System)

- Software package for fitting atomic structural models ("crystal structures") to single crystal and powder diffraction data.
- Use virtually any type of neutron or x-ray diffraction data as input
- Wide range of constraints and other features useful for complex problems.
- GSAS includes a number of plotting and utility tools.
- GSAS runs on Windows, Linux and Macintosh.



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**What is EXPGUI?**

**EXPGUI** is a graphical user interface to GSAS.

- Intuitive access to only a small range of the GSAS capabilities,
  - much of what is needed for Rietveld analysis
  - Full range of GSAS capabilities still available through command-line type (EXPEDT) interface.
- EXPGUI also provides many useful utilities for viewing fits and refinement results.
- Distributions of EXPGUI include GSAS to simplify installation
- Available for Windows, Linux and Macintosh.



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## Why use GSAS?

**There are many Rietveld packages available.**  
**GSAS (with EXPGUI), FULLPROF & TOPAS have the widest usage**

DANSE survey of Rietveld users (140 people):

- GSAS: 75% (94 of 105 use EXPGUI)
- FULLPROF: 39%
- Only 10% do not use either GSAS or FULLPROF
  - Distribution of respondents:
    - US: 26%
    - UK: 16%
    - France: 9%, Germany: 8%, Italy: 9% (Europe: 34%)

## What does GSAS do?

- GSAS supports all types of x-ray & neutron crystallography instruments
  - TOF & CW neutron
  - Lab & synchrotron & energy dispersive x-ray
  - X-ray & neutron single crystal
- GSAS has special features not found in most packages:
  - Rigid bodies, distance & compositional constraints
  - Several profile & preferred orientation functions
  - Protein refinements
- Supported: Bugs get fixed (usually quickly)

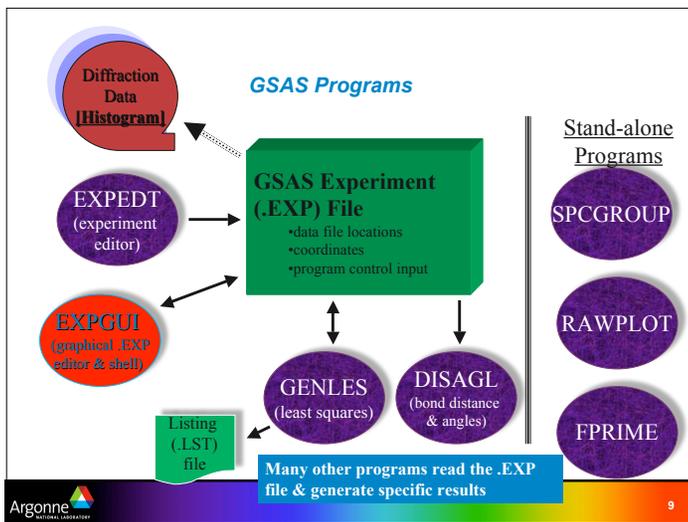
## Terminology

- GSAS uses Histogram to mean a collection of observations: a data set
- Q (momentum transfer):
  - The preferred unit for diffraction “angles”  
 $Q = 2\pi/d = 4\pi \sin\theta/\lambda$   
big Q => “high angle”  
can be used to compare data from different sources

## GSAS: capsule history

- GSAS – conceived in 1982- 1983
  - by A. C. Larson & R. B. Von Dreele
- 1st version released in Dec. 1985
  - Only TOF neutrons (& buggy)
  - Designed to run only on VAX computers
    - later for SGI, then MS-DOS (now windows) & then LINUX
      - (At one time ULTRIX & HP Unix versions existed)
    - 2003 ported to Mac OS X
- Designed from the start for:
  - multiple datasets & multiple phases
  - single crystal & TOF powder
- Later – CW neutron & CW x- ray powder data
- Basic structure & user interface is essentially unchanged from 1980's





### Core GSAS programs

- Use EXPEDT to set up Experiment file
  - (or EXPGUI, to be covered later)
- Use POWPREF to map reflections to data
- Use GENLES to compute pattern/refine

rerun POWPREF when reflection positions must be updated, due to changes in:

- cell parameters/zero correction
- profile/sample displacement
- data range
- phases or data sets are added

### Partial list of other GSAS programs

- POWPLOT: plot observed vs. computed pattern
- FOURIER, FORSRH, FORPLOT: compute Fourier map, find peaks & plot
- BIJCALC: analyze anisotropic displacement parameters
- ORTEP, VRSTPLOT: plot structures
- DISAGL: distances & angles
- HSTDUMP, TCLDUMP, REFLIST: list powder & reflection intensities
- PUBTABLE: tabulate results
- GSAS2CIF: create CIF's with results (rewritten!)
- RCALC: compute reflection R-factors (RF & RF2)
- GEOMETRY: compute from fitted parameters: Rigid bodies, L-S planes, error estimates on parameter sums.
- PC-GSAS: a windows program used to invoke other GSAS programs.  
 N.B. also possible to use right-click on .EXP files

### Stand-Alone GSAS programs

- RAWPLOT: plot observed data
- FPRIME: compute anomalous dispersion ( $f'$  &  $f''$  vs  $\lambda$ )
- SPCGROUP: space group info, including magnetic operations

## Powder Diffraction Data files for GSAS

Two input data files are needed:

- Raw **Histogram** (contains intensities & optionally  $2\theta$ , etc. or s.u.)
  - **Instrument parameter** file: defines data type ( $\lambda$ , x-ray/neutron, expected profile, ...). (create/edit with INSTEDIT in EXPGUI)
- GSAS has many different **histogram** formats (see manual!)
    - GSAS is pretty picky on data formatting
  - Instrument parameter files are tricky to make
    - needed only when data are added initially or plotted
    - try to use an example or get one for your instrument
    - EXPGUI can create/edit them!
  - Input files must be 80 chars/line + CR + LF (82/line)
    - GSAS will usually fix this
    - EXPGUI will always fix this



## EXPGUI, a graphical user interface for GSAS

Note that EXPGUI is a separate "add-on" for GSAS (Different author). GSAS works fine without EXPGUI.



## Obtaining EXPGUI

- Documentation
  - <http://www.ncnr.nist.gov/xtal/software/expgui/expgui.html>
  - Please read the installation and customization pages
- Tutorials (following tutorials in GSAS manual, but using EXPGUI)
  - Alumina (CW Neutron): <http://www.ncnr.nist.gov/xtal/software/expgui/tutorial3>
  - Nickel (TOF): <http://www.ncnr.nist.gov/xtal/software/expgui/tutorial1>
  - Garnet (CW Neutron): <http://www.ncnr.nist.gov/xtal/software/expgui/tutorial2>
- Mailing List
  - I keep a mailing list notice of updates & discussion of new features. The mailing list is inactive at present, but may be resumed. E-mail [Brian.Toby@ANL.gov](mailto:Brian.Toby@ANL.gov) to join.
- Distributions
  - See <http://www.ncnr.nist.gov/xtal/software/downloads.html>

## A Tour of EXPGUI

- EXPGUI is a "shell" that is used to call the various GSAS programs
  - Configurable (you can change menus & buttons -- see web pages)



## Least squares controls



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## Phase and atom parameters



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## Diffraction Data (Histogram) Parameters



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## Histogram parameter submenus



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## Phase & Histogram Scaling

home/toby/test/INRS.EXP

File Options Powder Xtal Graphs Results Calc Import/Export Help

expnam expedit genles powpref powplot lstview liveplot

LS Controls Phase Histogram Scaling Profile

Scale Factor: 43.353 Refine  Damping 0

Phase Fractions

Phase 1 fraction: 0.50010 Refine  Damping 0

Phase 2 fraction: 0.49990 Refine  Damping 0

hi	type	bank	ang/wave	title
1	NT	3	1.88.29	0001021 SI/N
2	NT	2	88.05	0001021 SI/N

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## Profile terms

EXPGUI TBO02ASYM1.EXP

File Options Powder Xtal Graphs Results Calc Import/Export Help

expnam expedit genles powpref powplot lstview liveplot leBall

LS Controls Phase Histogram Scaling Profile Constraints MD Pref Orient

Select a histogram

Hist 3 -- Phase 1 (type 3)

Damping 9 Peak cutoff 0.00500 Change Type

GU 0.236374E+03 GV -0.283195E+00 GW 0.167512E+03

GP 0.000000E+00 LX 0.000000E+00 LY 0.000000E+00

SL 0.225327E-01 HL 0.126677E-01 trms 0.000000E+00

shft 0.000000E+00 stec 0.000000E+00 ptec 0.000000E+00

slcc 0.000000E+00

Change Profile Function

Change profile function for Histogram #1 Phase #1

Current function is type 1.

Set function to type 1

lbl	ref	next value	default	current	lbl	ref	next value	default	current
GU	354.03	354.03	354.27	F1	0.0	0.0	0.0	0.0	0.0
GV	-760.40	-760.40	-722.60	F2	0.0	0.0	0.0	0.0	0.0
GW	651.59	651.59	646.09	Peak Cutoff	0.01	0.01	0.01	0.01	0.01
asym	0.0	0.0	0.0						

Set Quit Help

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## Atom/Profile Constraints

lsnr/people/toby/testdata/CONSTB.EXP

File Options Powder Xtal Graphs Results Calc Import/Export Help

expnam expedit genles powpref powplot lstview liveplot leBall

LS Controls Phase Histogram Scaling Profile Constraints

#	Phase	Atom(s)	Variable	Multiplier	Atom(s)	Variable	Multiplier	Delete	
1	edit	1	2,3	UI50	x 1.0000			<input type="checkbox"/>	
2	edit	1	4,5	UI50	x 1.0000			<input type="checkbox"/>	
3	edit	1	3	FRAC	x -1.0000	2	FRAC	x 1.0000	<input type="checkbox"/>
4	edit	1	5	FRAC	x -1.0000	4	FRAC	x 1.0000	<input type="checkbox"/>
5	edit	1	ALL	UI50	x 1.0000			<input type="checkbox"/>	
6	edit	1	1-6	X	x 1.0000			<input type="checkbox"/>	
7	edit	1	1,1	U22	x 1.0000			<input type="checkbox"/>	
8	edit	1	1	U33	x 0.1000	2	U33	x 0.2000	<input type="checkbox"/>
		3	U33	x 0.3000	4	U33	x 0.4000	<input type="checkbox"/>	
		5	U33	x 0.5000	6	U33	x 0.6000	<input type="checkbox"/>	
		1	U33	x 0.7000				<input type="checkbox"/>	

New Constraint Delete

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## Preferred Orientation: March-Dollase

lsnr/people/toby/testdata/GARNET.EXP (modified)

File Options Powder Xtal Graphs Results Calc Import/Export Help

expnam expedit genles powpref powplot lstview liveplot leBall

LS Controls Phase Histogram Scaling Profile Constraints MD Pref Orient

March-Dollase Preferential Orientation

Phase	h	k	l	Ratio	Fraction	Damping
axis 1	1.00	1.00	1.00	1.000000	1.000000	0
axis 2	0.00	0.00	1.00	1.000000	1.000000	0

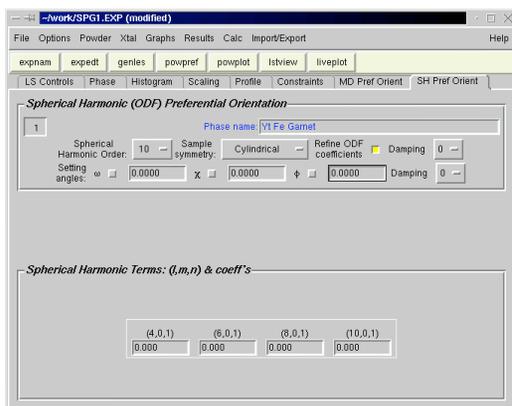
March-Dollase Preferential Orientation

Phase	h	k	l	Ratio	Damping
axis 1	1.00	1.00	1.00	1.000000	0

Where possible, EXPGUI hides irrelevant parameters. For example, Fraction is needed only with 2 or more M-D axes.

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## Preferred Orientation: Spherical Harmonics



## EXPGUI design features

- Unlike EXPEDT, edits are made in memory
  - file is not changed until File/Save is used (or a GSAS program is run)
- Invalid values are highlighted in red and are not saved

a	20.127581	b	19.949886	c	13.431625
$\alpha$	90.0000	$\beta$	90.0000	$\gamma$	90.0000

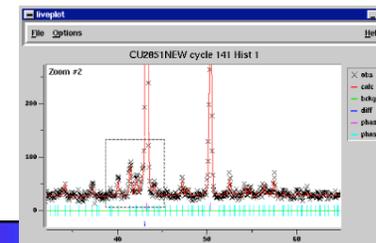
## EXPGUI Utilities

### Programs that add features not in GSAS.

- LIVEPLOT
  - Plot fit
- BKGEDIT
  - Manual background fit
- EXCLEDT
  - Edit data range & excluded regions
- Import/Export routines
  - GSAS2CIF
  - Import & write coordinates in multiple formats
- WIDPLT
  - Plot peak widths vs  $2\theta$
- LSTVIEW
  - Examine GSAS output listing (.LST file)
- FillTemplate & CIFSelect
  - Add descriptive info to CIF
  - Select publication flag for distances & angles
- INSTEDIT
  - edit instrument parameter files

## LIVEPLOT

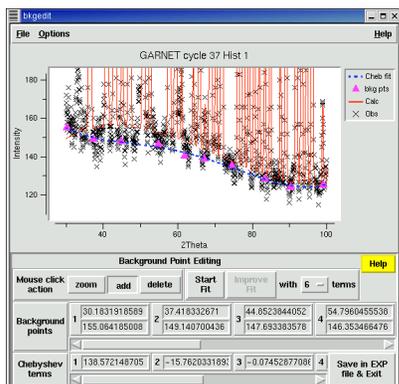
- “Zoomable” plot of obs/calc/bkg/diff
- tickmarks, label with  $hkl$  labels
- Optional: overlay with unit cell or ICDD entry
- Export to GRACE & .csv
- (obs-calc)/ $\sigma$
- Cumulative  $\chi^2$
- Shortcuts keys



## BKGEDIT

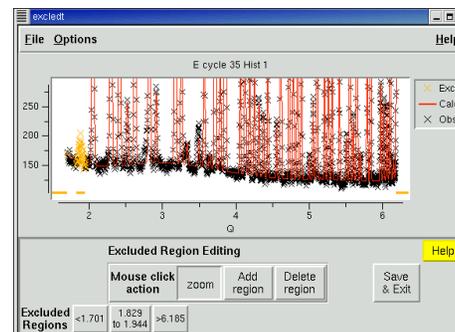
Background can be hard to fit, particularly when the structure is poorly modeled or when using a LeBail fit.

- Use of fixed background points is problematic
- BKGEDIT:
  - Fit most background functions to points input by user
  - Coefficients can be refined once model is complete
  - Compare functions (type #1 is best - BHT)



## EXCLEDT

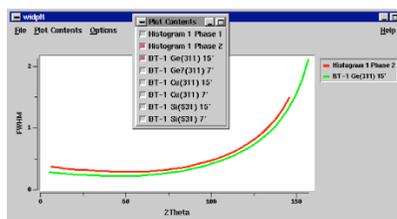
- Change data limits
- Add/delete excluded regions
- Work graphically in 2 $\theta$ , TOF, Q, (even d-space)



## WIDPLT

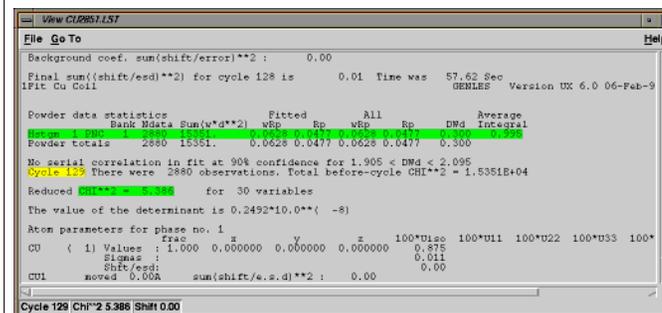
WIDPLT shows the FWHM as a function of 2 $\theta$ , Q, ... for a set of profile coefficients.

- Examine fit results to see that they make sense
- Compare values to predefined sets
- Look for hints of symmetry lowering



## LSTVIEW

- A Scrollable viewer for .LST file



## INSTEDIT

Allows instrument parameter files to be edited

- Save yourself some time:
  - make a file specific to your instrument or even each mode

The screenshot shows the 'Editing instrument parameter file' window. Key settings include:
 

- Select bank:** 1
- Data type:** CW neutron
- Radiation type:** Other
- Wavelength:** 1.54020
- Zero Correction:** 0.04000
- Profile type:** 1
- Peak cutoff:** 0.005000
- GU:** 0.596000E+02
- GV:** -0.163100E+03
- GW:** 0.166700E+03
- asym:** 0.871280E+01
- F1:** 0.000000E+00
- F2:** 0.000000E+00

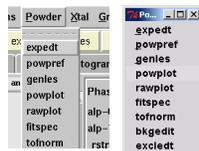
## Import/Export coordinates

Note that **you** can create import & export routines

The screenshots show the 'Import/Export' dialog box with various file format options. The 'PowderCell .CEL file' option is highlighted in both images. The second image shows the 'Adding atoms to phase #1' dialog box, also with 'PowderCell .CEL file' highlighted.

## EXPGUI: other features

- Detachable menus
  - (click on dashes)
- Archive/revert .EXP file
- Sort atoms/histograms
- Multiple histogram selection
  - Global changes
- CIF generation
  - Powder data
  - Customize from GUI



## Sort Atoms: Click on title bar to sort atoms by name, type, x,...

The screenshot shows the 'Sort Atoms' dialog box with the 'Sort by' dropdown set to 'Name'. The resulting atom list is shown below:

#	name	x	y	z	Occ	Usa	Use	Flag
1	Ti(1)	0.000000	0.000000	0.000000	16	1.0000	0.08979	
2	Ti(2)	0.500000	0.500000	0.500000	16	1.0000	0.08979	
3	O(3)	0.422403	0.125000	0.125000	40	1.0000	0.08880	
4	O(4)	0.125000	0.125000	0.125000	8	1.0000	0.00945	

### Multiple histogram selection: Click on the histogram title box

The screenshot shows the EXPGUI interface with a list of histograms on the left and a 'Selected Histograms' panel on the right. The list has columns for 'ht', 'type', 'bank', 'wpt/wave', and 'title'. The 'Selected Histograms' panel shows 'Selected Histograms: 2-31' and includes options for 'Background' (Globally Edit Background, Refine background, Damping) and 'Diffractometer Constants' (Refine wave, Set Wave Globally, Refine zero, Set Zero Globally, Damping).

- select all histogram types
- select only histograms of a single type

Also, sort histograms by clicking on header.

### More shortcuts:

- Mouse click modes in lists:
  - hold mouse button (drag) ==> select range
  - shift+click ==> select range
  - control+click ==> toggles single item
  - right-click ==> select all items in list

### What Can't EXPGUI do?

**EXPGUI has only a small fraction of the features of GSAS, but most of the commonly-used powder features**

#### Use EXPEDT for:

- set up single crystal refinements
- set up macromolecular phases
- soft constraints (perhaps someday)
- All other features not present in EXPGUI (e.g. Fourier maps, rigid bodies)

Note that EXPGUI & EXPEDT coexist well: EXPEDT can always be called to access features not implemented in EXPGUI

### Acknowledgements

EXPGUI was started as a hobby in ~1997

- Thanks to:
  - NIST Advanced Technology Program (1 year of support)
  - NIST Director's Reserve program in Materials Science & Engineering Laboratory (1 year of support)
  - Diane P. Toby, Ph.D. (forgiveness & understanding since 1991!)

**Please cite it if you use it!  
Please contribute source code!**

***Other free software from Brian Toby***

- CMPR  
General purpose powder diffraction tool (graphics, reflection generation, indexing, peak fitting, ICDD search)
  - CIFTTOOLS  
CIF editor & pdCIF viewer (please use when refereeing!)
- Also see web tools @ [www.ncnr.nist.gov/xtal](http://www.ncnr.nist.gov/xtal)