Introduction to GSAS & GSAS-II

R.B. Von Dreele, APS, Argonne National Laboratory, USA

vondreele@anl.gov

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A bit of history

GSAS – conceived in 1982-1983 by A.C. Larson & R.B. Von Dreele
1st version released in Dec. 1985

- **Designed for multiple data (histograms) & phases – "Premise of GSAS"**
- **Did single crystal & powders from start**
- **Only TOF neutrons (& buggy)**
- **Objective – a tool to give to users at LANSCE for diffraction – can take home & do it themselves!**
- **Only for VMS - VAXFortran**
- **Was "OOP" before OOP invented**
- **Coherent data structure (ISAM for EXP file)**
- **Complexity of multidata/phases – required a "smart" control file editor - EXPEDT**

A bit more of history

Later – add CW neutrons & CW x-rays (powder data)

- SGI unix version & then PC (MS-DOS) version
- also Linux version (briefly HP UX version)

2001 – EXPGUI developed by B.H. Toby

Recent – spherical harmonics texture & proteins

- New Windows, MacOSX, Fedora & RedHat linux versions
- All identical code – g77 Fortran; 50 pgms. & ~800 subroutines
- GrWin & X graphics via pgplot
- EXPGUI – all Tcl/Tk – user additions welcome

Basic structure is essentially unchanged 20+ yrs later

Structure of GSAS

1. Multiple programs - each with specific purpose
   editing, powder preparation, least squares, etc.
2. User interface – EXPEDT – control file complexity
   edit control data & problem parameters for calculations - multilevel menus & help listings
   text interface (no mouse!)
   visualize “tree” structure for menus
3. Common file structure – all named as “experiment.ext”
   experiment name used throughout, extension differs by type of file
4. Graphics - both screen & hardcopy
5. EXPGUI – graphical interface (windows, buttons, edit boxes, etc.); incomplete overlap with EXPEDT but with useful extra features – by B. H. Toby

GSAS & EXPGUI interfaces

GSAS – EXPEDT (and everything else):

```
EXPEDT data setup option (<?>,D,F,K,L,P,R,S,X) >
EXPEDT data setup options:
 <?> - Type this help listing
 D   - Distance/angle calculation set up
 F   - Fourier calculation set up
 K n - Delete all but the last n history records
 L   - Least squares refinement set up
 P   - Powder data preparation
 R   - Review data in the experiment file
 S   - Single crystal data preparation
 X   - Exit from EXPEDT
```

On console screen
Keyboard input – text & numbers
1 letter commands – menu help
Layers of menus – tree structure
Type ahead thru layers of menus
Macros ($M, $R & $X commands)

Numbers – real: ‘0.25’, or ‘1/3’, or ‘2.5e-5’ all allowed
Drag & drop for file names

EXPEDT – very complex; error checking; ask questions ONCE; & don’t ask what user shouldn’t have to know (symmetry operators, form factors, etc.) – result of the “Premise”

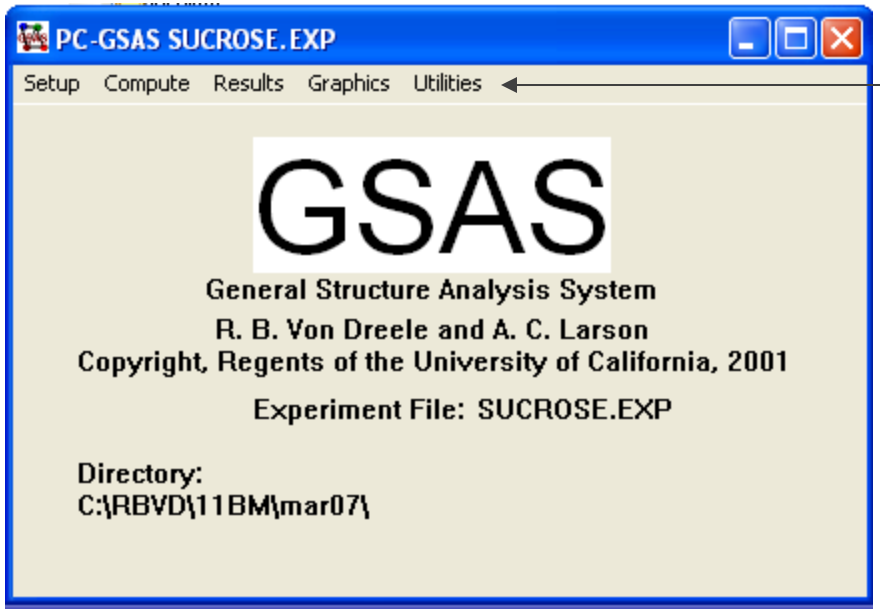
GSAS Macro files (example)

Add some atoms in expedt – starts at opening prompt & ends by terminating expedt; includes setting scale factor & some other stuff → A bit cryptic?

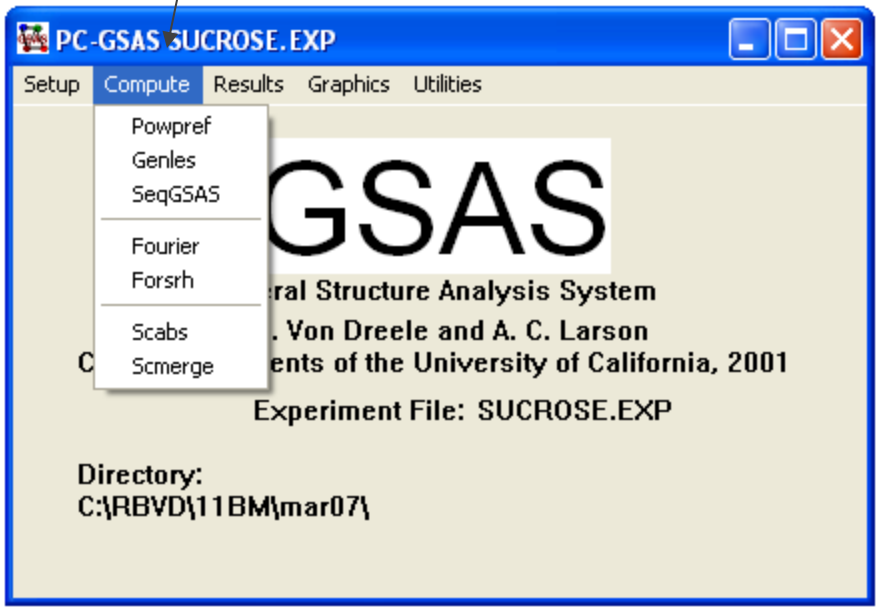
```
k l a                                !We need to insert the atoms
i 10 sb 0 0 0 1 Sb i /               !Enter the Antimony atom
i n o 1/4 1/4 1/4 1 O i /            !Enter the Oxygen atom
i n f .064 .136 .394 1 F i /         ! and the Fluorine atom
v 10:12 x u                          !Refine both position and Thermal motion
x                                    !We are finished with the atoms
o h                                  !Let's set the histogram scale factor up properly
c .4                                 !Change it to .4
x x                                  !Exit back to the main LS menu
l                                    !Edit the LS control data
c 5                                  !Run 5 cycles
f n                                  !Refine on F, not FSQ
s 1.5  /                             !Limit the data to F>3Sig(F)
n 5                                  !Set Rfree on 5% of data
x                                    !We are done with the LS control editing
x                                    !We are done with the LS data editing
x                                    !Exit from EXPEDT
```

Comments on each line after "!"

PC-GSAS – GUI only for access to GSAS programs



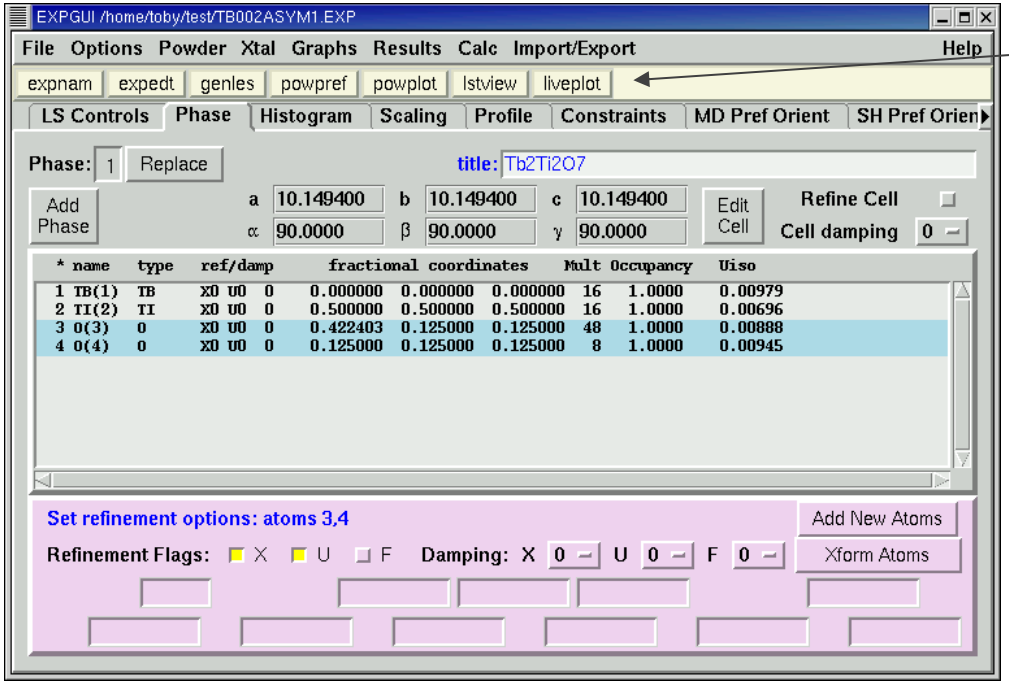
pull down menus for GSAS programs



(Windows only - not linux)

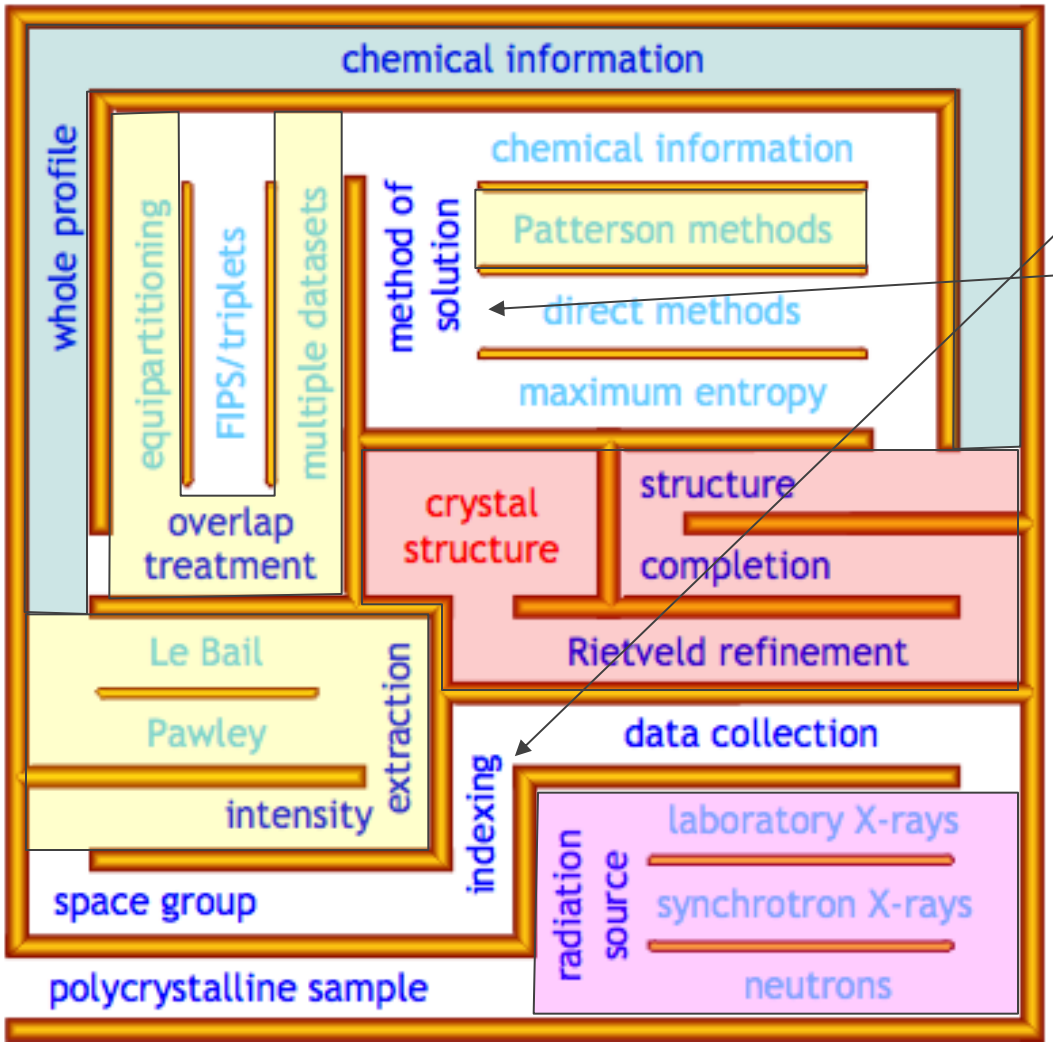
GSAS & EXPGUI interfaces

EXPGUI:



Access to GSAS
Typical GUI – edit boxes, buttons, pull downs etc.
Liveplot – powder pattern

GSAS-II: A fresh start



Fill in what's missing from GSAS:

- Indexing

- Structure solution

Base code – python

Mixed in old GSAS Fortran

Graphics – matplotlib,OpenGL

GUI – wxPython

Math – numpy,scipy

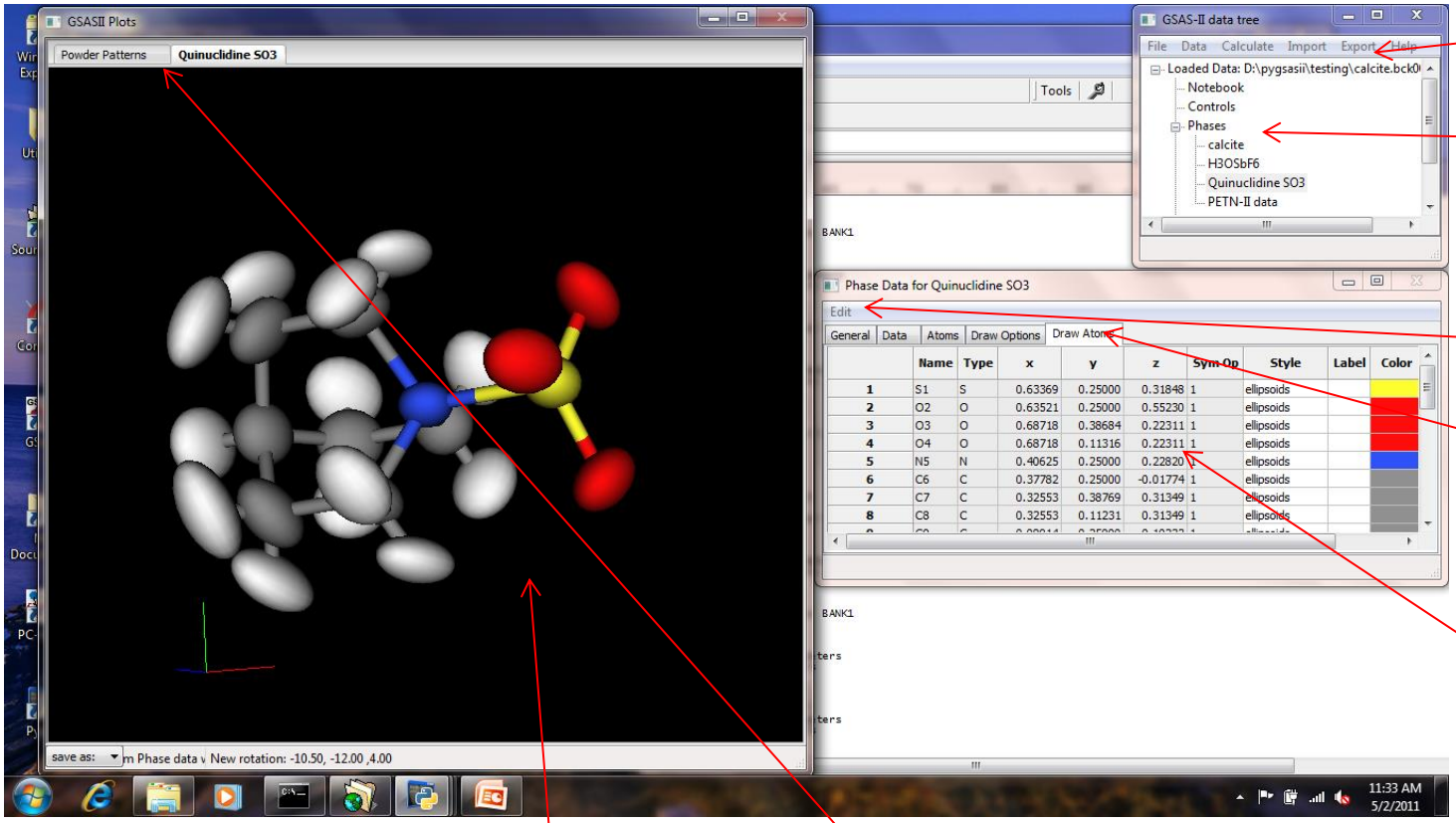
Current: python 2.6 & 2.7

Brief demo?

GSAS-II: A new General Structure Analysis System

- **Goals:**
  - **Cover crystallographic data analysis from raw data to final result**
  - **Same premise as for GSAS; combined data analysis**
  - **A complete system in a modern, easily accessible computer language – Python**
  - **Modern Graphical User Interface (GUI)**
  - **Open source – Python**
  - **All modern platforms (Windows, Linux & Mac OS10+) – Python**
  - **Reuse a bit of old GSAS – Fortran; e.g. space group stuff**
  - **Presently aimed at x-ray scattering : include neutrons in future**
  - **More “General” – include small angle, PDF, reflectrometries**

GSAS-II: A screen shot - 3 frame layout



Main menu

Data tree

Submenu

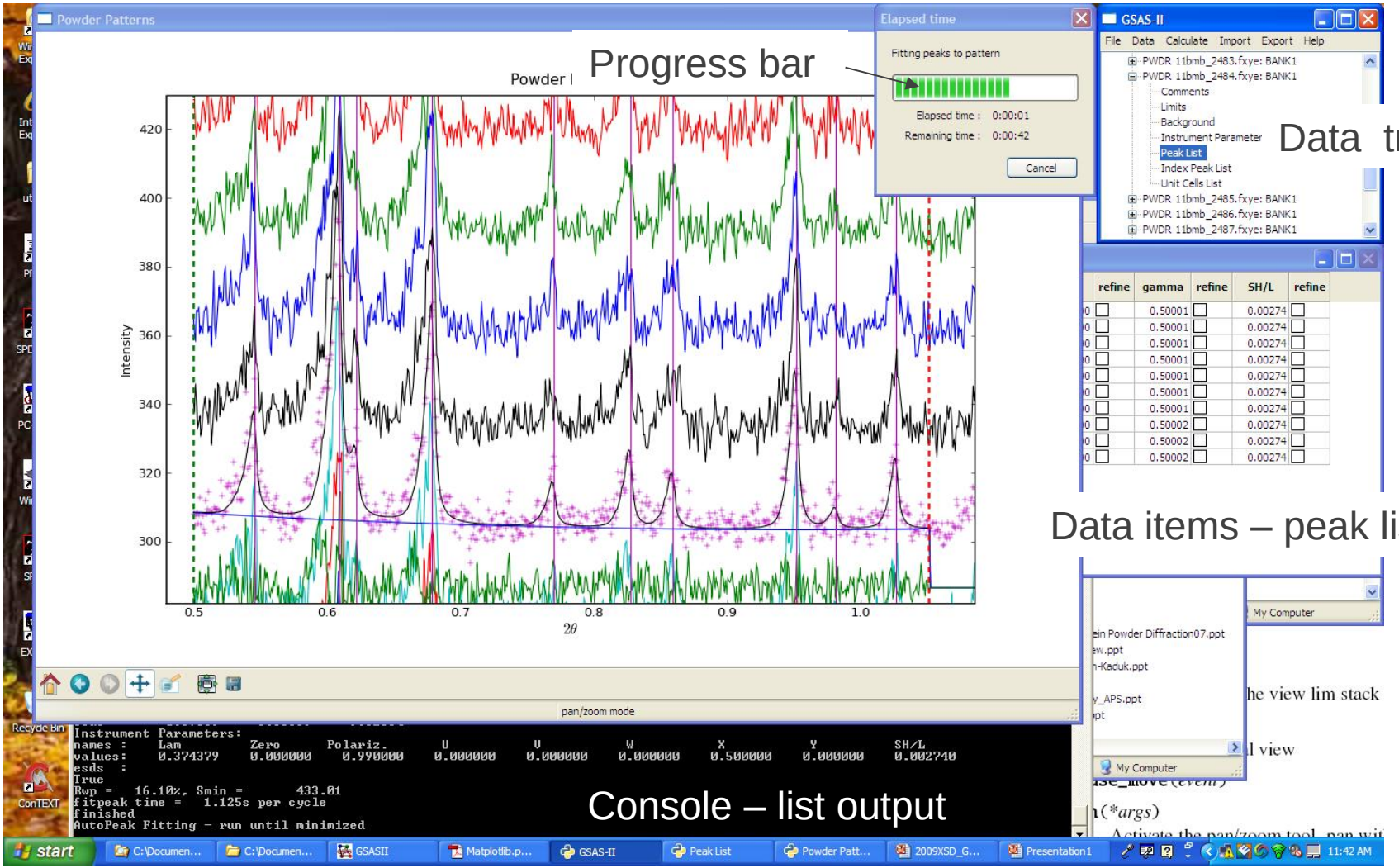
Data tabs

Data window

Drawing tabs

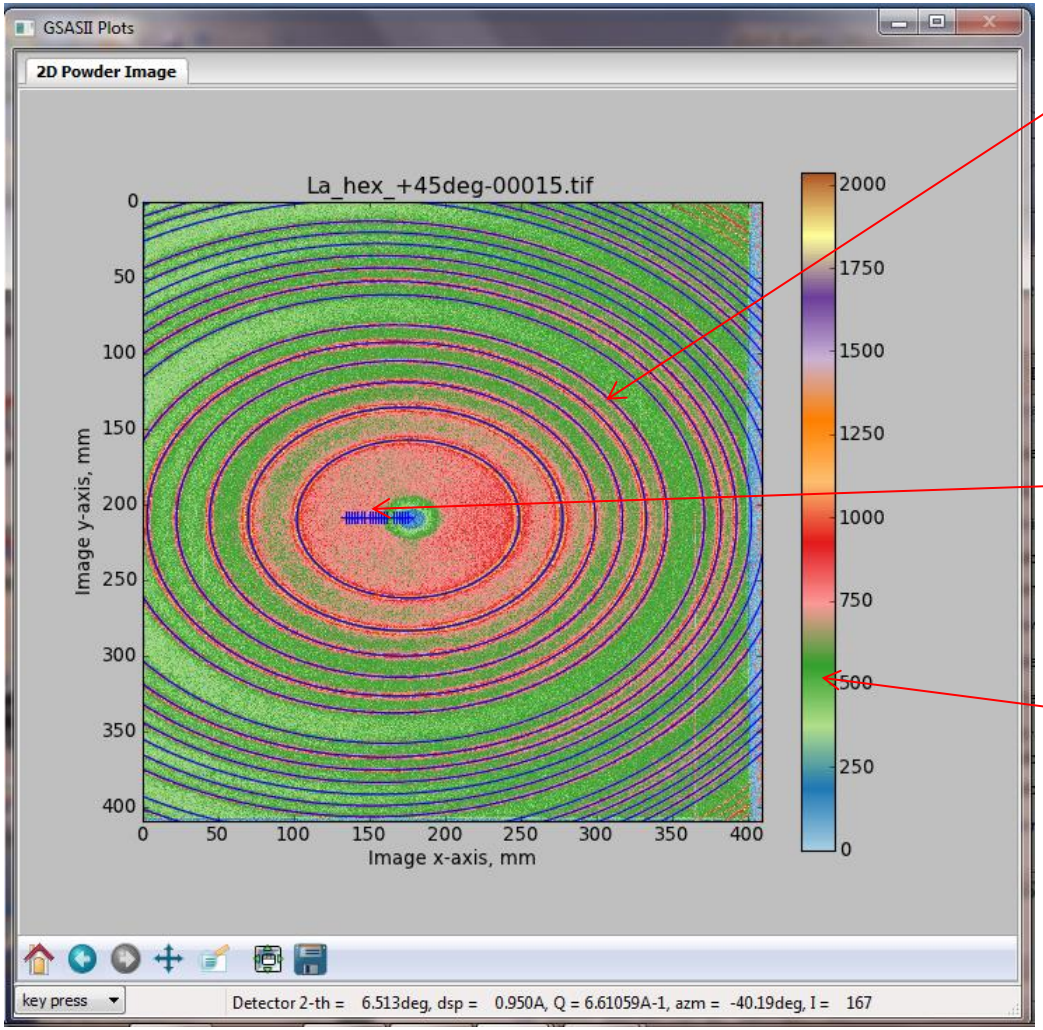
Graphics window

Another screen shot of GSAS-II - multipattern peak fitting



GSAS-II Current capabilities: 2D images

Calibration – tilted detector (e.g. 45° about vertical axis)



Ellipses – sections of Debye-Scherrer cones

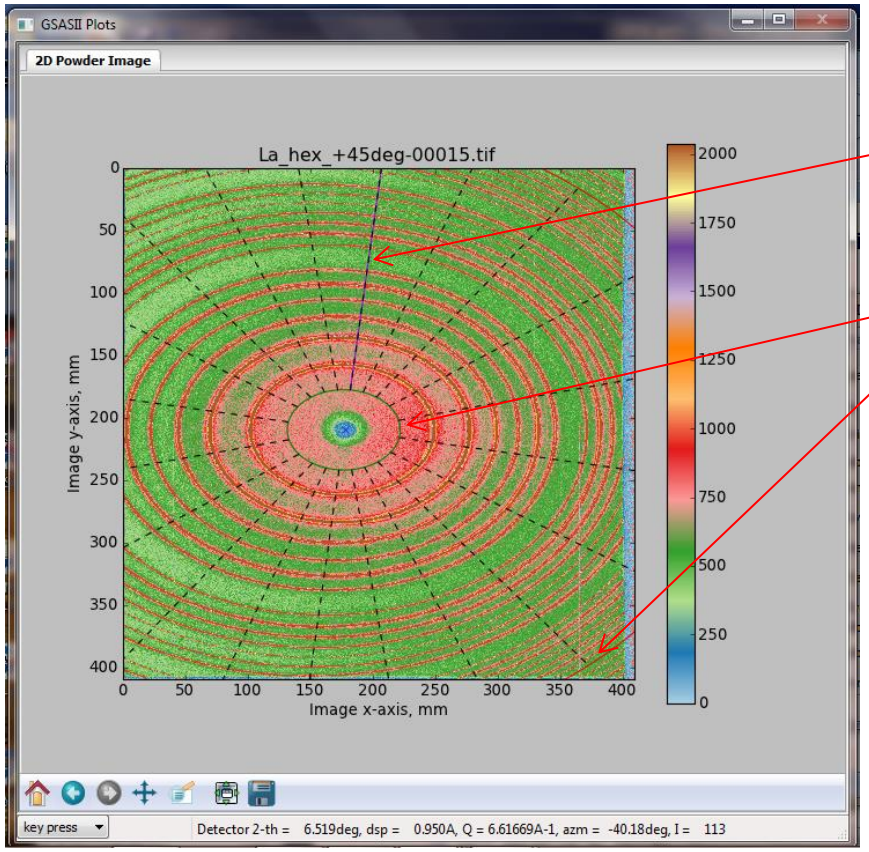
Ellipse centers – not on beam center!

Fitting only requires material (LaB_6) and λ (e.g. don't need to know distance – get that from fit)

Choice of color scheme – "Paired" is shown

GSAS-II Current capabilities: 2D images

Integration

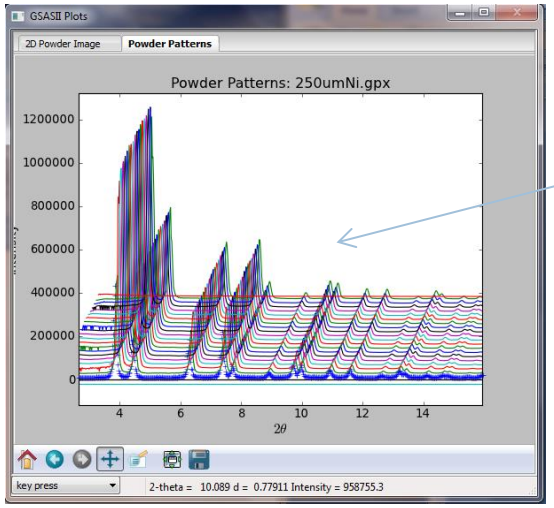


Multiple pie shaped sections with definable starting azimuth

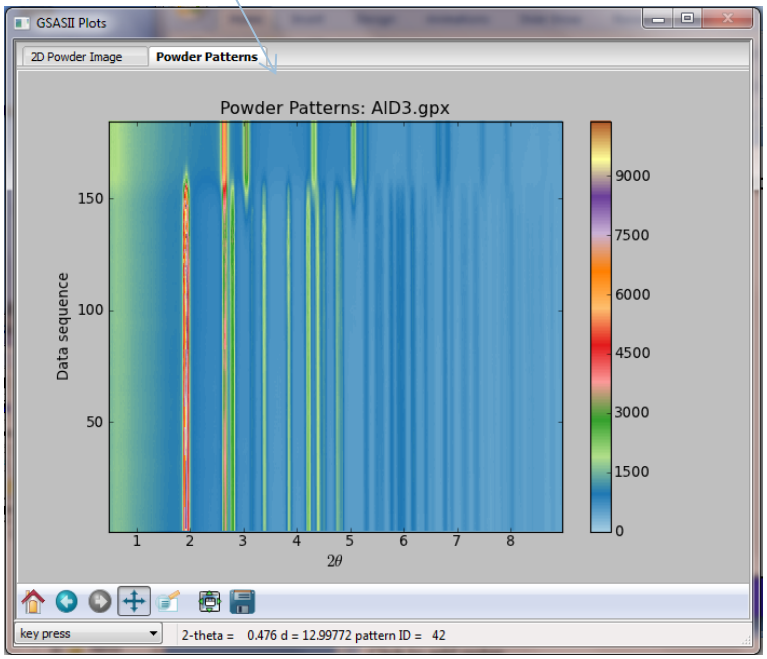
Lower & upper limits on 2Θ
Masks – spots, arcs, rings & polygons (not shown)
Effective replacement for Fit2D

Unlimited workspaces – as many images as you want.
Image combination – sum/difference
Image formats – tiff, MAR345, e.g. all I could find at APS.

GSAS-II Current capabilities: Powder patterns

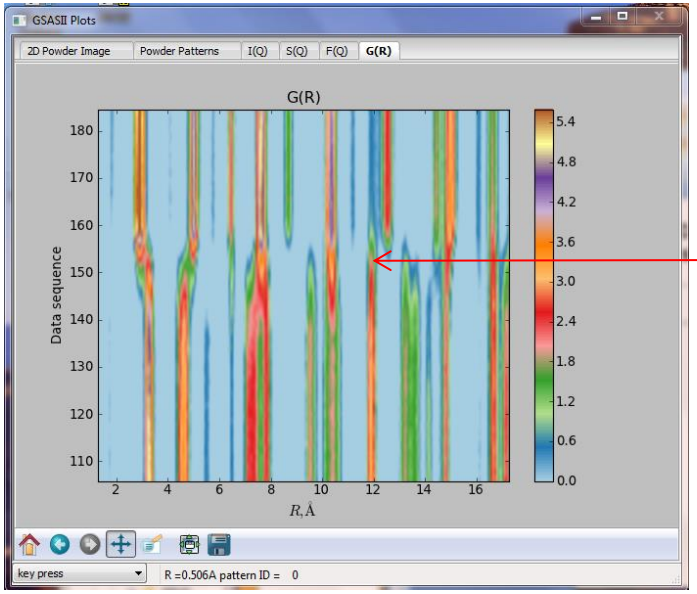


Waterfall plots or contour plots



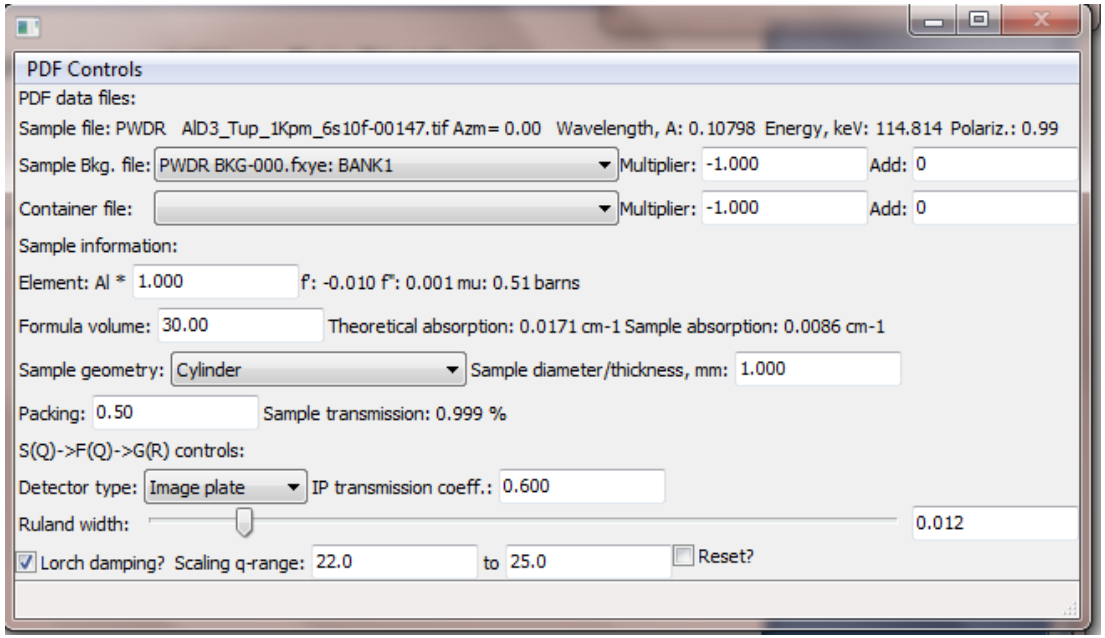
Peaks can be selected/fitted & indexed to identify lattice – modification of algorithm by A. Coelho.

GSAS-II Current capabilities: Pair Distribution Functions

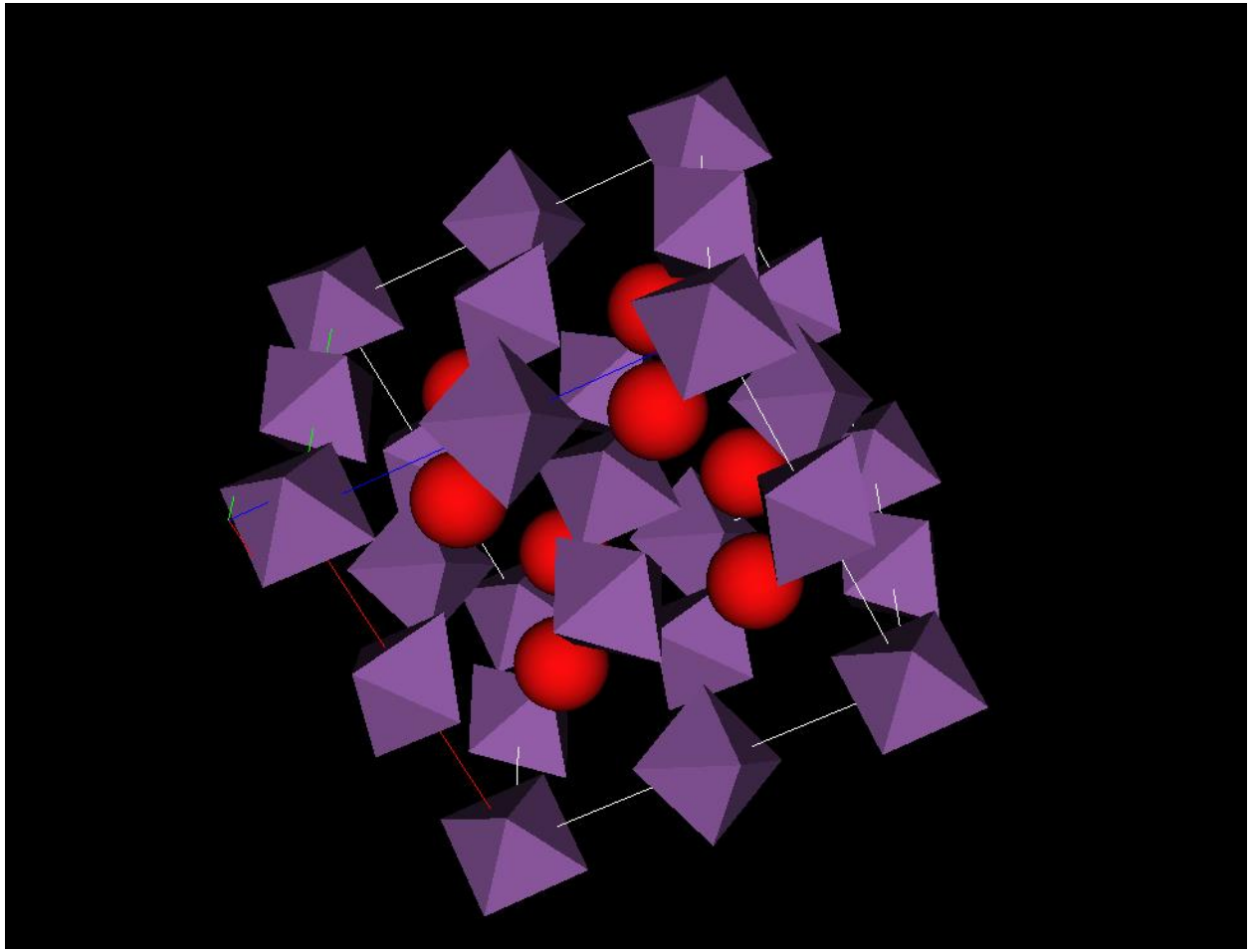


Multiple PDFs – example: 183 images/183 powder patterns/183 G(R)s calculated
Shows transition as T varied

Simple interface – one for each PDF; easy controls

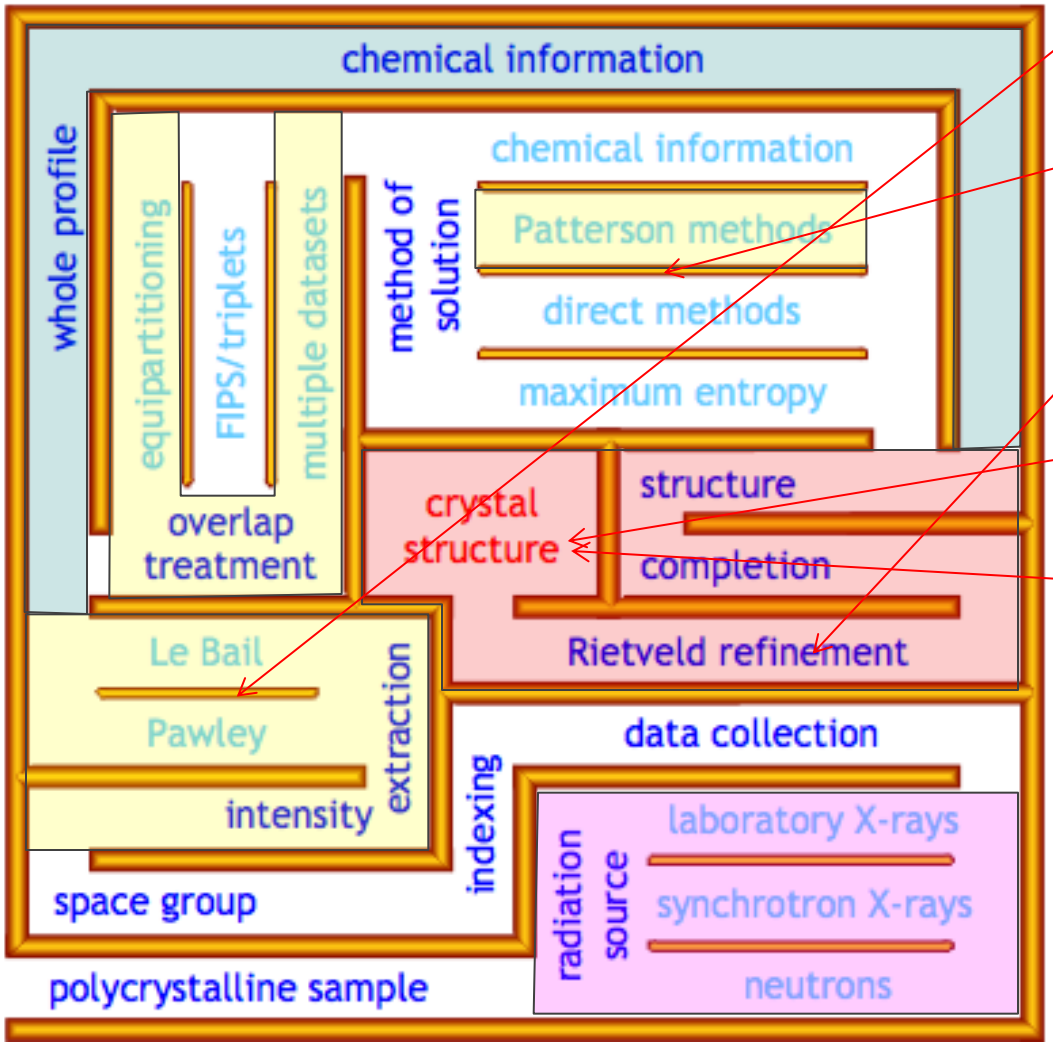


GSAS-II More capabilities: Structure drawing



Polyhedra
Van der Waals
Balls & sticks
Thermal ellipsoids
All selectable by atom

GSAS-II Future – fill in rest of the maze



- Pawley/le Bail refinement
- Charge flipping
- Monte Carlo/Simulated Annealing
- Rietveld refinement
- Result Analysis
  - Bonds & angles
  - Validation
- CIF Publication
- Other scattering
  - PDF (done)
  - Small angle
  - Reflectometry

NB – nonatomistic models

GSAS & GSAS-II Availability

- Subversion server at Argonne: https://subversion.xor.anl.aps.gov
- GSAS & EXPGUI: find it under EXPGUI (don't go to GSAS – that's source for us only); easy installation/upgrade
- Erice - //ERICE_SERVER/GSAS – Win, Linux & Mac OSX
- pyGSAS/trunk & pyGSAS/Examples
  - But not much instruction for downloading/installing/running; hopefully soon
  - You will need python 2.6-2.7, matplotlib, numpy, scipy, pyOpenGL, wxPython – easy from Enthought
- Also Fprime & Absorb: find under pyFprime
- A plug for APS & 11BM – go to http://11bm.xor.aps.anl.gov

12 detector/analyzer diffractometer with mail-in program…