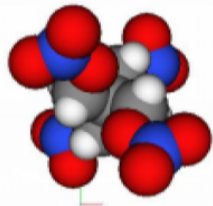


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**GSAS-II:  
WHAT IS NEW?  
SEQUENTIAL REFINEMENTS**

**GSAS-2**



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**IMPROVEMENTS TO THE GUI**

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## COMBINE DATA TREE AND DATA EDITING WINDOWS

New branch (new bugs!)

The screenshot shows the GSAS-II interface. The main window displays a powder pattern plot for 'PWDR OH\_00.fxye Bar'. The data tree on the right shows the project structure, including 'Project: AlternatelyScu', 'Notebook', 'Comments', 'Limits', 'Background', 'Instrument Parameters', 'Sample Parameters', 'Peak List', 'Index Peak List', 'Unit Cells List', and 'Reflection Lists'. A 'Help' window is open in the foreground, showing search results for 'Switch to test (2frame) GSAS-II version'.

Help

Search |

Check for updates

Regress to an old GSAS-II version

Switch to test (2frame) GSAS-II version

Tutorials

Help on Data tree

Help on current data tree item

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## SPEEDING UP REFINEMENTS

## MULTICORE GSAS-II

Attempts to spread computations over multiple cores has not yet resulted in speedups

Profiling code did spot some places for improvements. Particularly a change in derivative computations:

- T3R3 (protein):
  - before 195 sec/cycle
  - now 57 sec/cycle
  
- Jaderite (complex material/11-BM):
  - Before 8.3 sec/cycle
  - Now 7.2 sec/cycle

## SEQUENTIAL REFINEMENTS

## SEQUENTIAL REFINEMENT

### Initial implementation: $n$ datasets with same parameters

Background: GSAS-II (& GSAS) have three types of parameters

- Phase parameters (atom positions, unit cell constants,...)
- Histogram parameters (scale factor, instrumental profile terms,...)
- Phase/Data (histogram) parameters:
  - Phase fractions
  - Lattice distortions
  - Size/strain (sample) profile

## SEQUENTIAL REFINEMENT

### Sequential refinement performs a separate refinement on each histogram in a series

Two modes:

- Copy-forward: parameters from a previous histogram are used in the next
- Use previous: histogram & Phase/Data parameters from last saved values (previous fit) as starting point

Note: There is only one set of Phase parameters. At present, they are not changed by the sequential fit.

## SEQUENTIAL REFINEMENT

**Initial implementation:  $n$  datasets with same parameters**  
**Now allows phase changes, new variables**

- Multiple bugs fixed (many!)
- Plot updated to show last refined, updated on row selection
- Ability to hide columns in Sequential Results Table
- Export of multiple phases in CIF
  
- Requested: “movie” of structural changes

## DISCUSSION TOPICS FROM MEETING

- Enhancements:
  - Export to XYE
  - Enhancement: Export contour plot to Origin, etc.
  - Seq. Ref.: how to change use flag for multiple entries at once
  - Save window positions
  - Use right-click on tree item to bring up item-specific menus
  - Image masking: fill polygon excluded region with a partly transparent color
- Problems:
  - phase/data histogram list only shows used histograms. How to add unused?
  - Seq. ref.: data panel not updating after variable add, etc.
  - Polygon masking not working conveniently