

Problem 3: Getting better graphics with GSAS

- Observed & computed diffraction patterns with LIVEPLOT
 - LIVEPLOT cute tricks
 - Exporting from LIVEPLOT
 - Publication quality graphics from GRACE (Mac/Unix)
- Using CMPR to access diffraction patterns
- Plotting structures in DRAWxtl

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3.1A LIVEPLOT Graphics

- Useful short cuts: press keys in window to...
 - N -- plot next histogram
 - 1 -- tickmarks for phase 1 (likewise 2-9, for other phases)
 - H -- labels hkl values of tickmarks near mouse
 - A -- labels hkl values for all tickmarks (use D to clear)
 - Arrow keys move zoom window (small jumps)
 - Control-arrow makes big shifts in zoom window
 - Z -- set zoom region manually
 - L -- displays position of mouse
- LIVEPLOT can also
 - Plot in Q or d-space
 - Plot the "cumulative χ^2 " or (obs-calc)/ σ

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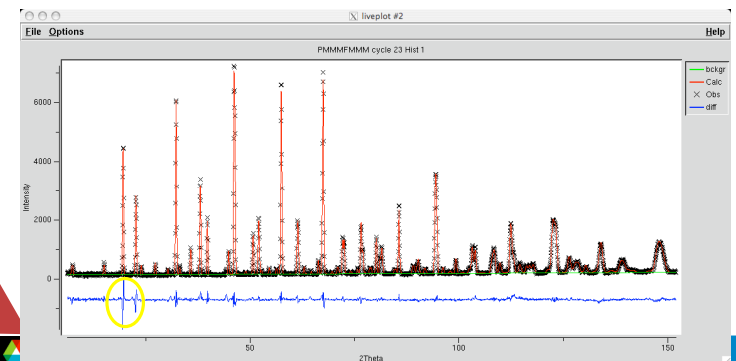
3.1B LIVEPLOT Graphics

- What is "cumulative χ^2 " or (obs-calc)/ σ ?
 - Usual Rietveld "difference plot" tends to visually overstress minor differences in strong reflections.
 - Weighting differences by σ reduces this.
- Approach 1: weighted difference plot
 - Plot (obs-calc)/ σ
 - positive/negative peaks show areas of worst fit
- Approach 2: Cumulative χ^2 (W.I.F. David)
 - Plot running sum of [(obs-calc)/ σ]²
 - produces a line that rises fastest where fit is worst
 - Integrates area under peaks -- so shows impact of misfit regions
- Approaches are pretty much equivalent -- select according to your own preference

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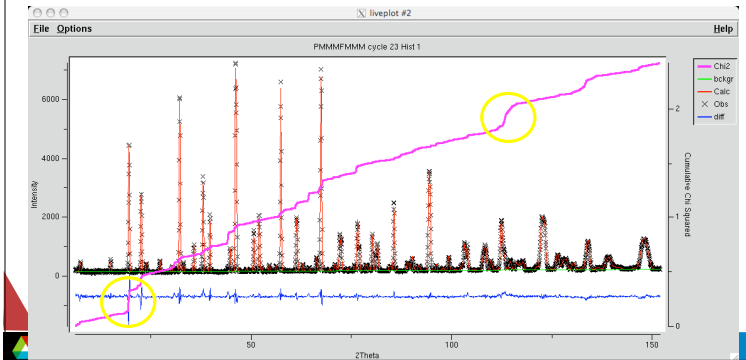
3.1C LIVEPLOT Graphics

Note: the common obs-calc plot implies that the minor misfit at $\sim 20^\circ$ is by far the worst-fit part of pattern



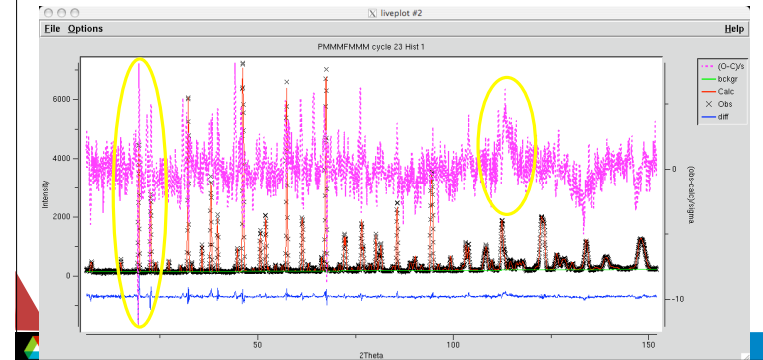
3.1D LIVEPLOT Graphics

- Cumulative χ^2 plot shows misfit at $\sim 100^\circ$ is same severity as $\sim 20^\circ$ region.



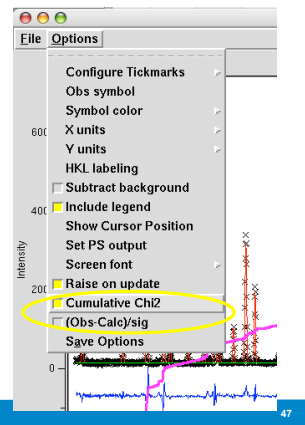
3.1E LIVEPLOT Graphics

- The (obs-calc)/ σ plot also shows the relative severity of different misfit regions



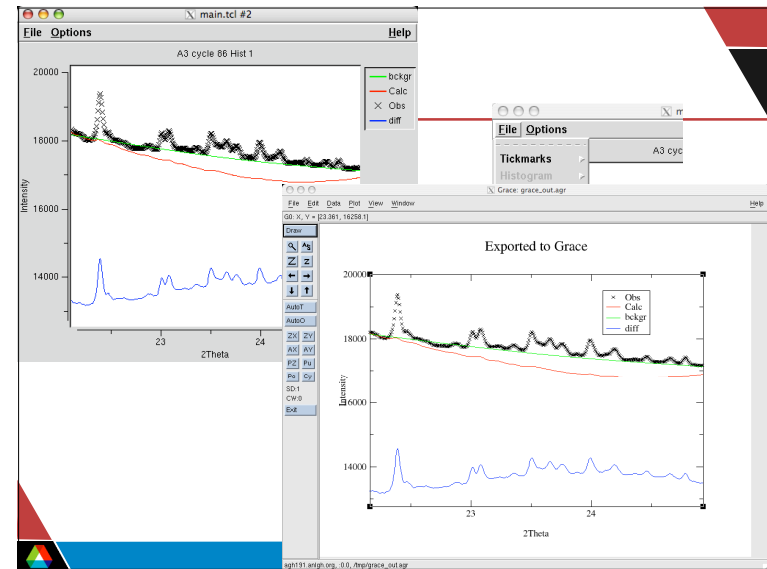
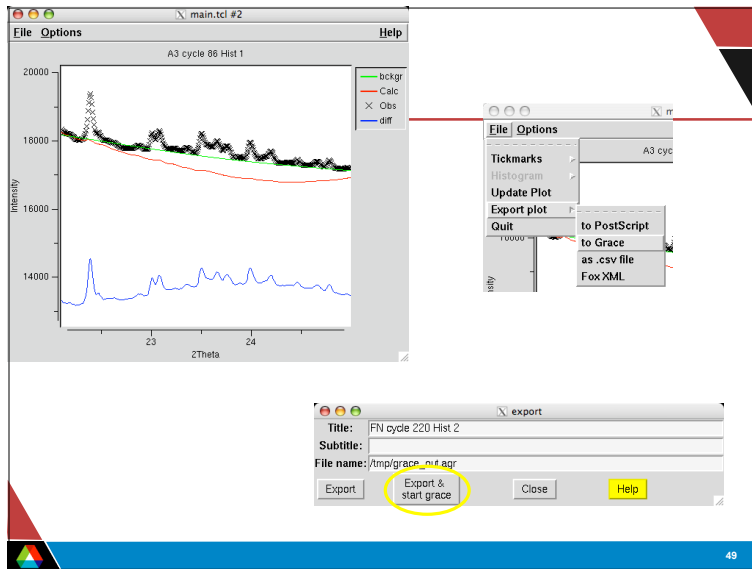
3.1F LIVEPLOT Graphics

- Turn on/off display of the Cumulative χ^2 or (obs-calc)/ σ from the Options menu



3.2 Exporting LIVEPLOT Graphics

- LIVEPLOT results can be exported pretty much WYSIWYG to the GRACE (a.k.a. xmgrace & xmgr) program
 - GRACE runs very well in Unix & on the Mac and is easy to install, but appears to be hard to set up in Windows.
 - GRACE plots can be edited to add annotations, change symbols & line types, etc & produces high-quality graphics in several formats.
 - Windows users can use the Export to Grace file and then move that file to a Linux or Mac computer to produce publication-quality output.
- LIVEPLOT also exports to FOX. Useful because BKGEDIT or Le Bail fit can be used to set up background for FOX
- LIVEPLOT export to PostScript is pretty low quality
- For Windows, graphics can be constructed from the .csv export.
 - I am looking for a good Windows-friendly graphics program that accepts ASCII input and ASCII control instructions (or someone willing to write DDE control code).



3.3 Accessing GSAS results from CMPR

When GSAS & CMPR are installed in the same place, CMPR can use a routine in GSAS to read powder diffraction data from GSAS binary files

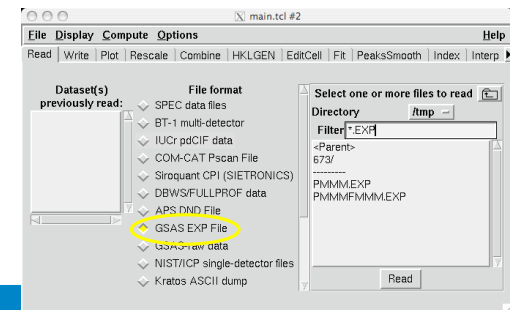
- i.e.* install in C:\GSAS & C:\CMPR (default)
- or* C:\MyProgs\GSAS & C:\MyProgs\CMPR
- or* /usr/local/gsas & /usr/local/cmpr

(it is possible to let CMPR know where to find GSAS in other ways; read <http://www.ncnr.nist.gov/xtal/software/cmpr/cmprdoc.html>)

This is useful as CMPR can be used to do useful manipulations/conversions of GSAS results

3.3A Accessing GSAS results from CMPR

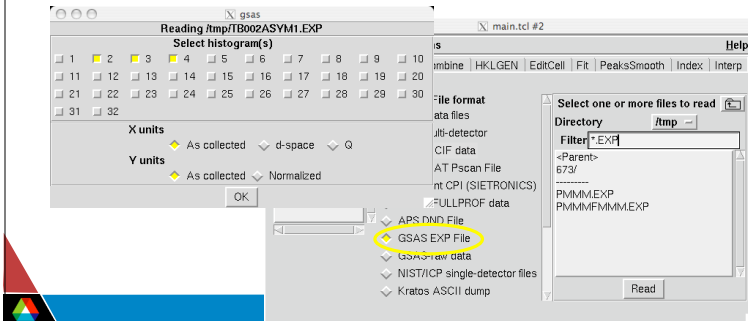
When CMPR finds GSAS, the option to read from "GSAS EXP File" appears in the menu of formats:



3.3B Accessing GSAS results from CMPR

When CMPR finds GSAS, the option to read from "GSAS EXP File" appears in the menu of formats:

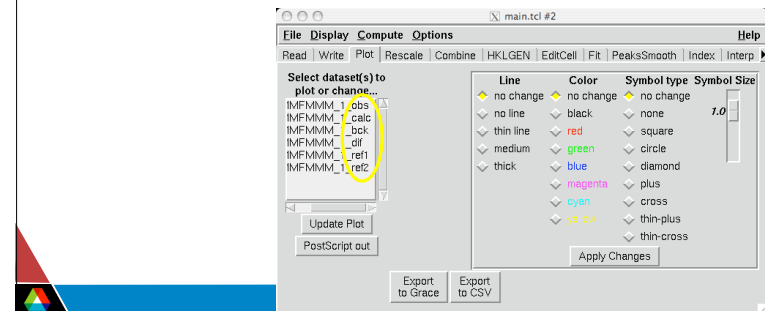
When multiple histograms are present, CMPR allows histogram selection:



3.3C Accessing GSAS results from CMPR

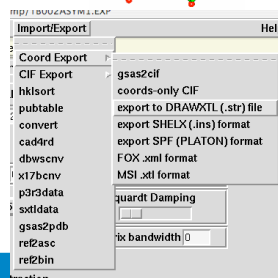
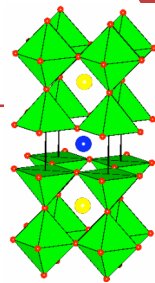
CMPR reads the observed, calculated, background, and difference patterns

It also reads in peak positions for each phase

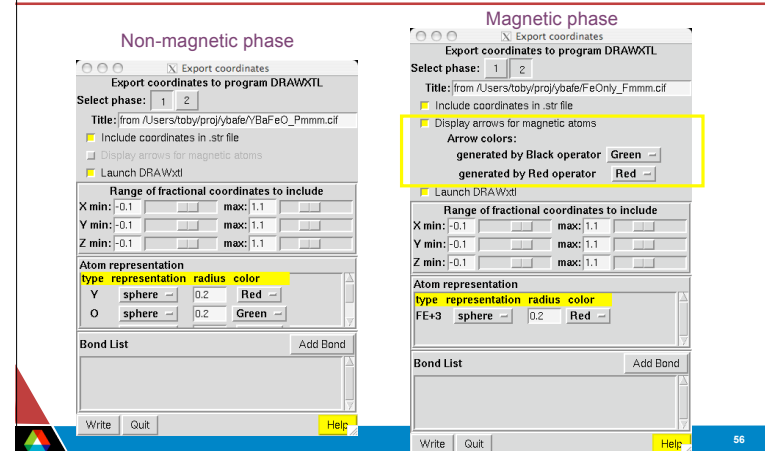


3.4 EXPGUI can export to & start DRAWxtl

- DRAWxtl is an open-source molecular drawing program that runs on Windows, Mac, Linux
 - It is available in GUI and non-GUI versions
 - View structures in OpenGL (real time rotation)
 - Produces ray-traced (POVRAY) WYSIWYG output
 - Also creates VRML (v1 & v2) input files
- EXPGUI interface to DRAWxtl is found in the Coordinate Export submenu of the Import/Export menu
 - Note that other formats are available here

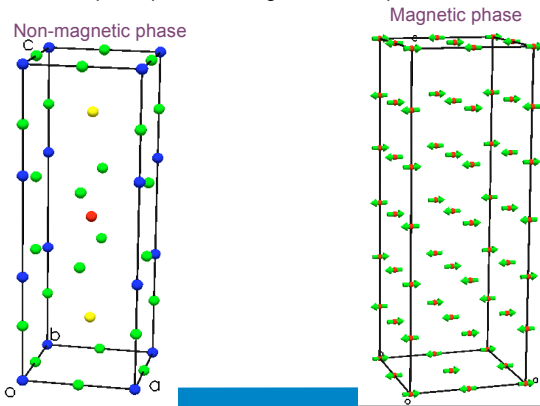


3.4A EXPGUI Interface for DRAWxtl



3.4B EXPGUI Interface for DRAWxtl

- Default EXPGUI options produce boring but useful representations



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3.4C Interface to DRAWxtl options

- Playing with options in the interface can create more interesting figures

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3.4D Interface to DRAWxtl options

- Playing with options in the interface can create more interesting figures

3.4E DRAWxtl Internal GUI

- There are many more options within DRAWxtl's GUI and even more in the control (.STR) file
- Manual tweaking of the POVRAY file can produce professional-quality graphics

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