Argonne NATIONAL LABORATORY

... for a brighter future

U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by The University of Chicago

An Overview of GSAS and EXPGUI

Brian H. Toby

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

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.

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.

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”

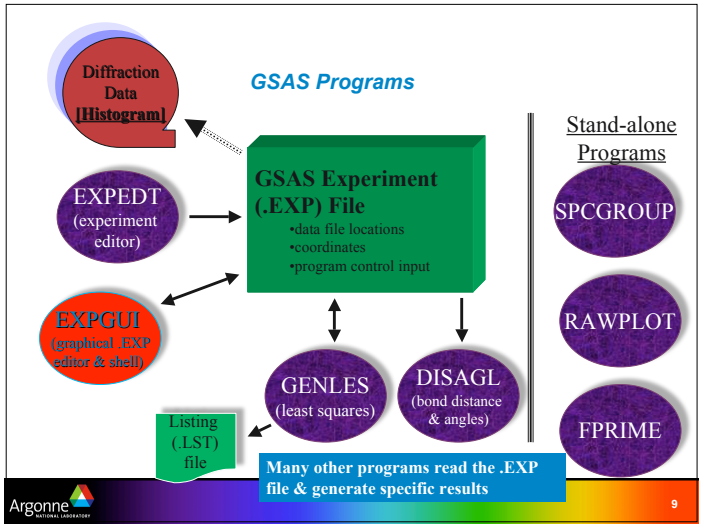
    can be used to compare data from different sources

GSAS: capsule history

- GSAS – conceived in 1982- 1983
  - by A. C. Larson & R. B. Von Dreele

LANSCE
Los Alamos Neutron Science Center

- 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 λ)
- SPCGROUP: space group info, including magnetic operations

Powder Diffraction Data files for GSAS

Two input data files are needed:
- Raw Histogram (contains intensities & optionally 2θ, etc. or s.u.)
- Instrument parameter file: defines data type (λ, 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

Argonne NATIONAL LABORATORY
... for a brighter future

U.S. Department of Energy
THE UNIVERSITY OF CHICAGO
Office of Science
A U.S. Department of Energy laboratory managed by The University of Chicago

EXPGUI, a graphical user interface for GSAS

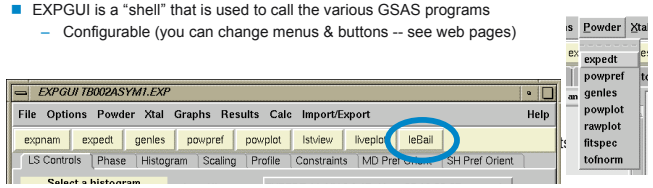
Note that EXPGUI is a separate "add-on" for GSAS (Different author). GSAS works fine without EXPGUI.

Obtaining EXPGUI

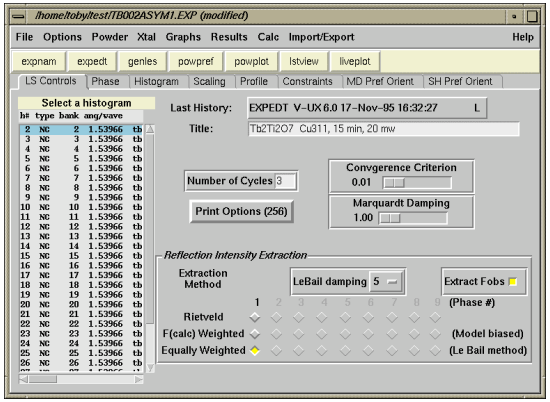
- Documentation
  - http://www.ncnr.nist.gov/xtal/software/expgui/expgui.html
  - Please read the installation and customization pages
- Tutorials (following tutorials in GSAS manual, but using EXPGUI)
  - Alumina (CW Neutron): http://www.ncnr.nist.gov/xtal/software/expgui/tutorial3
  - Nickel (TOF): 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 to join.
- Distributions
  - See http://www.ncnr.nist.gov/xtal/software/downloads.html

A Tour of EXPGUI

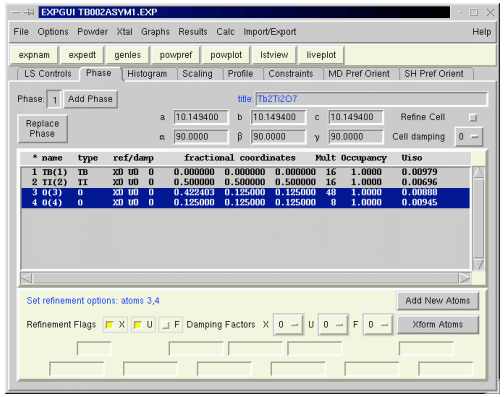
- EXPGUI is a "shell" that is used to call the various GSAS programs
  - Configurable (you can change menus & buttons -- see web pages)



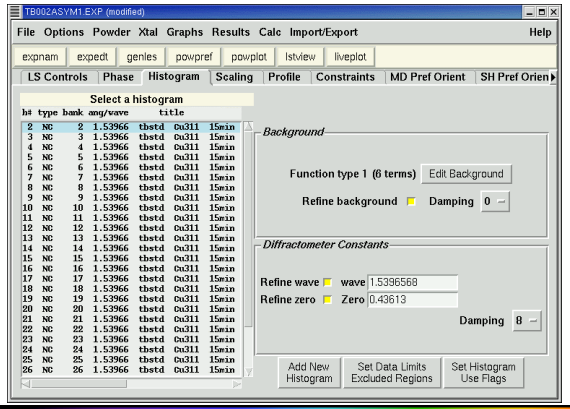
Least squares controls



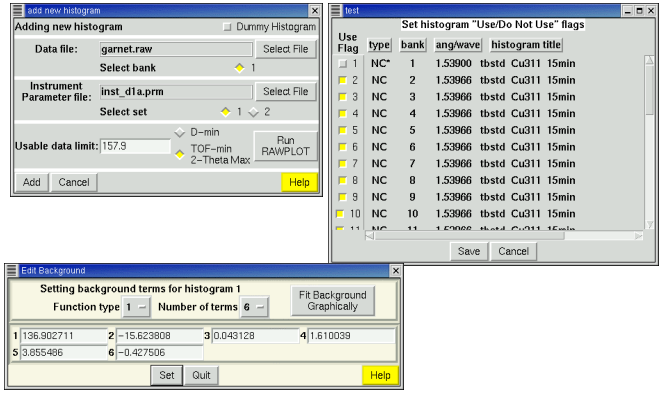
Phase and atom parameters



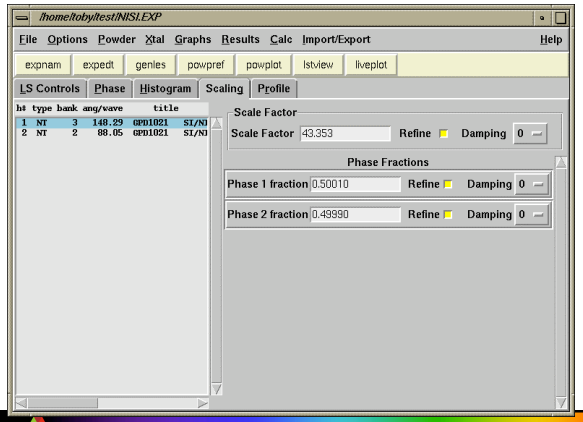
Diffraction Data (Histogram) Parameters



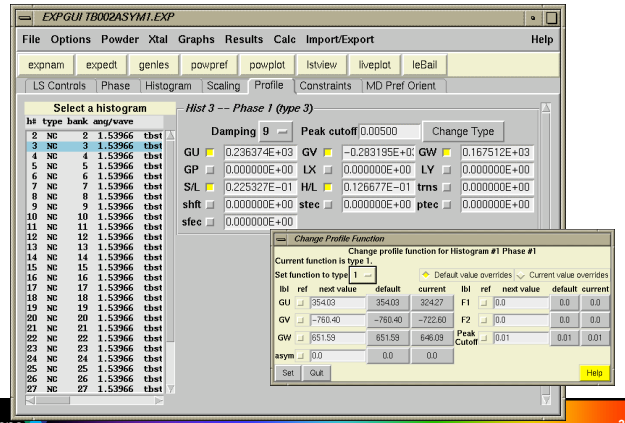
Histogram parameter submenus



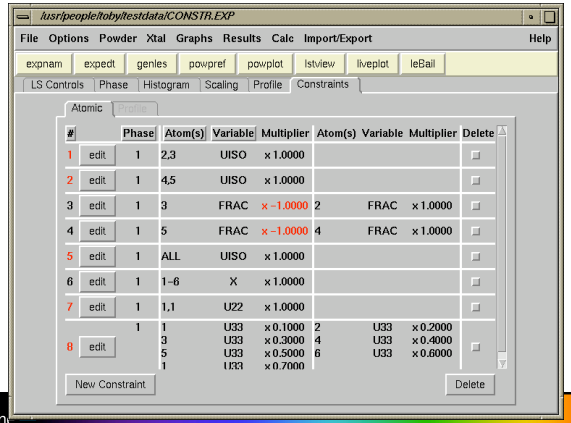
Phase & Histogram Scaling



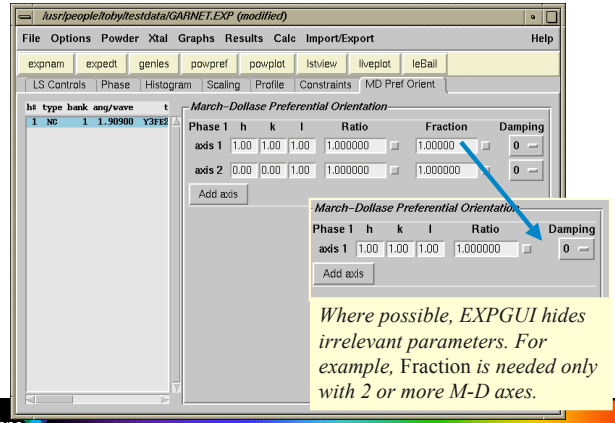
Profile terms



Atom/Profile Constraints

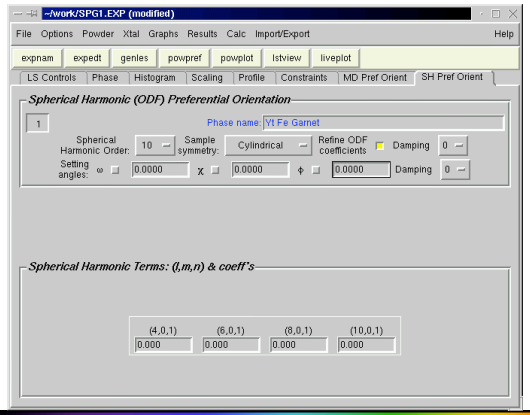


Preferred Orientation:March-Dollase



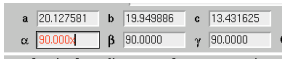
Where possible, EXPGUI hides irrelevant parameters. For example, Fraction *is needed only with 2 or more M-D axes.*

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



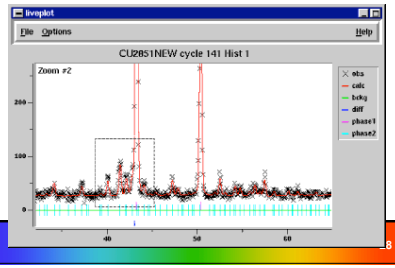
EXPGUI Utilities

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 2θ
- 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)/σ
- Cumulative χ^2
- Shortcut keys



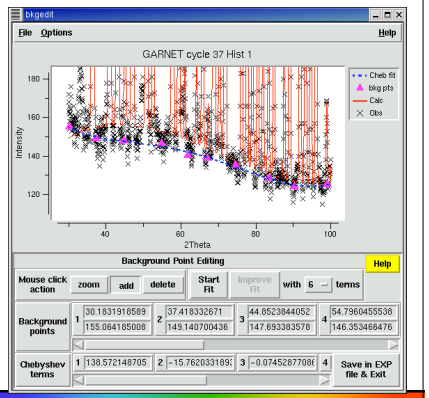
BKGEDIT

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

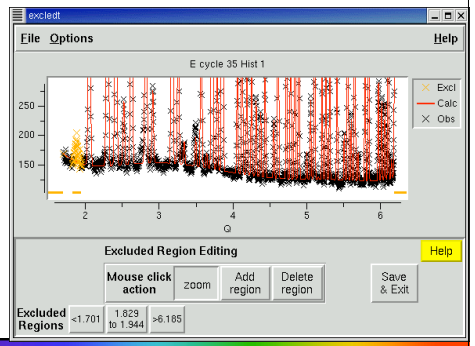
BKGEDIT:

- 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

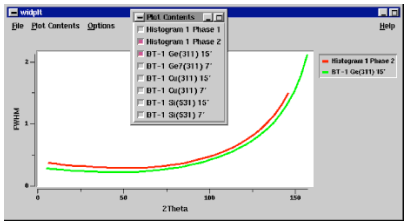
- Change data limits
- Add/delete excluded regions
- Work graphically in 2θ, TOF, Q, (even d-space)



WIDPLT

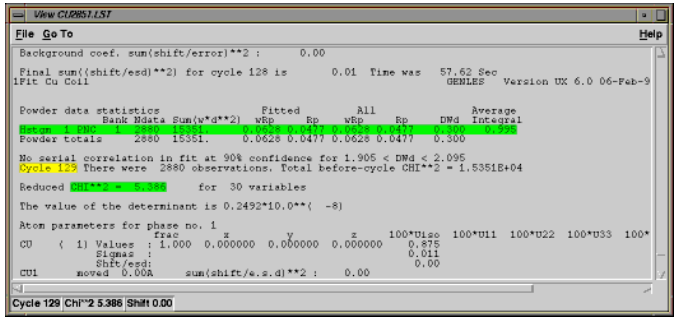
WIDPLT shows the FWHM as a function of 2θ, Q,… for a set of profile coefficients.

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



LSTVIEW

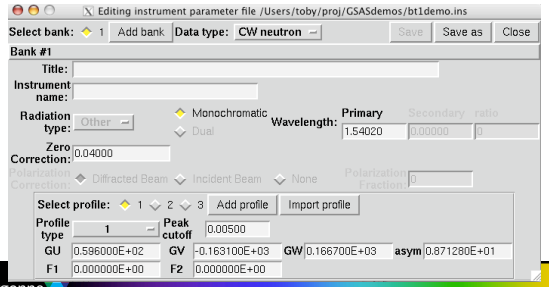
- A Scrollable viewer for .LST file



INSTEDIT

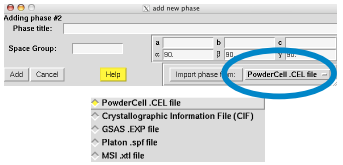
Allows instrument parameter files to be edited

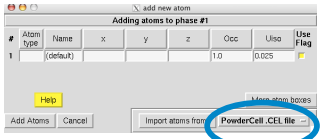
- Save yourself some time:
  - make a file specific to your instrument or even each mode



Import/Export coordinates

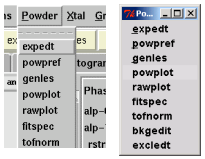
Note that ***you*** can create import & export routines



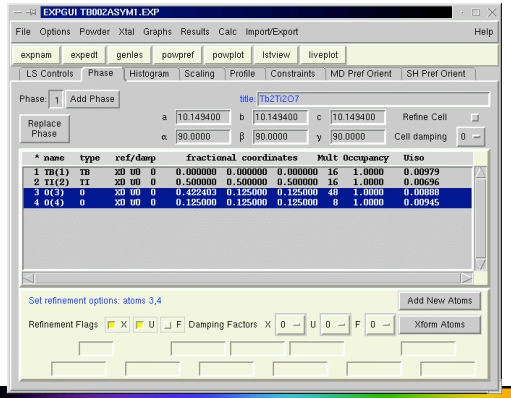


EXPGUI: other features

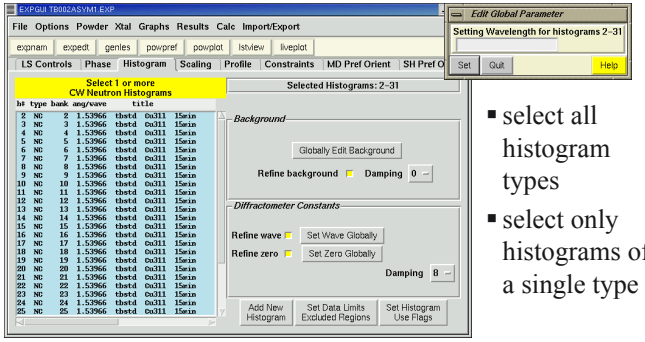
- Detachable menus
  - (click on dashes)
- Archive/revert .EXP file
- Sort atoms/histograms
- Multiple histogram selection
  - Global changes
- CIF generation
  - Powder data
  - Customize from GUI



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



Multiple histogram selection: Click on the histogram title box



- 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)
- CIFTOOLS
  CIF editor & pdCIF viewer (please use when refereeing!)

Also see web tools @ www.ncnr.nist.gov/xtal