DANSE Diffraction sub-group report

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Diffraction methods

- Single crystal diffraction
  - TOPAZ
- Powder diffraction
  - POWGEN3, VULCAN, NOMAD, SNAP
- Total scattering
  - POWGEN3, NOMAD, SNAP
- (macromolecular diffraction)

Frontiers of Structural Science

- Structure studies are ubiquitous: Whatever the scientific frontier in material science knowledge of structure is important
- Complex materials: the nanostructure problem
  - Structural fluctuations at the nanoscale
  - Nanoparticles
  - Inhomogeneous systems, intercalated nanoporous systems
- Materials science through diffraction
  - Grain structure
  - Texture
  - Particle size
  - Thin films
- Materials in action
  - Parametric studies
  - Combinatorial studies
  - Materials under extreme conditions
- (Mechanical properties through diffraction)

Complex modeling for Complex structures

REVIEW

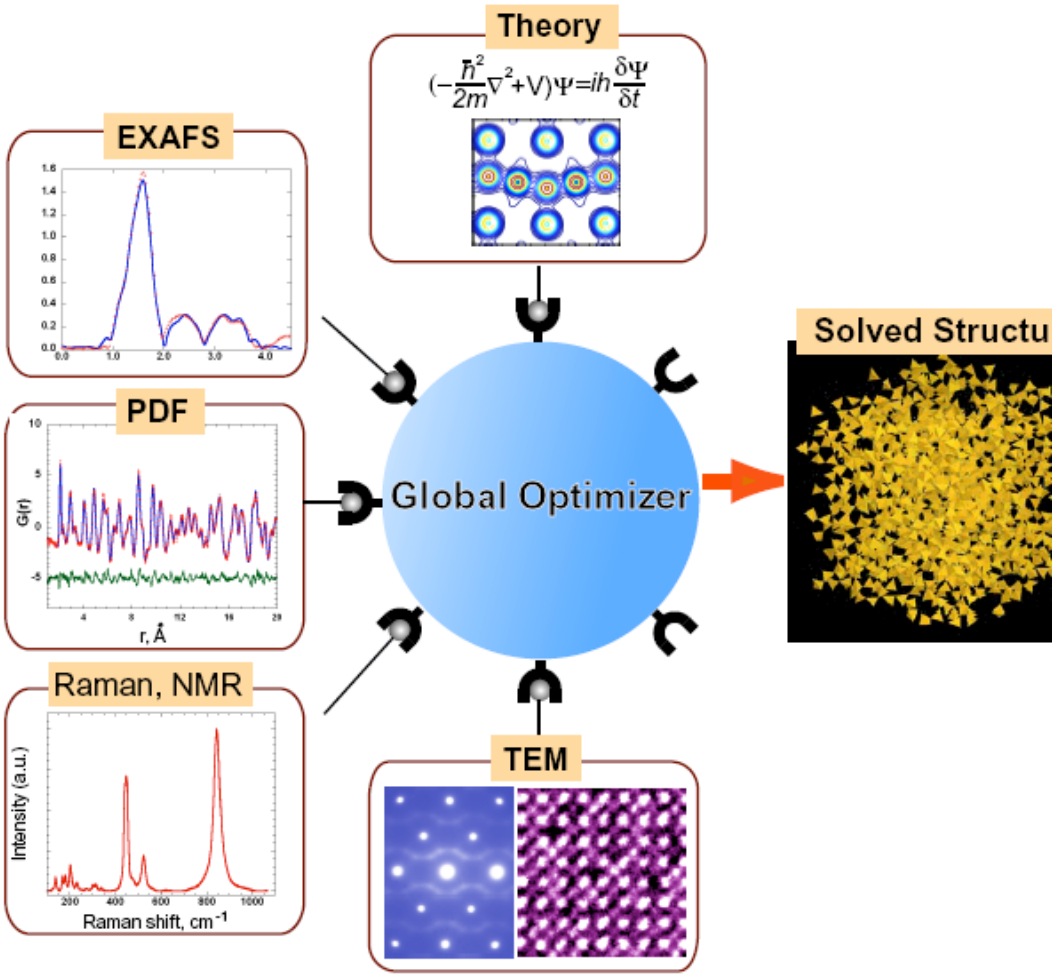
The Problem with Determining Atomic Structure at the Nanoscale

Simon J. L. Billinge[1]* and Igor Levin[2]

- Solve the inverse problem
  1. Regularize the problem (more constraints/restraints than degrees of freedom)
  2. Develop algorithms to solve it

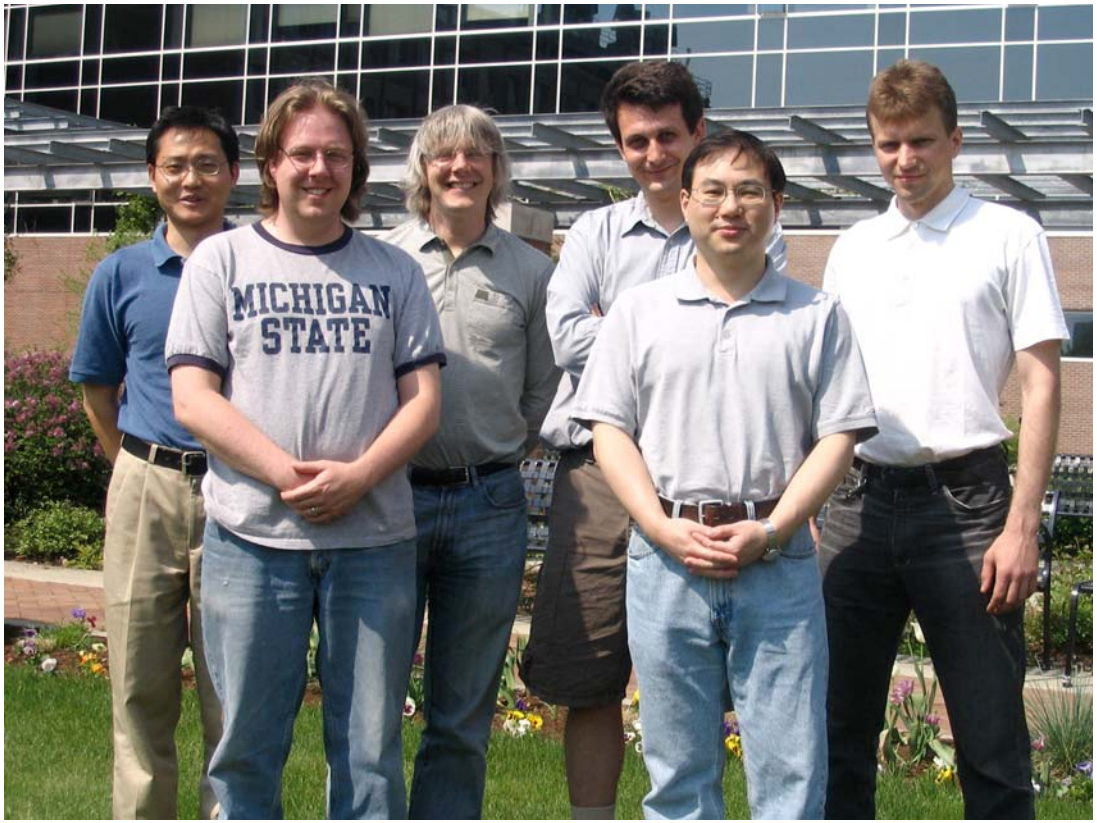
DANSE is ideally suited for this kind of application

DiffLAB task

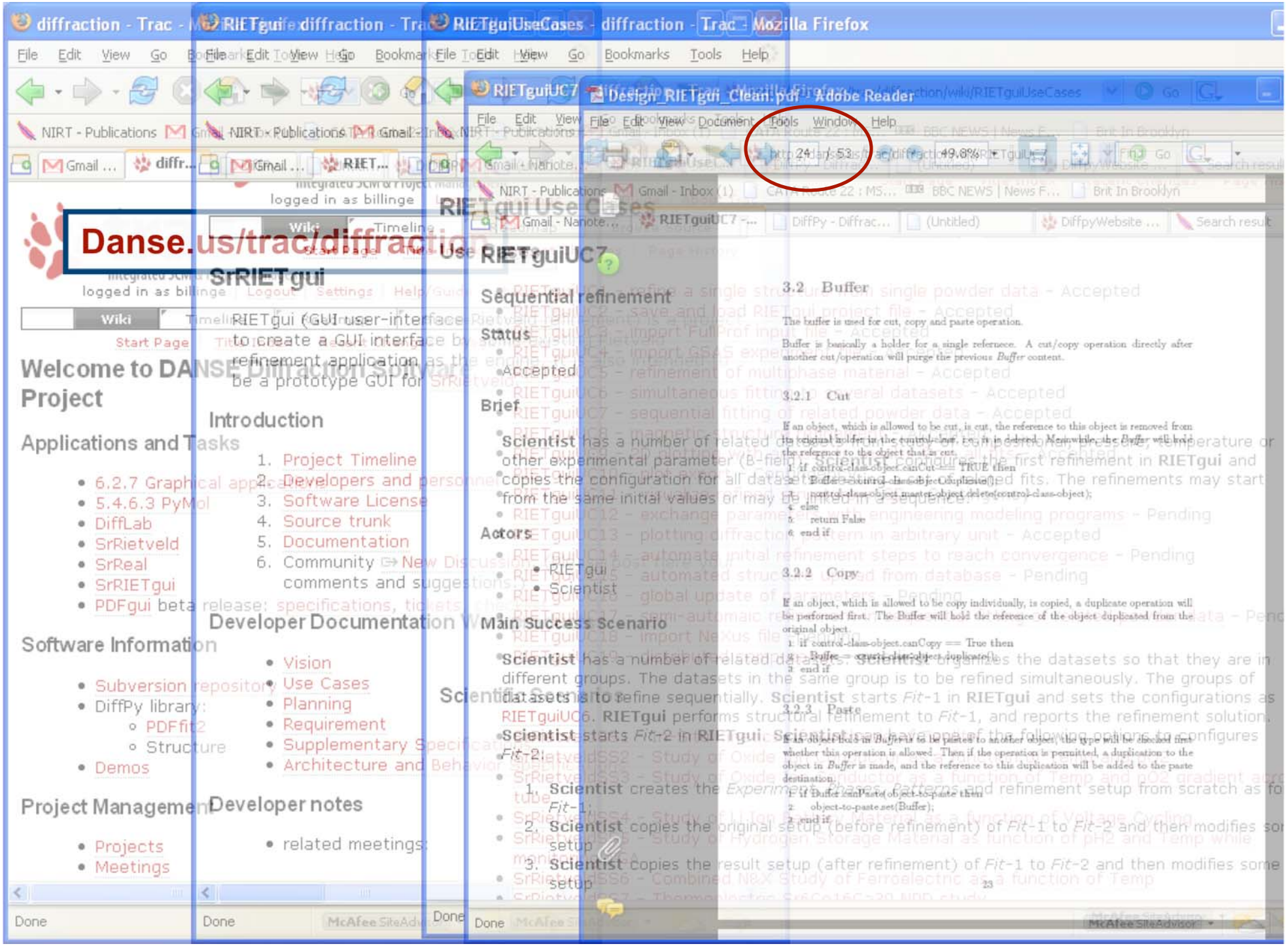


- Thanks to Igor Levin for help producing the figure

Group



- Pavol Juhas (PD – part time)
- Wenduo Zhou (PD – full time)
- Emil Bozin (PD – part time)
- Jiwu Liu (GS – part time)
- Chris Farrow (GS – part time)
- Dmitriy Bryndin (not show GS full time)
- Simon Billinge (PI)


diffraction - Trac - Mozilla Firefox
RIETguiUseCases - diffraction - Trac - Mozilla Firefox
RIETguiUC7
Design_RIETgui_Clean.pdf - Adobe Reader
Danse.us/trac/diffraction
Welcome to DANSE Diffraction Software Project
Applications and Tasks
Software Information
Project Management
Introduction
Developer Documentation
Developer notes
SrRIETgui
RIETgui (GUI user-interface
to create a GUI interface
refinement application
be a prototype GUI for
RIETgui Use Cases
Use RIETguiUC7
Sequential refinement
Status
Accepted
Brief
Actors
Main Success Scenario
3.2 Buffer
3.2.1 Cut
3.2.2 Copy
3.2.3 Paste

Software enabling new science from SNS

- New science by enabling expert scientists, non-expert scatterers
  - Get scientists closer to what they do: the science
  - Expanding the range of problems that utilize neutron diffraction, expanding the user base of non-experts
- New science by enabling expert scatterers
  - More powerful, flexible configurable software
    - E.g. complex modeling paradigm
    - Rich (and growing) libraries of components
- New science by extending software capabilities
  - New algorithms, new methods

Flagship Applications

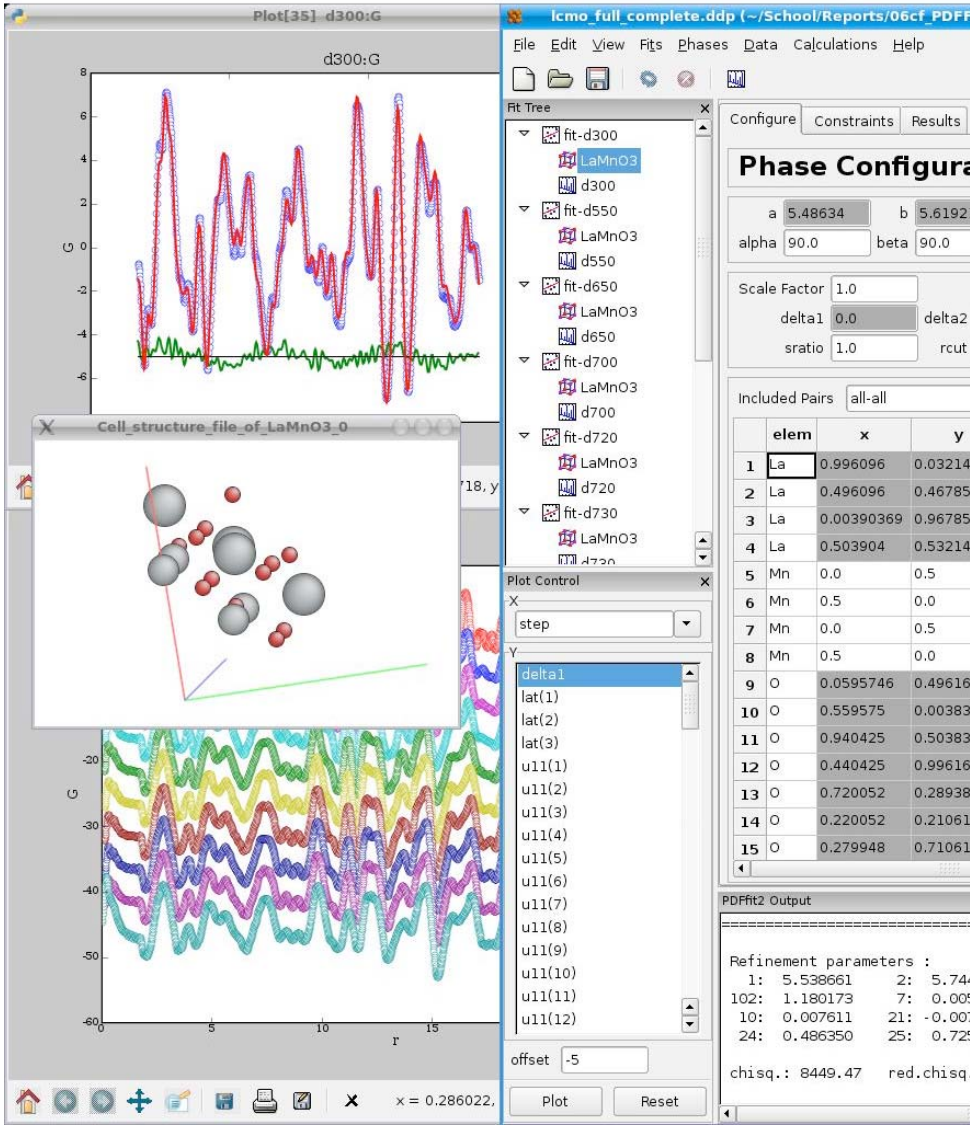
- PDFgui/SrReal – Enabling scientists
  - Enhanced real-space analysis capabilities
  - PDFgui uses existing PDFfit2 engine. 1.0beta is released
  - SrReal is our holding name for the replacement built on refactored library routines
- SrRietveld – Enabling scientists
  - Enhanced powder diffraction/Rietveld refinement capabilities
  - Initially with an existing engine (Fullprof), later using library routines
  - Design foci are to optimize for
    - Get the scientist closer to the science: Automation, visualization
    - Real-time operation: will require distributed implementation
    - Scalable and optimized for parametric refinements of multiple datasets

- Diffpy – Expert scatterers
  - Modular libraries of diffraction components that are available in Python and in Pyre
- DiffLab – Expert scatterers
  - Application for building (and executing) “complex modeling” refinement applications on the fly using the Diffpy library
    - User designs her own refinement program depending on what information is available
  - Extensible: grows in power as the libraries grow

Progress: PDFgui v1.0beta: www.diffpy.org

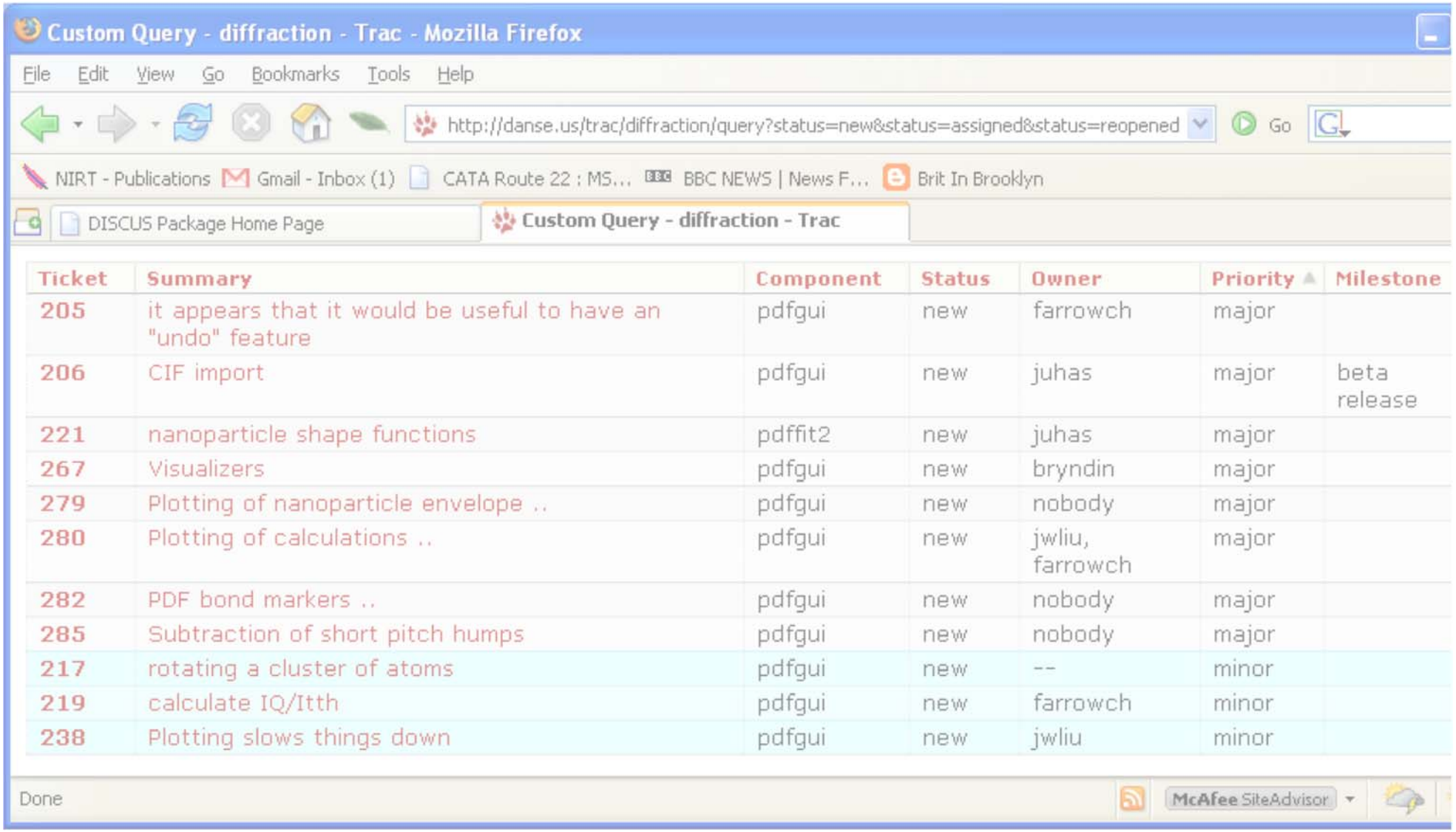
Adopted by Thomas Proffen for his instrument, currently being used in a PDF workshop in Canada

- New features:
  - Dynamic memory allocation
  - Supports space-groups
  - Supercell expansion
  - Spherical nanoparticle form-factor implemented
  - Supports xyz, CIF, PDB file formats (expanded from discus)
  - Automatically generates
    - Symmetry constraints
    - Analytic derivatives of user and symmetry constraint equations
  - Live plotting
  - Structure visualization
  - Parametric plotting
  - Macro language for T-series, doping-series, r-series
  - Smart extraction of meta-data from files and file-names
  - User requested usability features such as fit summary and automated updating of inputs
  - Built-in bug-reporting



Enabling new science

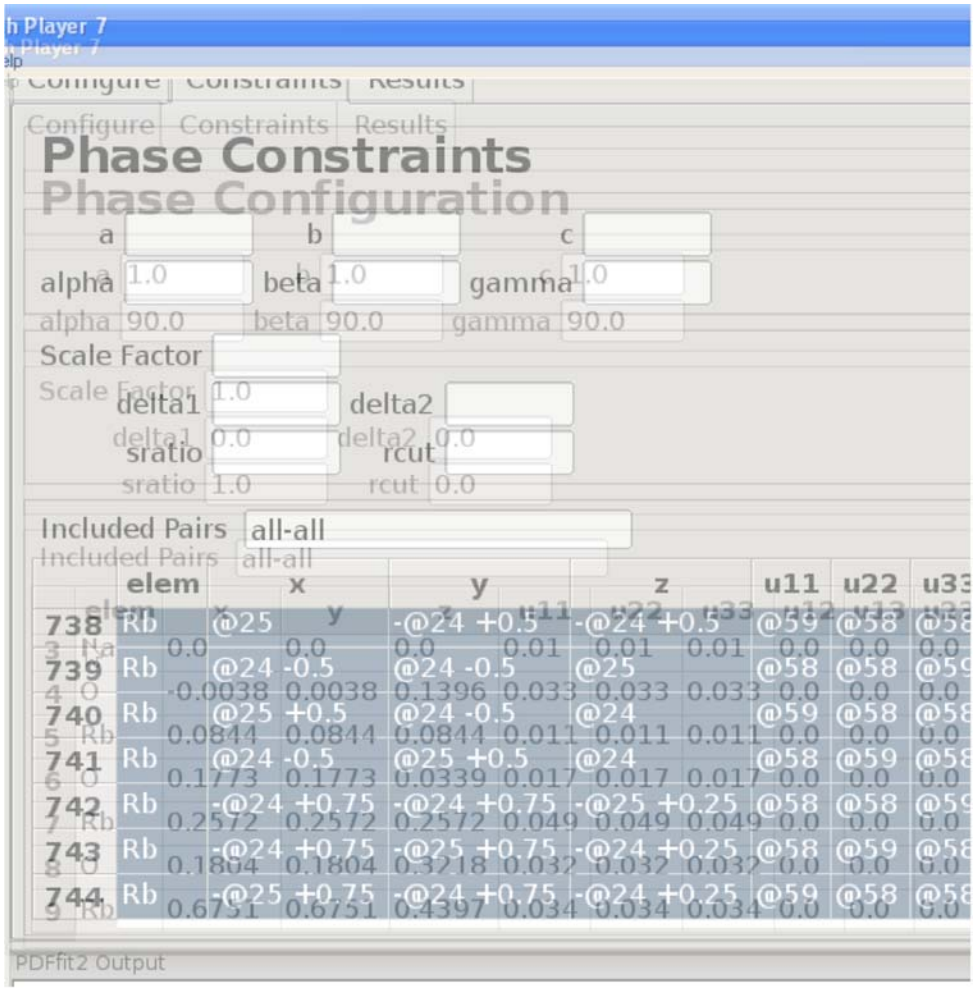
- Real-time analysis at the beamline (faked example, but it has really been used in this way at GPPD)
- Temperature series of $LaMnO_3$ from 15K to 300K
- Quick to set up and refine structure at each point while visualizing a refined parameter



Ticket	Summary	Component	Status	Owner	Priority	Milestone
205	it appears that it would be useful to have an "undo" feature	pdfgui	new	farrowch	major	
206	CIF import	pdfgui	new	juhas	major	beta release
221	nanoparticle shape functions	pdffit2	new	juhas	major	
267	Visualizers	pdfgui	new	bryndin	major	
279	Plotting of nanoparticle envelope ..	pdfgui	new	nobody	major	
280	Plotting of calculations ..	pdfgui	new	jwliu, farrowch	major	
282	PDF bond markers ..	pdfgui	new	nobody	major	
285	Subtraction of short pitch humps	pdfgui	new	nobody	major	
217	rotating a cluster of atoms	pdfgui	new	--	minor	
219	calculate IQ/Itth	pdfgui	new	farrowch	minor	
238	Plotting slows things down	pdfgui	new	jwliu	minor	

Enabling new science

- Student: HyunJeong Kim
- Large zeolite structure with Se chains or rings inside
- Would never have been attempted with the old program
  - Structure too large without special version of the code compiled
  - Asymmetric unit would have had to be expanded by hand from 9 to 750 atoms!
  - Constraint equations due to the crystal symmetry coded by hand



Year 1 Summary

- DiffDANSE team in place (not quite finished yet)
- Learned a lot about software engineering
- Put in place a software development process that we are happy with
- Put in place an EVR reporting process that we are happy with
- Released first full-featured software application to the community
- Begun planning and design for Rietveld and DiffLAB Complex modeling applications

Next Year forecast

- PDFgui is now shipped. We will maintain but not develop it further (http://www.diffpy.org)
- SrRietveld
  - Focus on PDFgui type functionality in a Rietveld code with an existing Rietveld engine that will be operating on POWGEN3 by the end of the year
  - Engine will be replaced gradually in out years
- DiffLAB
  - Working version of Difflab
  - Collaborate with Michael Aivazis to ensure that Pyre has the functionality to support this
- Begin the task of creating diffpy libraries
  - Basic design and API's will be an early focus
  - Support for needs of Engineering Diffraction will be an early focus

DiffDANSE outreach

- Software support and research-community engagement
  - Described in the research part of the talk
- Education
  - Developing K12 science curricula: PI now has an active role in the PROMSE project at MSU – can PROMSE/DANSE activities leverage each other?
  - Developing University nanoscience and scientific software curricula and content – scheduled for later in the project
- Broadening participation
  - Individual efforts of the group members to recruit underrepresented persons
    - e.g., female high-school student will join us for 6 weeks in the summer
    - PI has an active relationship with a science teacher Scott Goodman at Everett high-school. Very interactive, but less active this year due to reprioritization of efforts of Scott due to some personal reasons

Single Crystal Support

- We are very interested in single crystal diffraction but this was largely descoped from the original DANSE WBS. Why?
  - Existing scope is already large
  - Many of the existing single crystal requirements that we identified could be satisfied with existing software once integrated intensities are extracted from the data
  - Novel uses of single crystal data (e.g., analyzing diffuse scattering) are very exciting but still very much at the research stage. These were in the WBS as research grade, not production grade, tasks and were descoped when we were over-budget
  - Our expectation is that most of the data-reduction tasks to obtain integrated intensities will be handled by the SNS data reduction group
  - Our knowledge of single crystal is lower
- Therefore, the only tasks that remained in DiffDANSE were interfacing SNS reduction routines to the DANSE framework.

New Possibility

- Funding request to DMR from Dennis and Ruth Mikkelson and Tibor Koritsanszky to support single crystal developments
- Proposal to integrate these with DANSE and SNS developments
- DiffDANSE proposal: This development can be integrated into the DiffDANSE software development process
  - Use the same svn and Trac infrastructure
  - Development software engineering work-products synchronized with DiffDANSE standards will ease releases and transition to SNS
  - Ensure interoperability of single crystal components with other DiffDANSE and DANSE modules by tighter integration into the DiffDANSE group