SrRietUI

DANSE Team
Michigan State University
Why SrRietUI?

• There are famous GSAS, FullProf, ...

• But at SNS
  – data comes quickly
  – large data files generated
  – refinement setup really complicated
  – parametric studies in many points
  – current codes do not interpret in 3rd party software, e.g. EngMod
What SNS Needs?

• Rapid and flexible setup of multiple connected refinement;

• Rietveld refinement is in quasi real-time (experimentalist leaves with 2000 refined structures, not 2000 data sets)

• Easy to use by non-programmers

• Codes can inter-operate with third party codes
SrRietUI's Solution (Vision)

- Scripting interface for manipulating refinement setup
- Distributed computation
- Rietveld–API
- Automated refinement
- [ GUI ]
Scripting Interface

- Currently using Python
- Sequential fitting
- Able to support various Rietveld refinement engines
- Supporting NeXus
- Python binding to FullProf/GSAS?
Rietveld API

- Is FullProf better than GSAS?
- If there is an API that is independent of Rietveld refinement engine ...

-- this is “Rietveld API”

- Increase user community of SrRietUI
- Structure refinement API
Other Features

- **Distributed Computation**
  - parallel refinement for multiple refinements
  - Use Pyre services when they are ready

- **Automated Refinement**
  - automatic refinement control

- **GUI**
  - for most users
Planning

• ~ 2007–08–20 alpha–0 release
  WBS Task “Reciprocal–space Model Refinement Launcher”

• ~ 2007–09–15 alpha–1 release
  Sequential fitting

• ~ 2007–10–10 alpha–2 release
  WBS Task “Reciprocal–space Model Refinement UI”

• ~ 2007–12–31 alpha–3 release
  WBS Task “Automated Feedback Refinement Control”
  POWGEN3 related tasks
Rietveld Refinement Setup
**Code Structure**

- **Online Documentation**
  
  http://nirt-pc.pa.msu.edu/diffdocs/SrRietUI/inherits.html

- **Self-defined Data Type**
  
  boolean, enumerate, float, integer, refine, string

- **Unified definitions for all parameters**
  
  name, definition, data type, valid range, default value
Rietveld Parameters

Categorizing Rietveld Parameters to A Hierarchal Structure
**Base Structure of a Class**

- **3 types of variables**
  - Parameter
    (Example: \((x,y,z)\) of an atom)
  - Subclass (1-to-1)
    (Example: thermo factor of an atom)
  - Container (1-to-many)
    (Example: a phase containing atoms)

- **Dictionaries for definition**
  - Too many and too complicated parameters in Rietveld refinement
  - The refinement engines are updated frequently
  - A neat way to organize the parameters, subclasses and containers
  - Good documentation!
What's in alpha-0 Release?

• The core of SrRietUI
  – creation of data structure
  – basic methods to access the data structure
  – translate between SrRietUI data structure and FullProf input file

• Use cases: set up a Rietveld refinement

• Usability:
  – Scripts to demonstrate the use cases

• Tutorial