

Lecture goal

- Introduce advanced & less obvious features of EXPGUI
- Lecture format: Problems & Solutions

Prerequisites:

- Crystallography
- Some experience with GSAS & EXPGUI
- Desire to learn new tricks & easier approaches

This lecture will not introduce GSAS or EXPGUI

Note

- Everything presented works the same on Windows, Macintosh or Linux unless noted otherwise
- Some tricks are for CW fits only

3

Software is free & on web

- GSAS + EXPGUI
<http://www.ncnr.nist.gov/xtal/software/downloads.html>
- GSAS updates
<http://www.ccp14.ac.uk/ccp/ccp14/ftp-mirror/gsas/>
- EXPGUI updates
<ftp://ftp.ncnr.nist.gov/pub/cryst/gsas/>
- CMPR
<http://www.ncnr.nist.gov/xtal/software/downloads.html>
- DRAWxtl
<http://www.lwfinger.net/drawxtl>
- GRACE (aka xmgr & xmgrace) -- **not windows friendly**
 - <http://plasma-gate.weizmann.ac.il/Grace/>
 - For Mac, use FINK (<http://fink.sf.net>)

4

Remember to say "thanks"

- If you use the software, please cite it:
 - A.C. Larson and R.B. Von Dreele, *General Structure Analysis System (GSAS)*. Report LAUR 86-748, Los Alamos National Laboratory (2000).
 - B.H. Toby, "EXPGUI, a Graphical User Interface for GSAS". *Journal of Applied Crystallography*. **34**: p. 210-3 (2001).
 - B.H. Toby, "CMPR - a powder diffraction toolkit". *Journal of Applied Crystallography*. **38**: p. 1040-1 (2005).
 - L.W. Finger, M. Kroeker, and B.H. Toby, *Home Page for DRAWxtl*. <http://www.lwfinger.net/drawxtl> (2005).
 - Stambulchik, E., *Grace Home Page*, <http://plasma-gate.weizmann.ac.il/Grace/> (2000).

5