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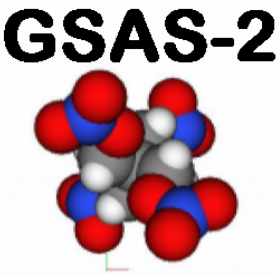
GSAS-II: WHAT IS NEW? SEQUENTIAL REFINEMENTS



ROBERT B. VON DREELE BRIAN H. TOBY

IMPROVEMENTS TO THE GUI

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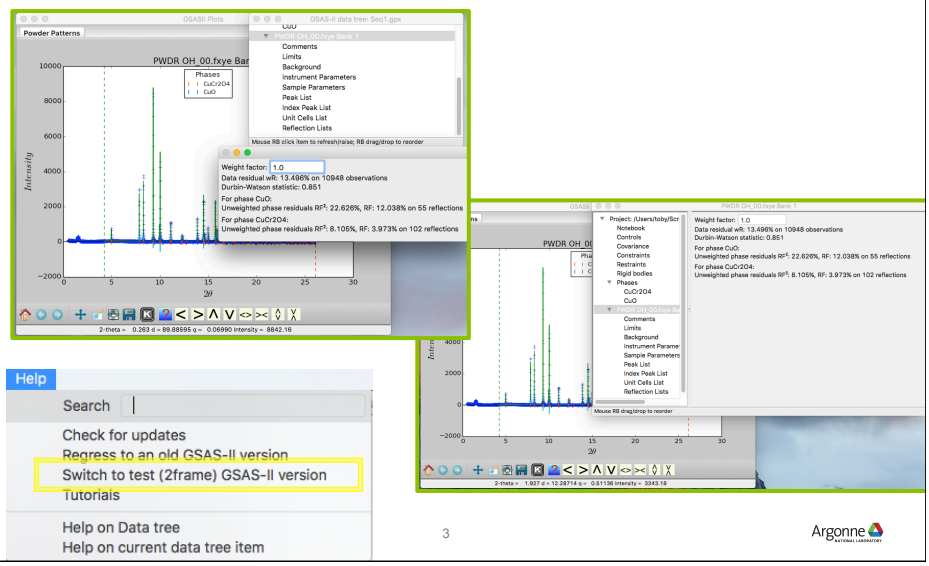
COMBINE DATA TREE AND DATA EDITING WINDOWS

New branch (new bugs!)



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SPEEDING UP REFINEMENTS

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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

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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

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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.

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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 selectrion
- Ability to hide columns in Sequential Results Table
- Export of multiple phases in CIF

- Requested: “movie” of structural changes

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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

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