



# DANSE Diffraction Software for the SNS: DiffDANSE

**S.J.L. Billinge**

*Dept. Physics and Astronomy  
Michigan State University*



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

## DiffDANSE goals

- Make diffraction data analysis software that SNS users (and other people) want to use!
- Make sure that it has a long life
- Have fun doing it



## DiffDANSE goals

- Make diffraction data analysis software that people want to use!
  - Solves people's scientific problems, opens new scientific horizons
  - Shortens time to publication
  - Flexible
  - Easy to use
    - Good user documentation
  - Robust and Stable



## DiffDANSE goals

- **Make sure that it has a long life**
  - Maintainable (esp. by others, i.e., SNS!)
    - Good developer documentation
    - Requirements/use cases/tests stored with the code
  - Extensible
    - modular
  - Scalable
    - Dynamic memory allocation
    - Distributable/parallelizable
  - Quality controlled
  - Open source



# Outline

- Goals
- Progress
- Planning



# Progress

- Management and Organisation
- Software



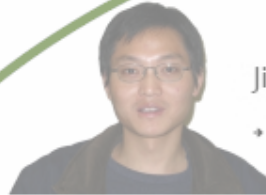
# Management and Organisation

- Sub-contracts
  - In place
  - MSU hasn't invoiced Caltech yet – need to clear up what to bill for
  - Second period – not in place, should be quick. Need to follow up after my trip to Europe
- Hiring
- Project controls
- Training
- Software process



# DiffDANSE development team

program in his own style while  
 assuring that the individual  
 parts of the final  
 program will work  
 together.

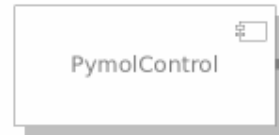


**Jiwu Liu – Grad Student**  
 → PDFControl, GUI, PDFPlot, PDFData

**Professor Simon Billinge**  
 → Project Manager



**Dmitriy Bryndin – Grad Student**  
 → PymolControl, PDFControl, GUI



3d plot manager



Server interface



**Chris Farrow – Grad Student**  
 → PDFProxy, PDFFitting

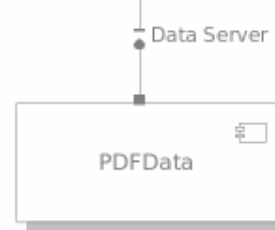
Plot manager



Fit manager



**Pavol Juhas – Postdoc**  
 → PymolControl, PDFData



Data Server

Contains PDF data,  
 structure data  
 and metadata.



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

# Management and Organisation

- Sub-contracts
- Hiring
- Project controls
  - Emil Bozin handling reporting functions
  - Use Google spreadsheets for collecting developer input
  - Cut and paste to MS excel for computing information to forward to Mike
    - Not completely trouble-shot, but hopeful that this will work well with little overhead for everyone. See Emil for demo.
- Training
- Software process



# Management and Organisation

- Sub-contracts
- Hiring
- Project controls
- Training
  - On-the-job training
    - Works ok because of interactive group
  - Pyre training is a priority. Working with MM and MA after this meeting to jump-start this
- Software process



# Management and Organization

- Sub-contracts
- Hiring
- Project controls
- Training
- Software process
  - Objective: satisfy the needs of
    - project reporting
    - the requirement of usable, extensible, maintainable code
    - quality assurance requirements
  - Requirements:
    - Minimize developer/management overhead



5.4.6.3PyMol - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/5.4.6.3PyMol

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Welcome to Gmail 5.4.6.3PyMol - diffraction - Trac Welcome to RESX



Search

[Login](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Title Index](#) | [Recent Changes](#) | [Page History](#)

## 5.4.6.3 PyMol

This task is to wrap the PyMol molecular structure viewer into the Pyre framework. More information about PyMol can be found [here](#). From the PyMol page: "PyMOL is a molecular graphics system with an embedded Python interpreter designed for real-time visualization and rapid generation of high-quality molecular graphics images and animations."

This task also includes developing a DANSE project API for structure-viewers that will be used also by other structure viewer software packages such as Atomeye.

### 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

- [Vision](#)
- [Use Cases](#)
- [Planning](#)
- [Supplementary Specifications](#)

Done McAfee SiteAdvisor

start 5.4.6.3PyMol - di... 3 Windows Expl... Microsoft PowerP... 96% 5:34 AM

SrRietveld - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/SrRietveld

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Gmail - Re: ICNS SrRietveld - diffraction - Trac Welcome to RESX

[Start Page](#) [Title Index](#) [Recent Changes](#) [Page History](#)

## SrRietveld

This is the main Rietveld application for DiffDANSE. It will support basic Rietveld functions found in GSAS, including some capability for magnetic refinements.

### Introduction

- [Project Timeline?](#)
- [Developers and personnel](#)
- [Software License](#)
- [Source trunk](#)
- [Documentation?](#)
- [Obtaining and building the code?](#)
- [Information for reviewers?](#)
- [Information for testers?](#)
- [Community discussion?.](#) (Please post here your comments and suggestions.)

### Developer Documentation Workproducts

- [Vision?](#)
- [Use Cases](#)
- [Planning?](#)
- [Supplementary Specifications?](#)

### Developer notes

- [Scratch place for old use cases](#)
- [design notes?](#)
- [process blog?](#)
- [related meetings: Meeting 2006-12-11 Meeting 2006-12-15 Meeting 2006-12-18](#)
- [Mike McKerns' useful process tutorial](#)

Edit this page Attach file Delete this version Delete page

Done McAfee SiteAdvisor

start 2 Firefox C:\WIN... 3 Win... Macrom... Microso... 100% 9:35 PM

5.4.6.3PyMol - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/5.4.6.3PyMol

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Welcome to Gmail 5.4.6.3PyMol - diffraction - Trac Welcome to RESX



Search

[Login](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

Wiki

Timeline

Roadmap

Browse Source

View Tickets

New Ticket

Search

[Start Page](#)

[Title Index](#)

[Recent Changes](#)

[Page History](#)

## 5.4.6.3 PyMol

This task is to wrap the PyMol molecular structure viewer into the Pyre framework. More information about PyMol can be found [here](#). From the PyMol page: "PyMOL is a molecular graphics system with an embedded Python interpreter designed for real-time visualization and rapid generation of high-quality molecular graphics images and animations."

This task also includes developing a DANSE project API for structure-viewers that will be used also by other structure viewer software packages such as Atomeye.

### 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

- [Vision](#)
- [Use Cases](#)
- [Planning](#)
- [Supplementary Specifications](#)

Done McAfee SiteAdvisor

start 5.4.6.3PyMol - di... 3 Windows Expl... Microsoft PowerP... 96% 5:34 AM

Firefox browser window showing the URL: <http://danse.us/trac/diffraction/browser/diffraction/StructureViewer/trunk/AUTHORS.txt>

Browser tabs: Welcome to Gmail, /diffraction/StructureViewer/trunk/..., Welcome to RESX


 Search

[Login](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

- Wiki
- Timeline
- Roadmap
- Browse Source
- View Tickets
- New Ticket
- Search

[Revision Log](#)

## root / diffraction / StructureViewer / trunk / AUTHORS.txt

View revision:

**Revision 704 (checked in by juhas, 3 months ago)** Better to have these files in package root directory as done in most of open source packages.

Line	
1	Simon Billinge
2	Emil Bozin
3	Dmitriy Bryndin
4	Chris Farrow
5	Pavol Juhas
6	Jiwu Liu
7	Wenduo Zhou

Note: See [TracBrowser](#) for help on using the browser.

**Download in other formats:**  
[Original Format](#)



Powered by [Trac 0.9.5](#)  
By [Edgewall Software](#).

Visit the Trac open source project at  
<http://trac.edgewall.com/>

Windows taskbar showing: Done, McAfee SiteAdvisor, 96% battery, 5:35 AM

Taskbar icons: start, /diffraction/Struc..., 3 Windows Expl..., Microsoft PowerP..., McAfee SiteAdvisor, 96% battery, 5:35 AM

5.4.6.3PyMol - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/5.4.6.3PyMol

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Welcome to Gmail 5.4.6.3PyMol - diffraction - Trac Welcome to RESX



Search

[Login](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Title Index](#) | [Recent Changes](#) | [Page History](#)

## 5.4.6.3 PyMol

This task is to wrap the PyMol molecular structure viewer into the Pyre framework. More information about PyMol can be found [here](#). From the PyMol page: "PyMOL is a molecular graphics system with an embedded Python interpreter designed for real-time visualization and rapid generation of high-quality molecular graphics images and animations."

This task also includes developing a DANSE project API for structure-viewers that will be used also by other structure viewer software packages such as Atomeye.

### 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

- [Vision](#)
- [Use Cases](#)
- [Planning](#)
- [Supplementary Specifications](#)

Done McAfee SiteAdvisor

start 5.4.6.3PyMol - di... 3 Windows Expl... Microsoft PowerP... 96% 5:34 AM

PyMolUseCases - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/PyMolUseCases

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Gmail - Re: ICNS PyMolUseCases - diffraction - Trac Welcome to RESX

## 5.6.4.3 PyMol Use Cases

### Use Cases

- [PyMolUC1-View a structure on screen](#) - Accepted
- [PyMolUC2-View multiple structures on screen](#) - Accepted
- [PyMolUC3-Save an image of a structure](#) - Rejected
- [PyMolUC4-Animate a series of structures](#) - Rejected
- [PyMolUC5-Save a movie of an animation](#) - Rejected
- [PyMolUC6-Change the style of plots](#) - Accepted
- [PyMolUC7-Change the color of plot elements](#) - Accepted
- [PyMolUC8-Change the view of plots](#) - Rejected
- [PyMolUC9-Import and export state of viewer](#) - Rejected

### Issues

[New Discussion](#)

- [#191](#) PyMOL exit "bug"
- [#192](#) PyMOL styles "bug"
- [#196](#) PyMOL serving as a viewer and a renderer

### Status

- Accepted - Use case will be implemented
- Rejected - Use case will not be implemented
- Contingent - Use case is accepted, but may not be implemented due to implementation risks or time constraints
- Pending - Use case is in review

[Back to PyMol](#)

Edit this page

Attach file

Delete this version

Delete page

Done

McAfee SiteAdvisor

start

2 Firefox

C:\WIN...

3 Win...

Macrom...

Microso...

100%

9:39 PM

PyMolUC3 - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/PyMolUC3

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Gmail - Re: ICNS PyMolUC3 - diffraction - Trac Welcome to RESX

 Search

logged in as [billing](#) | [Logout](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Title Index](#) | [Recent Changes](#) | [Page History](#)

## Save an image of a structure

### Brief

As [PyMolUC1](#) or [PyMolUC2](#), plus Scientist uses pymolControl to save visible structures to file in a common image format.

### Issues

[New Discussion](#)

[#196](#) PyMOL serving as a viewer and a renderer

[Back to PyMol Use Cases](#)

Edit this page

Attach file

Delete this version

Delete page

Download in other formats:

[Plain Text](#)



Powered by [Trac 0.9.5](#)  
By [Edgewall Software](#).

Visit the Trac open source project at  
<http://trac.edgewall.com/>

Done

McAfee SiteAdvisor

start 2 Firefox C:\WIN... 3 Win... Macrom... Microso... 100% 9:39 PM

SrRietveldUseCases - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/SrRietveldUseCases

Instant Message Customiz... NIRT - Publications Gmail - Inbox (1)

Gmail - Inbox (177) SrRietveldUseCases - diffraction - Trac Welcome to RESX



Search

logged in as [billinge](#) | [Logout](#) | [Settings](#) | [Help/Guide](#) | [About Trac](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Title Index](#) | [Recent Changes](#) | [Page History](#)

## SrRietveld Use Cases

### Use Cases

- [SrRietveldUC1 - refine a single structure from powder data](#) - Pending
- [SrRietveldUC2 - indexing from powder data](#) - Pending
- [SrRietveldUC3 - peak fitting from powder data](#) - Pending
- [SrRietveldUC4 - peak intensity extraction from powder data](#) - Pending
- [SrRietveldUC5 - structure solution from powder data](#) - Pending

### Issues

[New Discussion](#)

### Status

- Accepted - Use case will be implemented
- SFL - Save for later: Use case will not be implemented in DANSE
- Contingent - Use case is accepted, but may not be implemented due to implementation risks or time constraints
- Pending - Use case is in review

[Back to SrRietveld](#)

Edit this page

Attach file

Delete this version

Delete page

Done

McAfee SiteAdvisor

start 2 Firefox C:\WINDO... 3 Window... Macromedia ... 100% 9:22 PM

## Refine a single structure from powder data

### Brief

**Scientist** loads powder data from tof neutron powder diffractometer. Optionally, **scientist** graphically visualizes the loaded data. **Scientist** selects data channels and ranges to be used in the refinement. **Scientist** enters initial structural parameters for a periodic model. **Scientist** configures the fit. **Scientist** initiates refinement. **SrRietveld** saves refinement results, final profile and positions of Bragg peaks to output files. Optionally, **Scientist** graphically visualizes the fitting results. Optionally, **Scientist** graphically visualizes standard Rietveld statistics. Optionally, **Scientist** reconfigures and reruns the fit.

### Notes:

- **Configures the Fit:** Scientist selects and constrains the experimental, functional, and algorithmic parameters of the fit. Probably needs its own use case.
- **Graphically Visualizes ...:** Probably needs its own use case.
- **Standard Rietveld Statistics:** GSAS allows one to view a few standard plots:
  - Normalized error distribution:  $(I_0 - I_c)/\sigma(I_0)$  vs. TOF
  - Normal probability plot: See Section 4.3 of International Tables for Crystallography, Vol IV

### Actors

- [SrRietveld](#)
- Scientist

### Main Success Scenario

**Scientist** tells **SrRietveld** the source of the diffraction data. The optional choices are TOF Neutron powder diffractometer or local file. **SrRietveld** loads powder data from the specified location. Optionally, **scientist** graphically visualizes the loaded data. **Scientist** selects data channels and ranges to be used in the refinement. **Scientist** enters initial structural parameters for a periodic model, which includes space group and each site's atom type, fractional position, occupancy, and thermal parameter. **Scientist** enters the emission profile, instrument convolution information, intensity correction, background, zero error and the region for fitting. **Scientist** configures the fit by specifying the parameters to fit and setting up the constraints between parameters. **Scientist** initiates refinement. **SrRietveld** saves refinement results, final profile and positions of Bragg peaks to output files. Optionally, **Scientist** graphically visualizes the fitting results. Optionally, **Scientist** graphically visualizes standard Rietveld statistics. Optionally, **Scientist** reconfigures and reruns the fit.

### Issues

SrRietveld - diffraction - Trac - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://danse.us/trac/diffraction/wiki/SrRietveld

Instant Message Customize... NIRT - Publications Gmail - Inbox (1)

Gmail - Re: ICNS SrRietveld - diffraction - Trac Welcome to RESX

[Start Page](#) [Title Index](#) [Recent Changes](#) [Page History](#)

## SrRietveld

This is the main Rietveld application for DiffDANSE. It will support basic Rietveld functions found in GSAS, including some capability for magnetic refinements.

### Introduction

- [Project Timeline?](#)
- [Developers and personnel](#)
- [Software License](#)
- [Source trunk](#)
- [Documentation?](#)
- [Obtaining and building the code?](#)
- [Information for reviewers?](#)
- [Information for testers?](#)
- [Community discussion?.](#) (Please post here your comments and suggestions.)

### Developer Documentation Workproducts

- [Vision?](#)
- [Use Cases](#)
- [Planning?](#)
- [Supplementary Specifications?](#)

### Developer notes

- [Scratch place for old use cases](#)
- [design notes?](#)
- [process blog?](#)
- [related meetings: Meeting 2006-12-11 Meeting 2006-12-15 Meeting 2006-12-18](#)
- [Mike McKerns' useful process tutorial](#)

[Edit this page](#) [Attach file](#) [Delete this version](#) [Delete page](#)

Done McAfee SiteAdvisor

start 2 Firefox C:\WIN... 3 Win... Macrom... Microso... 100% 9:35 PM

# Progress

- Management and Organisation
- Software



# PyMol

- Mostly we used this to develop our software development process!
- However, software mostly done, Dmitriy waiting for some assistance with pyrolization
- Still not satisfied with all aspects such as documentation and review
- Attention focusing away a bit as one thing we learned from this is that such having such small “bite-sized” projects is not amenable to agile development and group activity
- Ask developers for more information



# PDFgui

- Prototype application
- Very successful from our perspective
  - Took one application “all the way” and learned a lot in the process
  - Resulting application we believe is good...
    - Meets the success definition
    - Expect that we can reuse much of the gui design
  - Excellent feedback from alpha-testers
- Status
  - Alpha0 and alpha1 releases were successful
  - Now have roughly 10 installations in different groups. Very positive feedback
  - Todo: beta by first week in April (documentation, windows)



PDFGui

File Edit Figs Calculations Phases Data Help

Configure Constraints Results

### Phase Configuration

a: 5.48634 b: 5.61921 c: 7.62821  
 alpha: 90.0 beta: 90.0 gamma: 90.0

Scale factor: 1.0  
 Correlation factor linear: 0.0 quadratic: 0.0  
 Low r sharpening: 1.0 up to Rcut: 3.5

	elem	x	y	z	u11	u22	u33	u12	u13	u23	occ
1	La	0.996096	0.0321494	0.25	0.00253993	0.00253993	0.00253993	0.0	0.0	0.0	1.0
2	La	0.496096	0.467851	0.75	0.00253993	0.00253993	0.00253993	0.0	0.0	0.0	1.0
3	La	0.00390369	0.967851	0.75	0.00253993	0.00253993	0.00253993	0.0	0.0	0.0	1.0
4	La	0.503904	0.532149	0.25	0.00253993	0.00253993	0.00253993	0.0	0.0	0.0	1.0
5	Mn	0.0	0.5	0.0	0.00065337	0.00065337	0.00065337	0.0	0.0	0.0	1.0
6	Mn	0.5	0.0	0.0	0.00065337	0.00065337	0.00065337	0.0	0.0	0.0	1.0
7	Mn	0.0	0.5	0.5	0.00065337	0.00065337	0.00065337	0.0	0.0	0.0	1.0
8	Mn	0.5	0.0	0.5	0.00065337	0.00065337	0.00065337	0.0	0.0	0.0	1.0
9	O	0.0595746	0.496164	0.25	0.0008201	0.0008201	0.0008201	0.0	0.0	0.0	1.0
10	O	0.559575	0.00383601	0.75	0.0008201	0.0008201	0.0008201	0.0	0.0	0.0	1.0
11	O	0.940425	0.503836	0.75	0.0008201	0.0008201	0.0008201	0.0	0.0	0.0	1.0
12	O	0.440425	0.996164	0.25	0.0008201	0.0008201	0.0008201	0.0	0.0	0.0	1.0
13	O	0.720052	0.289387	0.0311125	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
14	O	0.220052	0.210613	0.968887	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
15	O	0.279948	0.710613	0.531113	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
16	O	0.779948	0.789387	0.468887	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
17	O	0.279948	0.710613	0.968887	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
18	O	0.779948	0.789387	0.0311125	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
19	O	0.720052	0.289387	0.468887	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0
20	O	0.220052	0.210613	0.531113	0.00512371	0.00512371	0.00512371	0.0	0.0	0.0	1.0

Configuring a set of fits for a T-series on  $\text{LaMnO}_3$  data.



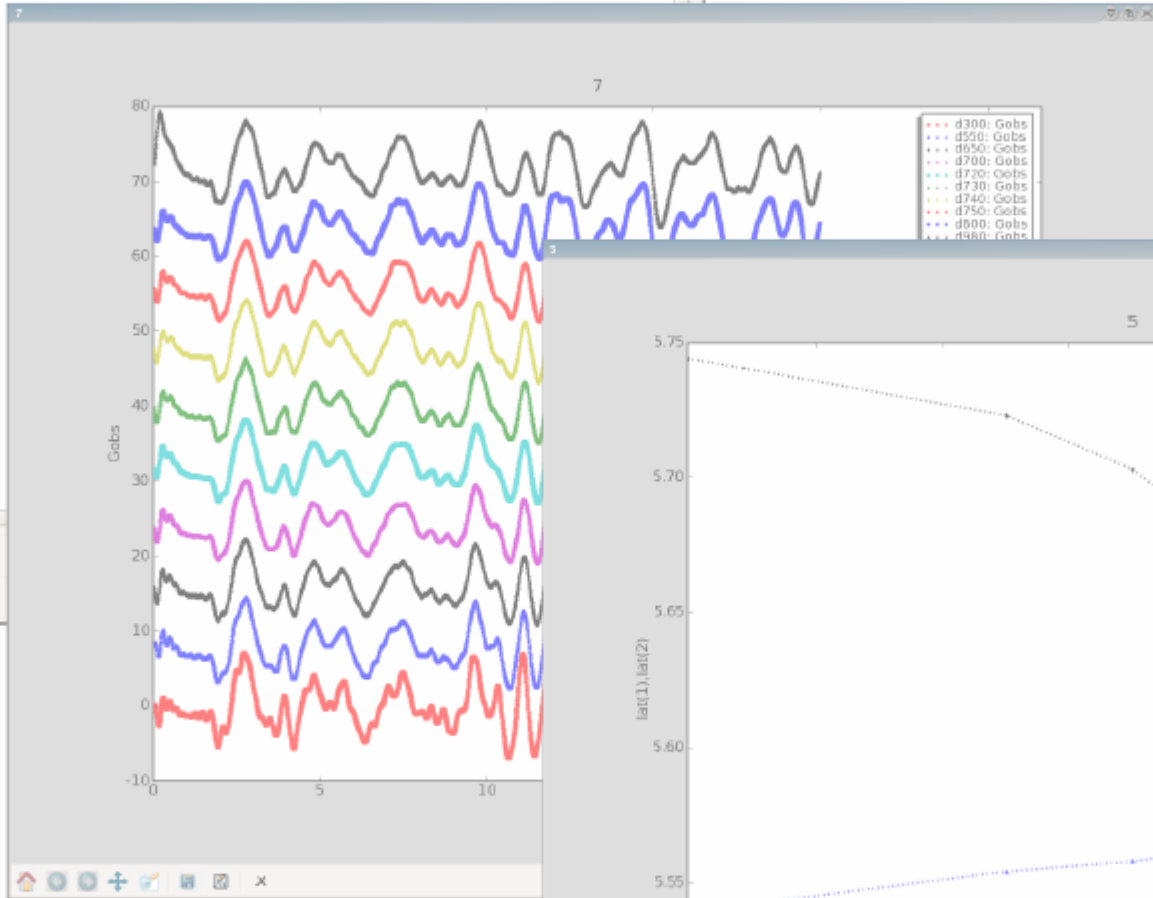
Quick Plot

X: step

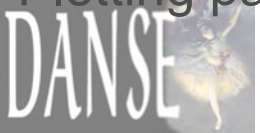
Y data:

- gamma
- lat(1)
- lat(2)
- lat(3)
- u1(1)
- u1(10)
- u1(11)
- u1(12)
- u1(13)
- u1(14)
- u1(15)
- u1(16)
- u1(17)
- u1(18)
- u1(19)
- u1(2)
- u1(20)
- u1(3)
- u1(4)
- u1(5)
- u1(6)
- u1(7)
- u1(8)
- u1(9)
- u2(1)
- u2(10)
- u2(11)
- u2(12)
- u2(2)

offset: auto



Plotting pane of PDFgui



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

# PDFgui

- Prototype application
- Very successful from our perspective
- Status
  - Alpha0 and alpha1 releases were successful
  - Now have roughly 10 installations in different groups. Very positive feedback
  - Todo: beta by first week in April (documentation, windows)
- Lessons learned
  - Too many to list; a very valuable experience
  - Need to work on build and release infrastructure now!



# Outline

- Goals
- Progress
- **Planning**



# Planning

- Management and Organization

- Hiring is ok for now
- Need a bit more work on project reporting etc., but getting close. Plan is to have it working smoothly by the end of March
- Software process:
  - Made a lot of progress. Need to consolidate what we have done and fine-tune it.
  - Need to work harder on software review and developer documentation. Not just passing external reviews but having developers work on each others code.
  - Seek to have it finalized by end of the semester
- Need better ways to do builds

- Software



# Planning

- Management and Organization
- Software
  - DiffPy
  - DiffLab
  - SrRietveld
  - SrReal



# DiffPy

- Python/Pyre component libraries for diffraction



# DiffLab

- Build your own application (Application Machine-tool Application)
  - Very much the motivation behind DANSE
  - This will be an application, initially, that just builds configurable regression modeling applications,
  - ....but it is extensible for other sub-groups

Basic idea:

model-centric modeling -> Cost-function-centric modeling  
drag and drop -> program introspection and resolution



# Modeling

- Need a model
  - Different models
- Need a cost function
- Need data
  - Different data



- Run DiffLab application

- DiffLab: What do you want in your cost function?
- DiffLab: Here are the possibilities that I can find
- Scientist: selects tof Neutron  $S(Q)$   $\chi^2$
- DiffLab: looks into this  $\chi^2$  module and checks for dependencies
- DiffLab: looks into DiffPy/DANSE libraries for all components that can satisfy those dependencies and presents a drop-down list of dependency resolutions
- Scientist selects desired component
- Repeat exhaustively to complete the tree



# Motivation

- Some motivating science problems in complex materials structure analysis:
- Molecules intercalated in zeolite
  - Z-matrix representation for molecules, periodic crystal for host
  - Two different models have to interact self-consistently
- Energy minimization in a regression loop
  - Nesting
- $\text{Cu}_3\text{Au}$ 
  - Monte Carlo ising-type moves then efficient relaxation steps
- Amorphous model builder...use energetics and relaxation in the model building process



# DIFF Lab 0.01



Configure

Runtime

Large empty gray area for configuration or runtime output.

- Data

Large empty gray area for data visualization or output.

Add

Remove

**click**

+ Model

+ Plotting

Cost function:

Run



Configure

Runtime

Presents a list of currently supported data types which is dynamically generated. User selects and next a list of required and optional configuration items is shown. This list is generated by looking for dependencies. Items with complete configuration are **green**, unfinished ones **red**. Items where defaults are used might have there own color.

- Neutron S(Q)
- Neutron G(r)
- X-ray constant wavelength Rietveld data
- ...

  
**click**

Data

Add

Remove



Model



Plotting

**Cost function:**

Run



Configure

Runtime

Neutron  $G(r)$  on the right is red...it has unresolved dependencies. DiffLab introspects to find these dependencies and makes a list below. The  $\oplus$  sign means that clicking on that will expand the tree in that direction, similar behavior to microsoft explorer file agent.

 $\oplus$  Data source $\oplus$  Cost function $\oplus$ ...**click**

Data

Neutron  $G(r)$ 

Add

Remove



Model



Plotting

Cost function:

Run



Configure

Runtime

By expanding Data source we see the suggestions that DiffLab makes for resolving the dependencies. It generates these lists dynamically by looking at the library to see what is available. The + sign changes to a minus sign (but I can't do it easily in ppt). The amber color (between red and green) means that the dependency will be resolved with user-input at run-time

- ⊕ Data source
  - ⊕ Local file
  - ⊕ Lujan PDF data server
  - ⊕ Enter manually
- ⊕ Cost function
- ⊕ ...

click

**Data**

Neutron G(r)

Add Remove

**Model**

**Plotting**

Cost function:

Run



Configure

Runtime

Selecting “read from file” causes “Data source” to turn green as this now has its dependencies resolved and can run (arguably the behavior just described is just a dialog between DiffLab and the user so maybe should take all take place at run-time and not at configuration time, but we can discuss that later. This at least illustrates the behavior). Now compress “Data source” (if you want) and expand “Cost function”...

- ⊕ Data source
- ⊕ Local file
- ⊕ Lujan NPDF dataserver
- ⊕ Enter manually
- ⊕ Cost function
- ⊕ ...

click

click

- Data

Neutron G(r)

Add

Remove

+ Model

+ Plotting

Cost function:

Run



Configure

Runtime

Let's do normal least squares,  $\text{SUM}(w_{ij}(G_{\text{calc}} - G_{\text{meas}})^2)$  so select CHI^2

⊕ Data source

⊕ Cost function

⊕ CHI^2

⊕ Bill David's Robust statistics

⊕ Custom

⊕...

click



Data

Neutron G(r)

Add

Remove



Model



Plotting

Cost function:

Run



Configure

Runtime

Only one thing left to get green so click it

- ⊕ Data source
- ⊕ Cost function
  - ⊕ CHI<sup>2</sup>
    - ⊕ Data
    - ⊕ Calculated function
    - ⊕ weights/errors
  - ⊕ Bill David's Robust statistics
  - ⊕ Custom
- ⊕...

click



Data

Neutron G(r)

Add

Remove



Model



Plotting

Cost function:

Run



Configure

Runtime

Again, DiffLab finds what is available and lists them. We want to fit a model which we do in the model tab on the right, so let's click it.

- ⊕ Data source
- ⊕ Cost function
  - ⊕ CHI<sup>2</sup>
    - ⊕ Data
    - ⊕ Calculated function
      - ⊕ Model (expand model at right)
      - ⊕ User supplied
    - ⊕ weights/errors
  - ⊕ Bill David's Robust statistics
  - ⊕ Custom
- ⊕ ...

click



Data

Neutron G(r)

Add

Remove



Model



Plotting

Cost function:

Run



Configure

Runtime

Cost function will now turn green when we satisfy all the “model” dependencies (maybe we need a different color as Amber means the program will run and will give a dialog box to get the user input. Here the color indicates that it is waiting for some dependencies to be resolved, but not in “Data” but in “Model”. Notice that Neutron G(r) has turned yellow as all it doesn’t need any more “configuring” from the user, so we can go on by adding another data-type (e.g., RAPDF G(r) or RAPDF F(Q)), or move to model...

- ⊕ Data source
- ⊕ Cost function
  - ⊕ CHI<sup>2</sup>
    - ⊕ Data
    - ⊕ Calculated function
      - ⊕ Model (expand model at right)
      - ⊕ User supplied
  - ⊕ weights/errors
- ⊕ Bill David's Robust statistics
- ⊕ Custom

- Data

Neutron G(r)

+ Model

+ Plotting

click

Cost function: **A1**\*[Chi2 Neutron G(r)]

Run



Configure

Runtime

Open the model pane and click add...

+ Data

- Model

Add Remove

+ Plotting

click

Cost function:  $\chi^2(\text{Neutron } G(r)) +$

Run



Configure

Runtime

Difflab looks for all the model possibilities and gives the list here.  
Let's make a PDFfit type program so we want crystal structure model:

- Crystalline structure (small unit cell, periodicity)
- Large box, periodic BC's
- Large box, hard boundary
- molecular (Z-matrix) **click**
- ...



Data



Model

Add

Remove



Plotting

Cost function:  $A1 + \text{CHI}^2(\text{Neutron } G(r)) +$

Run



Configure

Runtime

Difflab looks for all the model possibilities and gives the list here.  
Let's make a PDFfit type program so we want crystal structure model:

- Crystalline structure (small unit cell, periodicity)
- Large box, periodic BC's
- Large box, hard boundary
- molecular (Z-matrix) **click**
- ...



Data



Model

Add

Remove



Plotting

Cost function:  $A1 + \text{CHI}^2(\text{Neutron } G(r)) +$

Run



Configure

Runtime

Now, let's build PDFfit by clicking on Crystal model

+ Data

- Model

**Crystal model**  
click

Add

Remove

+ Plotting

Cost function:  $A_1 \cdot \chi^2(\text{Neutron } G(r)) + ..$

Run

# SrRietveld

- Status:
  - Collecting brief use-cases
  - Training Wenduo in Rietveld and profile fitting methods
  - Time to begin discussing more seriously with Jason Hodges and Engineering sub-group and other stake-holders
    - Had a visit from Jason, will follow up with more



# SrReal

- Real-space fitting clone of SrRietveld
  - May be combined into one application, or left separately as two
  - Replacement for PDFgui which is not modular and not using DiffPy libraries (though much of the PDFfit2 codes will be reused in DiffPy)



# PDFgui

- Make sure that it has a long life
  - Modular
  - Clear separation of gui from program logic. Interaction between the program and the gui through proxies
  - Team development results in code that is readable by more than one human being
  - Coding standards for docstrings and basic syntax structure
  - Project under subversion control under TRAC



Thanks!



---

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