

DANSE – DiffDANSE report and Community Engagement

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What is Diffraction?

- **Determination of the atomic-scale structure of materials**
 - Single crystal diffraction (crystallography)
 - Macromolecules
 - Small molecules
 - inorganics
 - Powder diffraction (Structure from crystalline powders)
 - Total Scattering and PDF studies (Nanostructure determination)
 - Disordered materials diffraction (amorphous materials and liquids)
- **Diffraction Instruments at SNS**
 - POWGEN3
 - NOMAD
 - SNAP
 - SCD

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Which scientific communities use diffraction?

- Materials scientists
- Chemists
- Condensed matter physicists
- Geologists, earth and planetary scientists
- Chemical engineers
- Molecular biologists
- ...

The community of people using diffraction is huge, though the number using neutron and synchrotron national user facilities is a rather small proportion of all these users

What are the frontiers in structure science and diffraction

- Complexity
- Nanostructure and the nanostructure problem
- Special environments, *in-situ* and *in-operando* measurements

Modern sources such as SNS are giving data of unprecedented quality

- data handling and modeling are currently the bottlenecks in most problems
- Algorithm development and implementation are required to solve problems such as the nanostructure problem

Goals of diffDANSE

To:

- Build an optimization framework for rapid prototyping of novel atomic-scale structure modeling and regression ideas
- Implement novel structure modeling approaches in the framework and released to the community allowing for new science
- Release software that addresses the scientific workflow problems of community scientists, especially handling large, and large numbers of, datasets
- Help solve the problems of SNS instrument scientists and leverage the use of SNS instrument time into better science
- Release software that lowers the learning curve for new users and increases participation in the community

Flagship Applications

- SrFit

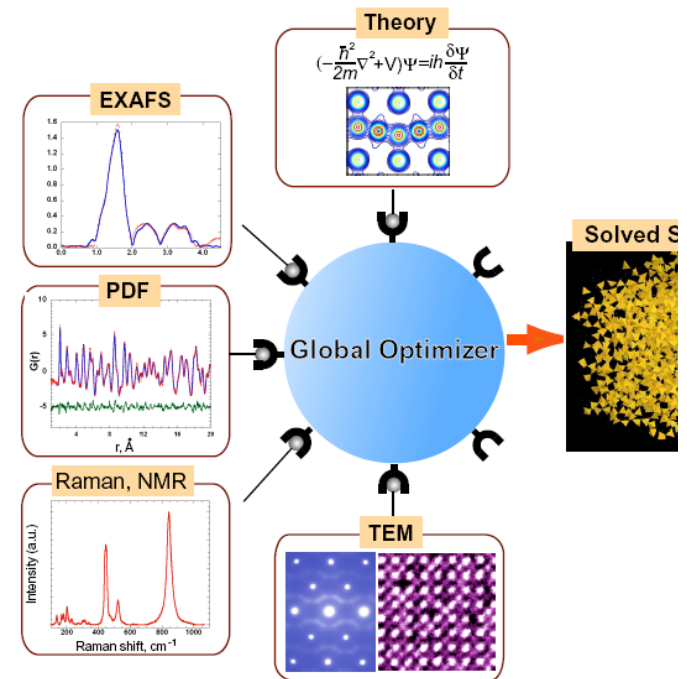
- optimization framework for rapid prototyping of novel structure modeling and regression ideas
- novel structure modeling approaches implemented, such as complex modeling (initially co-refinement of powder diffraction and PDF data)
- Status: working demonstration

- PDFgui/SrReal

- GUI-driven refinement of local and intermediate-range ordered structures to atomic pair distribution function data-sets

- SrRietveld

- Powerful Script-driven UI for rapid setup and easy to use Rietveld refinement of multiple powder diffraction data-sets
- Rietveld API separates the scripting layer from the engine allowing different engines to be used.



Billinge and Levin, Science, 2

Community engagement: requirements gathering and code development

How do we find out what the community/Instrument Scientists need

1. We already know what they want

- We are users!

2. Survey the existing software and usage patterns of the community

1. Online survey of usage
2. Conversations with people...what do they use for what, and why do they use that program?

10. total scattering/PDF data analysis

Crystallographica	- 9	12.86%
DISCUS	- 15	21.43%
ATLAS	- 2	2.86%
PDFGetX2	- 14	20.00%
PDFGetX	- 5	7.14%
RAD	- 10	14.29%
PDFgetN	- 12	17.14%
Gudrun	- 0	0.00%
ISAW	- 3	4.29%
Total Answers	- 70	

11. total scattering/PDF modeling

PDFFit	- 24	58.54%
RMC code (ISIS, cambridge)	- 8	19.51%
RMCPow	- 5	12.20%
EPSR	- 1	2.44%
Other - please write in at the end of the survey	- 3	7.32%
Total Answers	- 41	

Please indicate what software do you use for

12. data visualization/plotting

APD (Philips)	- 10	1.81%
Atoms	- 24	4.34%
CMPR	- 20	3.62%
Crystallographica	- 9	1.63%
Diamond	- 21	3.80%

<http://danse.cacr.caltech.edu/polls/results.php?sid=22>

Community engagement: requirements gathering and code development

How do we find out what the community/Instrument Scientists need

1. We already know what they want
 - We are users!
2. Survey the existing software and usage patterns of the community
 1. Online survey of usage
 2. Conversations with people...what do they use for what, and why do they use that program?
3. Ask them!
 - What are the limitations of the current software? What capabilities would they like

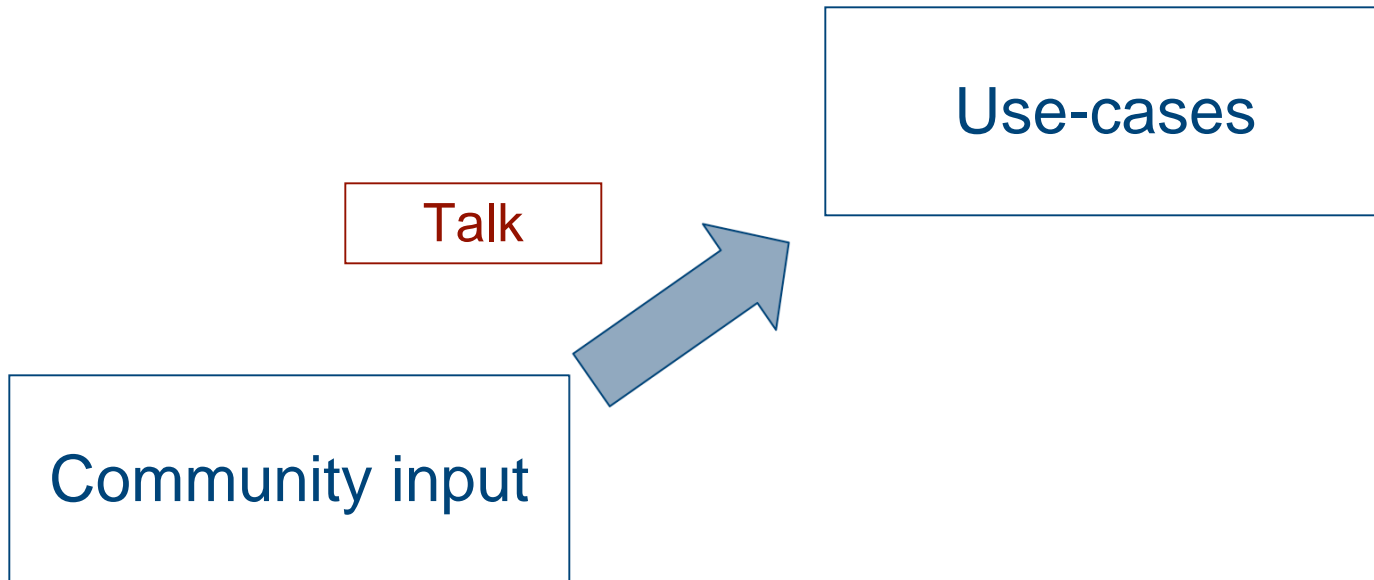
Problem!

We have learned that 2. and 3 yield imprecise information.

Solution:

Comes from our software development process that has been evolving over the initial 1.5 – 2 years of the project.

Community involvement: Requirements gathering





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Welcome to DANSE Diffraction Software Project

Google

Applications and Tasks

- [SrFit](#)
- [SrReal](#)
- [SrRietUI](#) current release user docs: [release information](#), [tutorial](#), [specifications](#), [tickets](#), [checklist](#)
- [PDFgui](#) beta release: [specifications](#), [tickets](#), [checklist](#)
- [6.2.7 Graphical applications](#)
- [SrRietveld](#)
- [5.4.6.3 PyMol](#)

Software Information

- [DANSE Release information](#)
- [Subversion repository](#)
- DiffPy library:
 - [PDFfit2](#)
 - [Structure](#)
- [Demos](#)

Project Management

- [Projects](#)
- [Meetings](#)
- [DANSE wiki](#)
- [Code Review Sessions](#)

Documentation

<http://danse.us/trac/diffraction>



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SrRietveld

This task is to create a model refinement user-interface (UI) for reciprocal-space fitting of powder data, or Rietveld fitting. The task is referred to as [SrRietveld](#), the target application. [SrRietveld](#) is to be a fully-functional user-friendly Rietveld application. [SrRietveld](#) is to be built using the Rietveld API, a general application programming interface for Rietveld fitting applications. Rietveld API will be general enough to interface with current Rietveld applications (Fullprof, GSAS). Rietveld API designed for application developers over application users.

Introduction

1. [Project Timeline](#)
2. [Developers and personnel](#)
3. [Software License](#)
4. [Source trunk](#)
5. [Documentation](#)
6. [Obtaining and building the code](#)
7. [Information for reviewers](#)
8. [Information for testers](#)
9. Community [discussion](#). (Please post here your comments and suggestions.)

Developer Documentation Workproducts

- [SrRietveld](#) encompasses the following WBS tasks
 - 6.2.7.5 Reciprocal-space Model Refinement Launcher

- 8. [Information for testers](#)
- 9. Community [discussion](#). (Please post here your comments and suggestions.)

Developer Documentation Workproducts

- [SrRietveld](#) encompasses the following WBS tasks
 - 6.2.7.5 Reciprocal-space Model Refinement Launcher
 - 6.2.1.3 Reciprocal-space model refinement
- [Vision](#)
- [Use Cases](#)
- [Supplementary Specifications](#)
- [Planning](#)
- [Architecture Specification](#)
- [Behavior Specification](#)

Reviews

- [Planning Review](#)
- [Design Review](#)

Releases ↑

⇒ [Spring 2008 DANSE Release](#)

Developer notes

- [Report progress on DANSE trac ticket](#)
- [Scratch place for old use cases](#)
- ⇒ [Link to DANSE site for this task](#)
- [design notes](#)
- related meetings: [2007-08-29](#), [2007-10-01](#), [Design Review](#)

SrRietveld Use Cases

Use Cases

Section 1: Pre-Rietveld Refinement

- [SrRietveld UC1-1 : indexing from powder data](#) - Pending
- [SrRietveld UC1-2 : peak fitting from powder data](#) - Pending
- [SrRietveld UC1-3 : peak intensity extraction from powder data](#) - Pending
- [SrRietveld UC1-4 : structure solution from powder data](#) - Pending
- [SrRietveld UC1-5 : check space group with The result of peak intensity extraction](#)- Pending

Section 2: Rietveld Refinement

- [SrRietveld UC2-1 : refine a single structure from powder data](#)- Accepted
- [SrRietveld UC2-2 : refine multiphase structure from powder data](#)- Pending
- [SrRietveld UC2-3 : refine a single structure from several powder data](#)- Pending
- [SrRietveld UC2-4 : refine magnetic structures from several powder data](#)- Pending
- [SrRietveld UC2-5 : import FullProf input file \(SrRietUI UC3\)](#)- Accepted - alpha 0
- [SrRietveld UC2-6 \(SrRietUI UC4\): import GSAS experiment file](#) - Accepted - ?
- [SrRietveld UC2-7 \(SrRietUI UC15\): automated structure upload from database](#) - Pending
- [SrRietveld UC2-8 \(SrRietUI UC20\): refine pattern data by using GSAS as the Rietveld refinement engine](#) - Accepted - 1
- [SrRietveld UC2-9 : pattern calculation](#)- Accepted - Beta Release
- [SrRietveld UC2-10 : particle size broadening](#)- Accepted-Beta Release

Section 3: Beyond Rietveld Refinement

- [SrRietveld UC3-1 : sequential fitting of related powder data \(SrRietUI UC7\)](#) - Accepted - alpha
- [SrRietveld UC3-2 : automatic background selection](#)- Pending
- [SrRietveld UC3-3 \(SrRietUI UC16\) : global update of parameters](#) - Pending
- [SrRietveld UC3-4 \(SrRietUI UC17\) : semi-automatic refinement in sequential fitting of related powder data](#) - Pending - alpha 2

Refine a single structure from powder data

Brief

Scientist loads powder data. Optionally, scientist graphically visualizes the loaded data in Plotter. Scientist selects data channels and ranges to be used in the refinement. Scientist enters initial structural parameters for a periodic model. Optionally Scientist graphically visualizes the initial structure in 3D Visualizer. Scientist configures the fit. Optionally, Scientist configures the minimization routine. Scientist initiates refinement. SrRietveld saves refinement results, final profile and positions of Bragg peaks to output files. Optionally, Scientist graphically visualizes the fitting results, and refined structure. Optionally, Scientist reconfigures and reruns the fit.

Expanded scenerio

- **Scope:** SrRietveld application
- **Level:** user goal
- **Primary Actor:** Scientist
- **Stakeholders and Interests:**
 - Scientist: Wants to determine the structure of a material on which he has diffraction data.
- **Preconditions:** Scientist has collected data and has a starting model in mind. Scientist knows the location of and has access to data.
- **Success Guarantee:** Refinement results are saved.

Main Success Scenario

1. Scientist starts the SrRietveld application.
2. Scientist configures the data.
 1. Scientist tells SrRietveld to load data from file.
 2. SrRietveld reads the file and collects data and metadata.
 3. Scientist selects channels to use in the fit
 4. For each channel, Scientist configures the phase.
 1. Scientist selects or specifies a peak profile function.



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refine a structure in 10 lines

Brief

Scientist starts with a cif file and data from a well-known diffraction beam line. In 10 lines (or less) of configuration, Scientist tells [SrRietveld](#) the instrument, loads the data, loads the cif file and starts the refinement. [SrRietveld](#) uses standard information about the instrument to configure the refinement. Optionally, Scientist informs [SrRietveld](#) how to deviate from the standard refinement procedure for the instrument.

Expanded scenerio

- **Scope:** SrRietveld application
- **Level:** user goal
- **Primary Actor:** Scientist
- **Stakeholders and Interests:**
 - Scientist: Wants to determine the structure of a material on which he has diffraction data without too much effort.
- **Preconditions:** Scientist has collected data and has a starting model in mind. Scientist knows the location of and has access to data. Scientist knows the instrument on which the data was collected.
- **Success Guarantee:** Refinement results are saved.

Explore metal-insulator transition of V2O3 in nano-particle sample

Brief

A scientist has diffraction data of V2O3 in both bulk sample and nano-particle sample at both low temperature (20K) and high temperature (300K). Scientist has diffraction data of V2O3 in nano-particle sample at transition temperatures. These data are not in full range of diffraction. Scientist uses [SrRietveld](#) to determine the lattice parameter, atoms' fractional coordinates and peak profile parameters of V2O3 with bulk sample data. Scientist uses [SrRietveld](#) to determine the size parameter of V2O3 with nano-sample data and with the lattice parameters, atoms' fractional coordinates and peak profiles parameter, which are determined by bulk sample, fixed. Scientist uses [SrRietveld](#) to explore the diffraction data of V2O3 in mixed phases at transition temperatures to calculate the fraction between two phases.

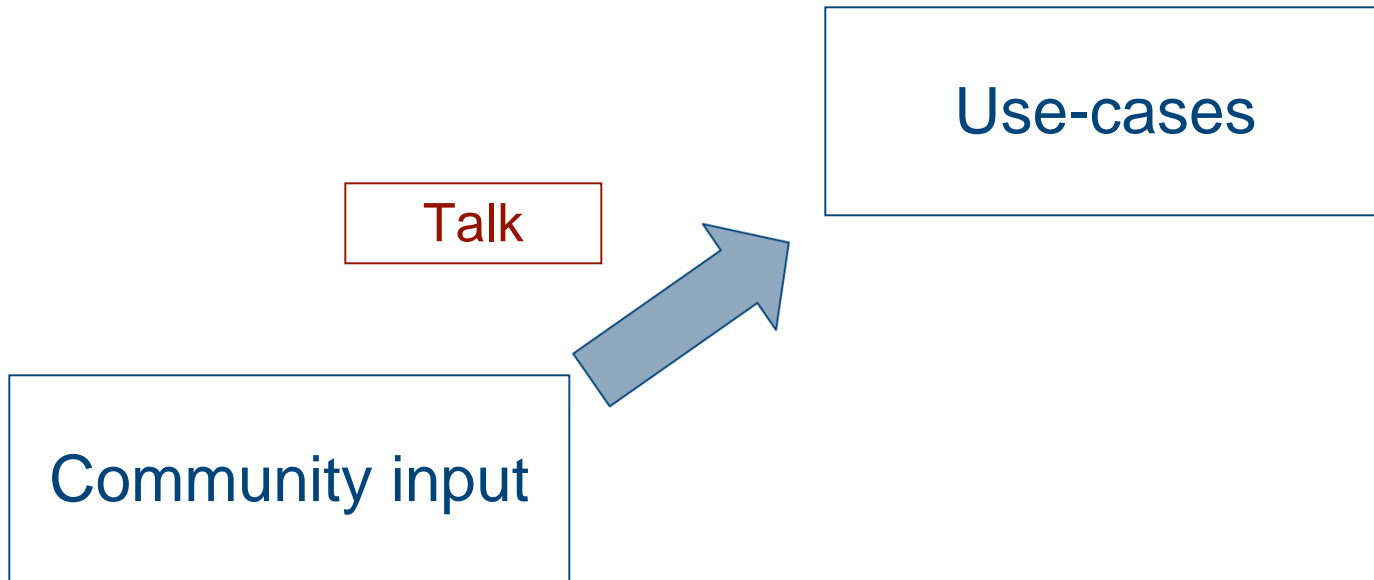
Expanded scenario

- **Scope:** [SrRietveld](#) application
- **Level:** user goal
- **Primary Actor:** Scientist
- **Stakeholders and Interests:**
 - Scientist: Wants to determine the structure of a material on which he has diffraction data.
- **Preconditions:** Scientist has collected data and has a starting model in mind. Scientist knows the location of and has access to data.
- **Success Guarantee:** Refinement results are saved.

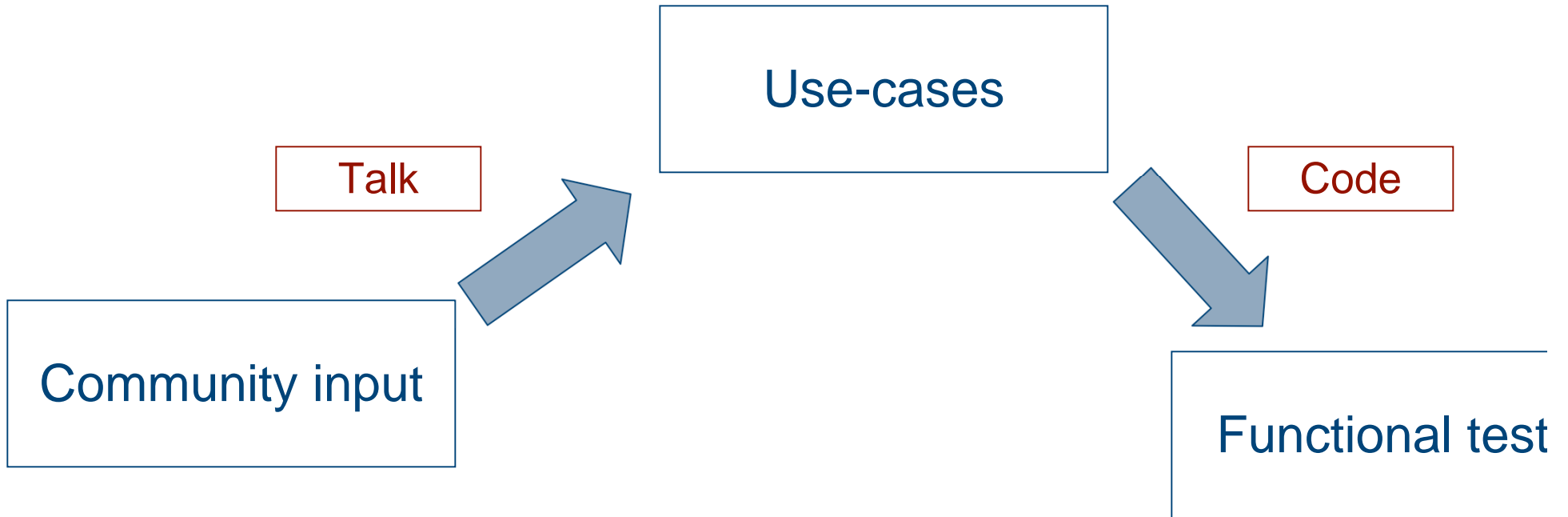
Main Success Scenario

1. Scientist uses [SrRietveld](#) to do LeBail to refine the lattice parameters and peak profile parameters of V2O3 at low-T (pure phase) and high-T (pure phase) in bulk sample;
2. Scientist uses [SrRietveld](#) to do Rietveld refinement on V2O3 at low-T (pure phase) and high-T (pure phase) in bulk sample to determine atoms' fractional coordinates, peak profile parameters;
3. Scientist adds the particle-size (50~100 nm) to [SrRietveld](#). [SrRietveld](#) do the Rietveld refinement on V2O3 at low-T (pure phase) and high-T (pure phase) in nano-particle sample to determine the parameters related to size effect.
4. Scientist uses [SrRietveld](#) to calculate the fraction of two phases of the diffraction data at transitional temperature (mixed phase). The diffraction is obtained on nano-particle sample, and in a limited range of 2-theta. It may not be appropriate for Rietveld refinement.

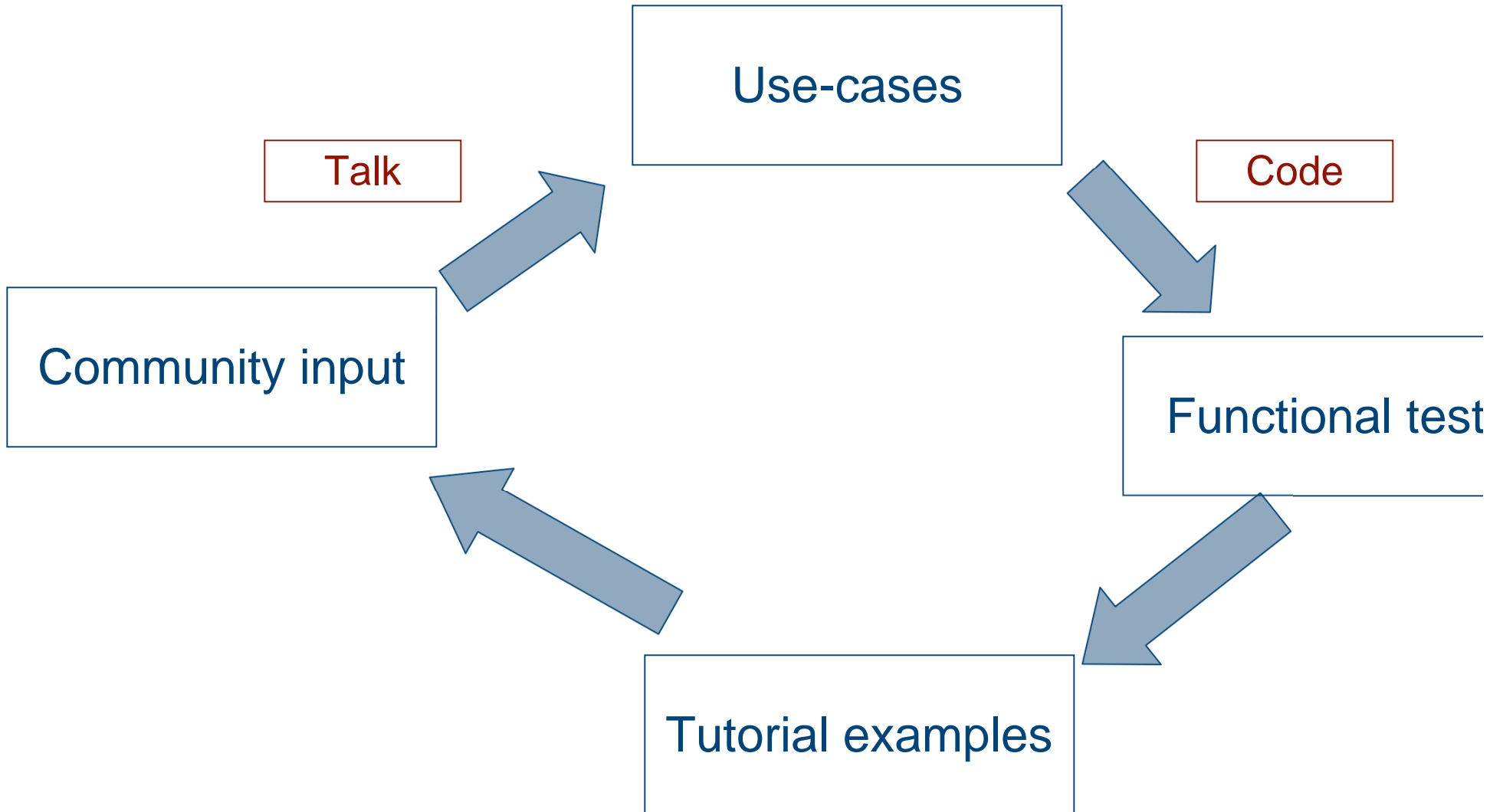
Community involvement in software development cycle



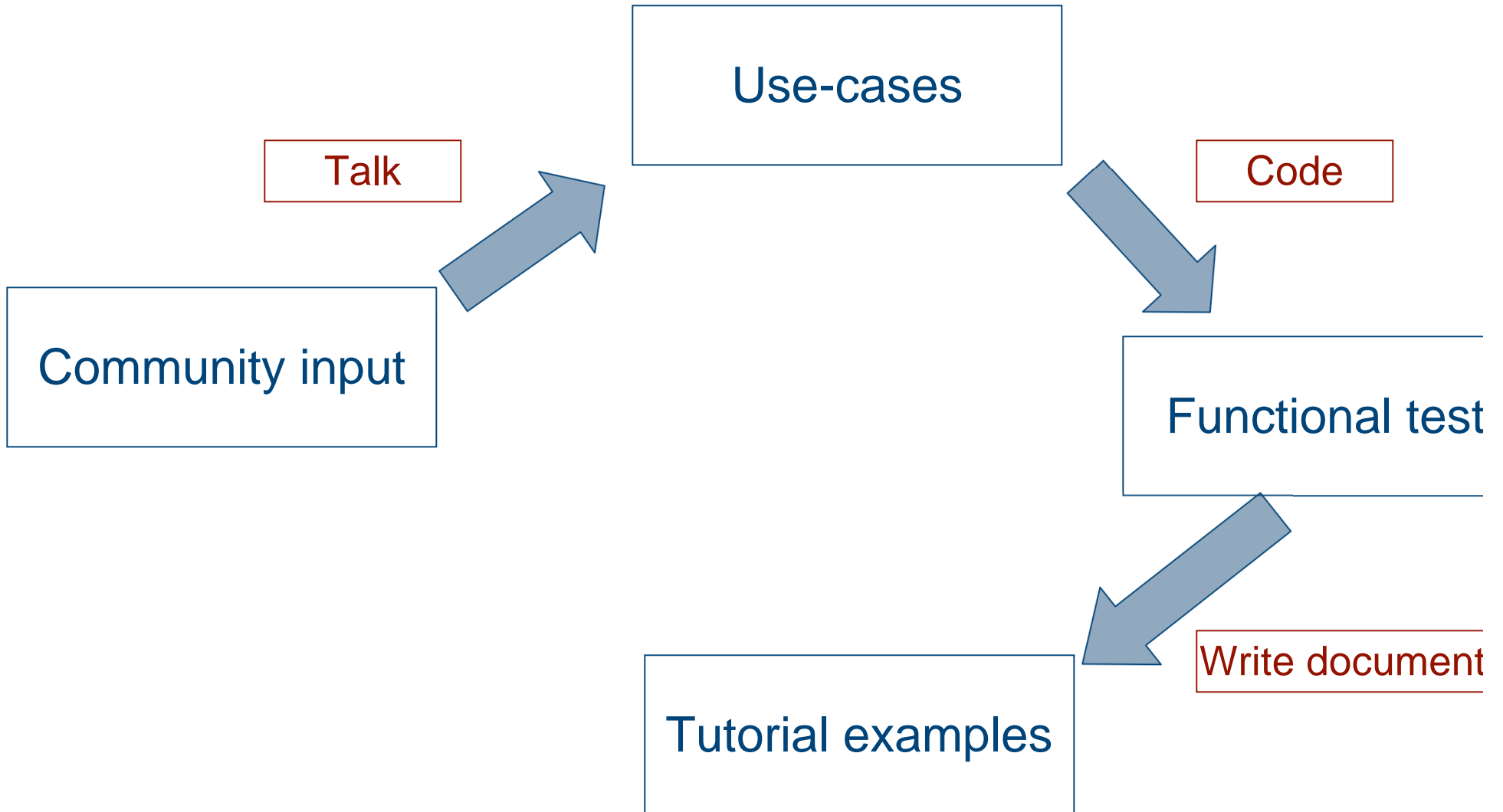
Community involvement in software development cycle



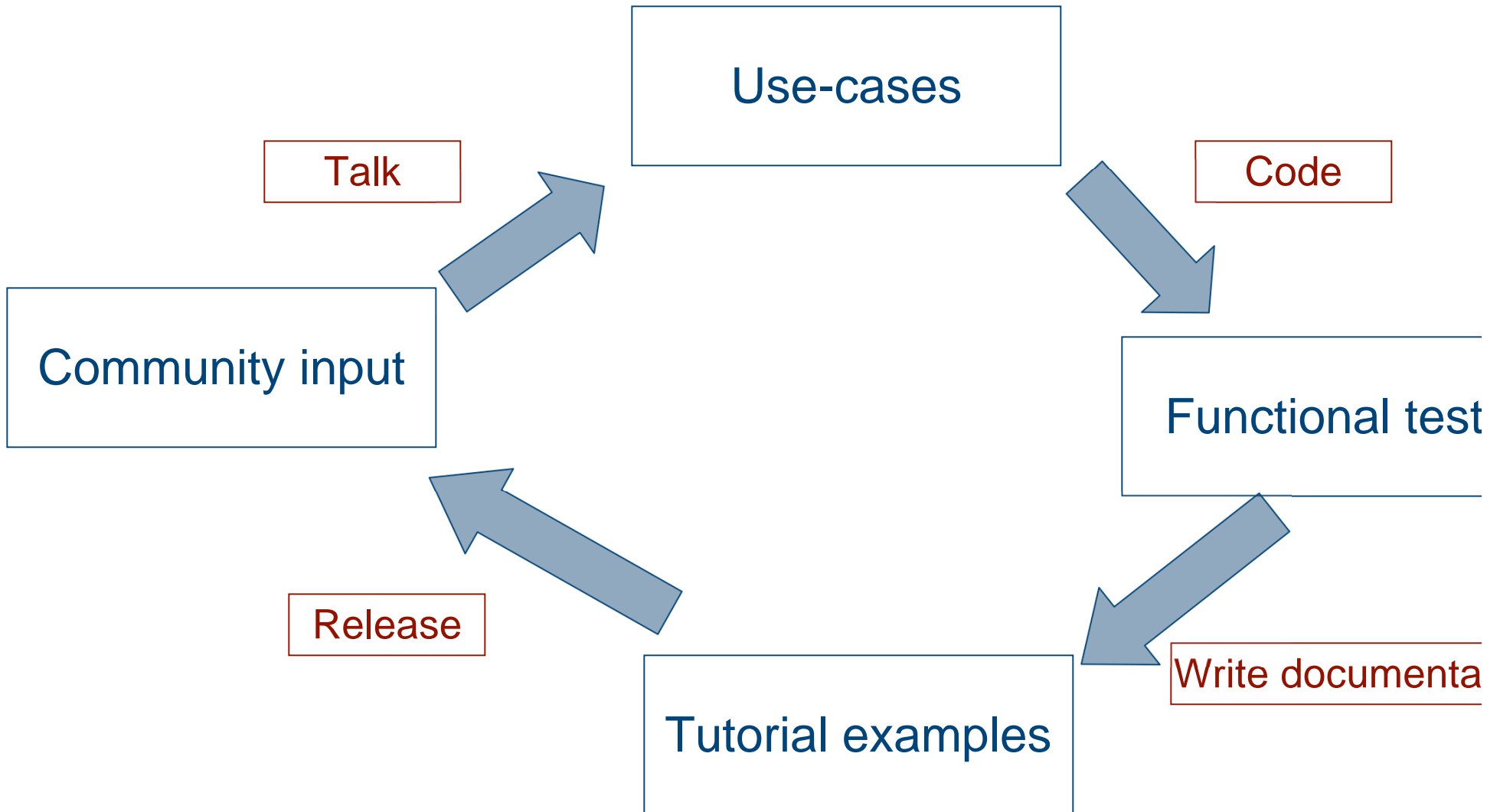
Community involvement in software development cycle



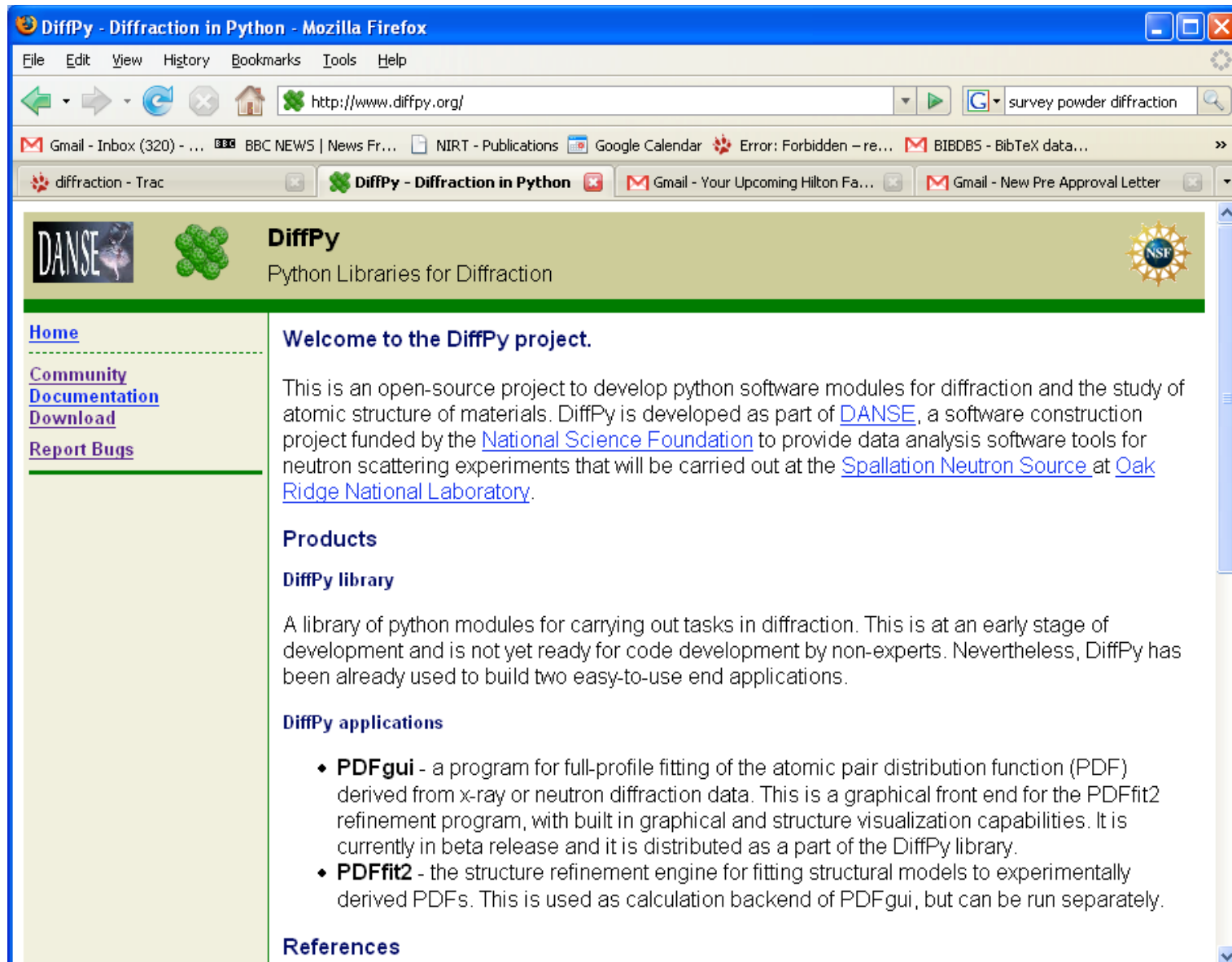
Community involvement in software development cycle



Community involvement in software development cycle



Community engagement: software releases



The screenshot shows a Mozilla Firefox browser window displaying the DiffPy website. The browser's address bar shows the URL <http://www.diffpy.org/>. The website header features the DANSE logo, the DiffPy logo (a cluster of green spheres), and the text "DiffPy Python Libraries for Diffraction". A navigation menu on the left includes links for Home, Community, Documentation, Download, and Report Bugs. The main content area is titled "Welcome to the DiffPy project." and contains the following text:

This is an open-source project to develop python software modules for diffraction and the study of atomic structure of materials. DiffPy is developed as part of [DANSE](#), a software construction project funded by the [National Science Foundation](#) to provide data analysis software tools for neutron scattering experiments that will be carried out at the [Spallation Neutron Source](#) at [Oak Ridge National Laboratory](#).

Products

DiffPy library

A library of python modules for carrying out tasks in diffraction. This is at an early stage of development and is not yet ready for code development by non-experts. Nevertheless, DiffPy has been already used to build two easy-to-use end applications.

DiffPy applications

- **PDFgui** - a program for full-profile fitting of the atomic pair distribution function (PDF) derived from x-ray or neutron diffraction data. This is a graphical front end for the PDFfit2 refinement program, with built in graphical and structure visualization capabilities. It is currently in beta release and it is distributed as a part of the DiffPy library.
- **PDFfit2** - the structure refinement engine for fitting structural models to experimentally derived PDFs. This is used as calculation backend of PDFgui, but can be run separately.

References

```
python setup.py install
```

The DiffPy subversion repository can be also browsed online [here](#).

DiffPy Releases

Please, join in the [community](#) forum for tips and tricks and feedback.

Name	Date	Size	Downloads
diffpy-1.0b.1792.exe	2007-12-18 20:39	20.4M	105
diffpy-1.0b.1792.tgz	2007-12-18 20:39	7.7M	42
diffpy-1.0b.1368.exe	2007-07-24 15:30	20.8M	255
diffpy-1.0b.1368.tgz	2007-07-24 15:30	7.4M	86
diffpy-1.0b.1351.exe	2007-07-06 16:30	20.8M	39
diffpy-1.0b.1351.tgz	2007-07-06 16:30	7.4M	25
diffpy-1.0b.1336.exe	2007-06-26 15:00	20.4M	22
diffpy-1.0b.1336.tgz	2007-06-26 15:00	7.9M	20
diffpy-1.0b.1309.exe	2007-06-17 18:00	20.4M	23
diffpy-1.0b.1309.tgz	2007-06-17 18:00	7.3M	21
diffpy-1.0b.1232.exe	2007-05-14 21:00	20.4M	47
diffpy-1.0b.1232.tgz	2007-05-14 21:00	6.9M	39
diffpy-1.0b.1218.exe	2007-05-07 11:00	20.4M	21
diffpy-1.0b.1218.tgz	2007-05-07 11:00	7.3M	24

If you have questions or remarks about this site, please contact [Simon J. Billinge](#).



DiffPy

Python Libraries for Diffraction



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Documentation

User manuals

PDFgui user manual formatted as [HTML](#), [PDF](#)

PDFfit2 Documentation is not yet available besides built-in help system. Since command and variable names are quite similar to the old PDFFIT, you can use this [manual](#) and [command reference](#) to get started with the program.

Reports

- 2007-08-27 - [NSF nugget](#) describing PDFgui.

Publications

1. C. L. Farrow, P. Juhas, J. W. Liu, D. Bryndin, E. S. Bozin, J. Bloch, Th. Proffen and S. J. L. Billinge, [PDFfit2 and PDFgui: computer programs for studying nanostructure in crystals](#), *J. Phys.: Condens. Matter* **19**, 335219 (2007)
2. Th. Proffen and S. J. L. Billinge, [PDFFIT a program for full profile structural refinement of the atomic pair distribution function](#), *J. Appl. Crystallogr.* **32**, 572 (1999)

If you have questions or remarks about this site, please contact [Simon J. Billinge](#).

3 Examples and tutorials

In this chapter we present series of examples and tutorials aimed at users already comfortable with the gui, to provide training in advanced gui features designed for most common modeling situations, such as building the structure from scratch, calculating the PDF based on a given structure, linking two fits, and creating and executing a series of fits on a sequence of data sets.

3.1 Building structure model using crystal symmetry

The purpose of this example is to demonstrate to the user the symmetry expansion capabilities of PDFgui. The goal is again to create a simple fit of Ni PDF, but this time from scratch rather than from a preexisting structure file. Further goal is to associate a dataset with the refinement, configure and execute a refinement, and display the result. The focus will be on the symmetry expansion features only, and the steps that are described earlier in [Section 2.2 \[Simple fit\], page 6](#) are left for the user to recreate. File to be used in this

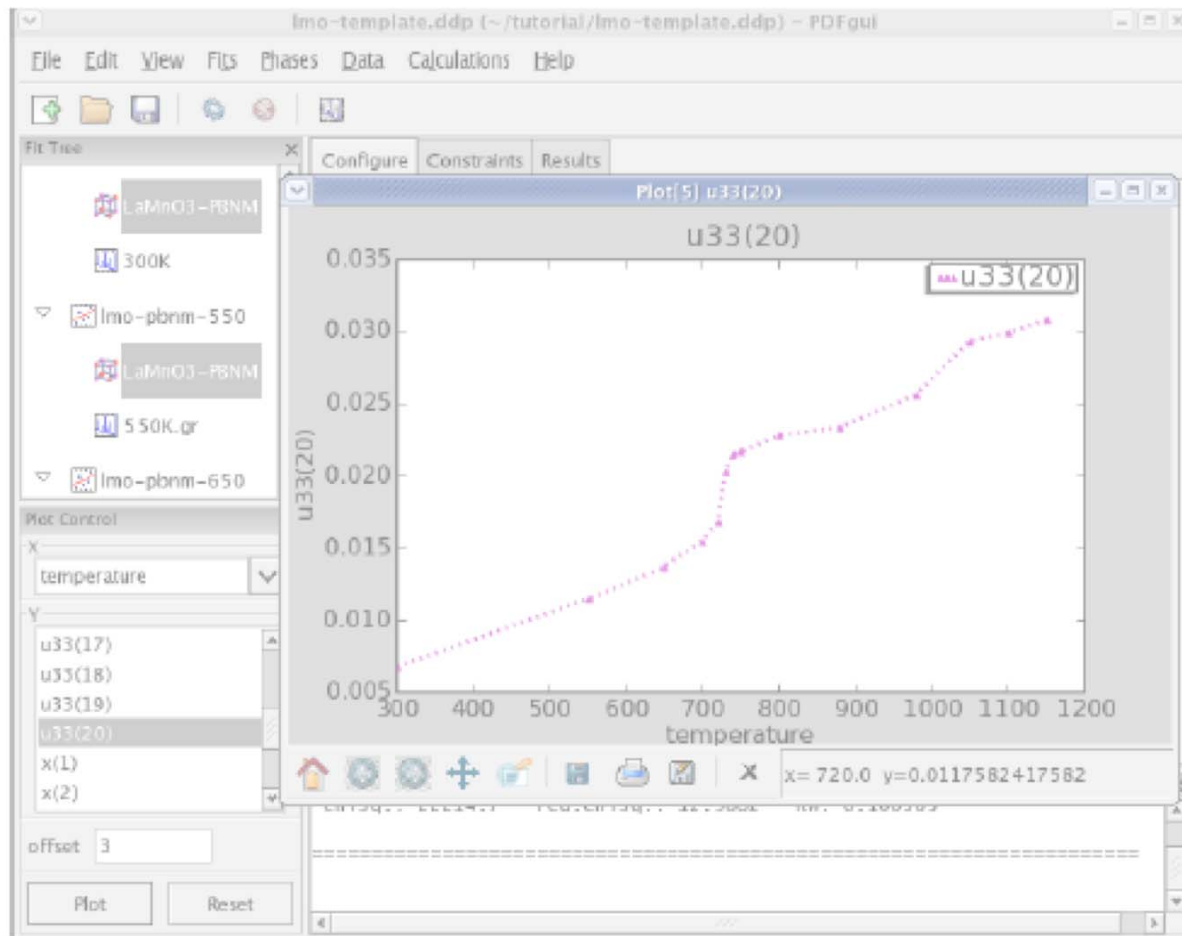


Figure 3.7: Displaying the refinement results as a function of external parameter: T-series refinement of LaMnO₃, example of isotropic ADP of oxygen atom on general position in *Pbnm* setting. Notable are the offsets just above 700 K (Jahn-Teller transition), and at around 1000 K when sample converts from orthorhombic to rhombohedral symmetry.

Despite quite high temperatures, an onset of the static offset above the transition temperature is clearly marked by this parameter, as apparent in Figure 2.7. Curious user could



DiffPy

Python Libraries for Diffraction



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Community

To ensure a bright future for the DiffPy project it is essential to build a strong community of users and contributing developers. There are several Google groups for support and development of DiffPy and related applications.

[diffpy-users](#)

Help on usage of PDFgui, PDFfit2 and other DiffPy components. This group should become a knowledge base for PDFgui user tips, tricks and troubleshooting. Feel free to ask your question here.

Subscribe email:

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[diffpy-dev](#)

For discussions about development and changes of PDFgui, PDFfit2 and DiffPy library in general. Materials scientists, chemists physicists, engineers - please contribute by telling us your needs or sharing your suggestions here.

Subscribe email:

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You can also share your comments, suggestions, praise or complaints by sending email to [Simone J. Billinge](#).

To report or browse bugs, please use the link at the sidebar of this page.



Home

New since last time: **3** members

Welcome to diffpy-users, a user help and discussion forum for PDFgui, PDFfit2 and other DiffPy components.

DiffPy software is part of an open source software development project, the diffraction sub-project of [DANSE](#), funded by the [National Science Foundation \(NSF\)](#).

Please, post your questions or comments about [DiffPy](#) software. We encourage you to join the group, but if you prefer to post without joining, just email diffpy-users@googlegroups.com.

Feel free to visit [diffpy-dev](#) for DiffPy development discussions.

[\[edit welcome message\]](#)**Discussions** 9 of 140 messages [view all »](#)[Exporting Structures](#)

By Chris Farrow - Apr 28 - 2 authors - 1 reply

[PDFgetX2 for windows](#)

By Pavol Juhas - Apr 16 - 3 authors - 3 replies

[copying structural parameters between datasets](#)

By Pavol Juhas - Feb 28 - 3 authors - 2 replies

[installation of PDFgui on SuSe 10](#)

By Pavol Juhas - Feb 23 - 1 author - 0 replies

[lattice parameter differences between PDF and Rietveld?](#)

By Simon Billinge - Feb 22 - 2 authors - 1 reply

[Isotropic displacement parameters and r-series fitting](#)

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Group info

Members: 56**Activity:** Low activity**Language:** English**Group categories:**[Science and Technology](#)[> Physics](#)[Computers > Software](#)[add a category](#)[More group info »](#)

diffpy-users

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plotting r-dependent series

Options

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[More options](#) Jan 25, 9:24 am

hi all,
I feel like a real idiot, but apparently I cannot plot the structural parameters in my r-dependent fit. I prepared the macro as usual, setting first r and then the increment. The fit starts nicely but then, if I want to look at the structural parameters as a function of r, I realise that r does not appear in the list of possible x in the plot control window. I tried selecting i) the fits, ii) the structures, iii) the data. At the end I gave up...
Can anyone help me? I'm using the windows version

cheers,
Monica

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[emil.bo...@gmail.com](#) [View profile](#)

[More options](#) Jan 25, 11:16 am

This is how to plot the refined parameters against "r" in r-dependent fit. Select all structures in the fit trees of your linked fits. In the plotting window select the desired parameter(s) that you want to plot. As a variable to plot against choose "index". This is an integer parameter that represents your r. Be aware of the fact that value in units of r has to be calculated by multiplying the index with the r-step size in your refinement. In other words, think twice before interpreting at which r (in Angstroms) something starts to happen, as

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[www.StatisticsSolutions.com](#)

interpreting at which r (in Angstroms) something starts to happen, as index is what it says - index, that enumerates steps in your r -dependent refinement, and knows nothing about the actual lengths. The reason this was set up like this is because you could use anything as your r_{\min} and any step size to determine your r_{\max} ; moreover, sometimes you may do a boxcar fitting where you keep the refinement range size fixed, but move both r_{\min} and r_{\max} simultaneously. In all these cases it is hard to predict what quantity and against which r user wants to plot the results. By having index as a variable, it allows you to see the trends, and then take your time to find the best way to interpret the result in the language of actual distances.

Cheers,

Emil

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[More options](#) Jan 25, 1:32 pm

Hi Monika,

You can select the structures and then choose index for x and the parameters you want to plot for y . This gives each of your r -fits a number on the x -axis, I think in the order they appear in your fit tree. I'm not sure if there is a way to plot the actual r value vs the parameters, but you can export this data and change the x -values in another program. It will probably still save you time.

Enabling this feature might be a nice suggestion for the developers.

Hope that helps!

Katharine

On Jan 25, 2008 5:24 AM, <mdapia...@gmail.com> wrote:

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--

Katharine Page
Graduate Student, Materials Department
University of California, Santa Barbara, CA 93106
Phone: (805) 893 5770, kp...@mrl.ucsb.edu

Science does not know its debt to imagination.
~Ralph Waldo Emerson

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Monica Dapiaggi [View profile](#)

[More options](#) Sep 30 2002, 7:56 pm

Hi Emil and Katharine,
thanks for the tip...I was actually wondering what was the meaning of
'index'!!!

It worked perfectly!

thanks again

Monica

At 17.16 25/01/2008, you wrote:

- [Show quoted text](#) -

Monica Dapiaggi
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Home

Welcome to diffpy-dev, a group for discussions on development and changes of PDFgui, PDFfit2 and [DiffPy](#) library in general.

DiffPy software is part of an open source software development project, the diffraction sub-project of [DANSE](#), funded by the [National Science Foundation \(NSF\)](#).

You can contribute by joining the group or by sending email to diffpy-dev@googlegroups.com. When reporting bugs, always give reproducible example and include software version and OS platform. Send us patches if you can!

For user help and discussions, visit [diffpy-users](#).

[\[edit welcome message\]](#)



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By Pavol Juhas - May 20 - 1 author - 0 replies

[PDFgui Not working no output](#)

By nmrg...@gmail.com - May 20 - 1 author - 0 replies

[BCA workshop feedback !](#)

By Pavol Juhas - Apr 10 - 4 authors - 5 replies

[Debye behavior of thermal parameters](#)

By email.bo...@gmail.com - Apr 10 - 1 author - 0 replies

[particle size function](#)

By dif...@pa.msu.edu - Apr 9 - 1 author - 0 replies

[Linux distributions ..](#)

By Pavol Juhas - Apr 9 - 2 authors - 1 reply

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Language: English

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can not open ppt file

[Options](#)★ 1 message - [Collapse all](#)[Pavol Juhas](#) [View profile](#)[More options](#) May 21, 2:20 am

- Hide quoted text -

On Thu, May 15, 2008 at 06:11:06PM -0400, dif...@www.diffpy.org wrote:

> reporter: hj...@lanl.gov

> summary: can not open ppt file

> description: I do not know what went wrong... this project file
> worked well and suddenly pdfgui can not open it any more... last
> thing I did on this ppt file are> 1. in one structure, I created one position for He atoms with very
> large occupancy (16000000)
> 2. in another structure, I inserted 1000 atoms sitting on the same
> position

> component: pdfgui

> version: 1.0b.1792

> traceback: {{{

> Traceback (most recent call last):

> File "diffpy\pdfgui\gui\mainframe.pyc", line 415, in _f
> File "diffpy\pdfgui\gui\mainframe.pyc", line 2186, in onOpen
> File "diffpy\pdfgui\control\pdfguicontrol.pyc", line 468, in load
> File "diffpy\pdfgui\control\fitting.pyc", line 203, in load
> File "diffpy\pdfgui\control\examiner.pyc", line 155, in load[Home](#)[Discussions](#)[+ new post](#)[Members](#)[Pages](#)[Files](#)[About this group](#)[Edit my membership](#)[Group settings](#)[Management tasks](#)[Invite members](#)[Sponsored Links](#)[Google Analytics](#)Get The Data You Need Faster With
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www.rockymountainlabs.com[Materials Analysis](#)Techniques- XRD, Microscopy, DSC/T
Radiography, Infrared, XRF, SEM
www.xrddiff.com

```
> File "diffpy\pdfgui\gui\mainframe.pyc", line 2186, in onOpen
> File "diffpy\pdfgui\control\pdfguicontrol.pyc", line 468, in load
> File "diffpy\pdfgui\control\fitting.pyc", line 203, in load
> File "diffpy\pdfgui\control\organizer.pyc", line 155, in load
> File "diffpy\pdfgui\control\fitstructure.pyc", line 706, in load
> File "diffpy\pdfgui\control\fitstructure.pyc", line 128, in readStr
> File "diffpy\Structure\pdfffitstructure.pyc", line 66, in readStr
> File "diffpy\Structure\structure.pyc", line 172, in readStr
> File "diffpy\Structure\Parsers\StructureParser.pyc", line 58, in parse
> File "diffpy\Structure\Parsers\P_pdfffit.pyc", line 104, in parseLines
> StructureFormatError: 5770: file is not in PDFfit format
> )))
```

Hi Hyunjeong,

I could reproduce the problem for step 1, but step 2 did not seem to cause any problem. I created a new ticket for this bug at <http://danse.us/trac/diffraction/ticket/361>, it should be easy to fix that.

Please, check if you can get invalid project file just by inserting 1000 atoms. If it is so, let me know how to reproduce this, or just email me the broken project. Thank you,

Pavol

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Community engagement: Education and outreach

- Hands on workshops
 - American Conference on Neutron Scattering, Santa Fe, NM, May 2008
 - 11th European Powder Diffraction Conference, Warsaw, Poland, Sept. 2008
 - British Crystallographic Association, March 2008

- Talks
- Posters



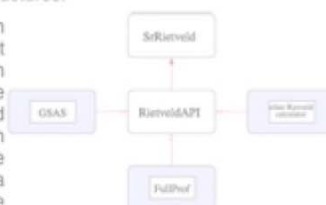
SrRietveld: Toward A Next-Generation Rietveld Refinement Program W. Zhou, C. L. Farrow, S. J. L. Billinge



The Rietveld Method and DANSE

Rietveld refinement [1] is used in the characterization of crystalline material. The neutron and X-ray diffraction of powder samples results in a pattern characterized by peaks in intensity at certain positions. The height, width and position of these peaks can be used to determine many aspects of the material structures.

DANSE (Distributed Data Analysis for Neutron Scattering Experiments) is a software development project on distributed data analysis for neutron experiments. The goal of the DANSE project are to build a software system that enables new and more sophisticated science to be performed with neutron scattering experiments, makes the analysis easier for all scientists and provides a robust software infrastructure that can be maintained in the future.



[1] H. M. Rietveld (1969). "A profile refinement method for nuclear and magnetic structures". *Journal of Applied Crystallography* 2: 65-71.

Features

SrRietveld provides intuitive Python commands to set up a complicated refinement configuration in a few steps for a specific diffractometer.

```
> myfit = simpleFit( Data = "mydata.dat",  
                    bgData = "mybackground.dat",  
                    Instrument = "POWGEN3",  
                    Model = ["structure1.cif"],
```

With SrRietveld's flexible and powerful plotting functionalities, users can

(1) observe the refinement result and (2) easily investigate the relationships among physical parameters with the flexible plotting tool.



SrRietveld - Script User Interface to Rietveld Refinement

SrRietveld is the Rietveld refinement application in the DANSE project. It is designed to facilitate new science that will be enabled by the powerful POWGEN3 diffractometer at the Spallation Neutron Source at Oak Ridge National Lab. It is also a general purpose application designed to solve contemporary scientific Rietveld refinement problems.

SrRietveld is written in the Python programming language and consists of a variety of modules for Rietveld refinement and related tasks, which are compiled from Fortran or C++. SrRietveld is built on top of a general application programming interface (API) for Rietveld refinement, referred to as RietveldAPI. RietveldAPI can be functionalized using different Rietveld refinement engines without modifying SrRietveld.

In the SrRietveld alpha release, FullProf is used as the Rietveld refinement engine. RietveldAPI allows the refinement engine to be changed. For example, implementing GSAS as a refinement engine would allow FullProf or GSAS, or both, to be selected for a particular refinement.

SrRietveld's alpha release is a demo release. We encourage interested developers to download it from <http://danse.us/trac/SrRietveld>

RietveldAPI





BCA workshop feedback !

[Options](#)[Home](#)★ 6 messages - [Collapse all](#)**Thomas E. Proffen** [View profile](#)[More options](#) Apr 8, 6:49 am

Hi developers ;-)

We have just finished the BCA PDFgui workshop, and there is a number of bugs and feature request coming from this group (due to internet security we could not use the build in submission feature). Here they are:

- (1) FEATURE: Is there a way to show error bars on the plots (e.g. ull as function of T). If not this should be added.
- (2) FEATURE: The option to plot R_w as function of T, x, r seems to be missing - would be nice if it could be added.
- (3) BUG: The 'spdiameter' should really be a property of the phase and not the dataset - think a mix of particles of two different sizes. I think this is how it was implemented in the old PDFFIT (possibly after the version Jaques used for pdfFIT2).
- (4) FEATURE/BUG: Most common error was to leave U_{ij} 's at zero. Better error message would be helpful - e.g. U_{ij} 's cannot be all zero !
- (5) BUG: The results panel of the phase tab did update to silly values if a fit was aborted. Should retain earlier values.
- (6) FEATURE: It would be nice to have a 'select all phases' or 'select a;;' datasets in the fit tree (may be I missed how to do it - all I can do is select all).

That is all. Business was great, nice and we got some positive feedback. To

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- Other activities
 - Contributing code to external open source projects



Community involvement in software development cycle

