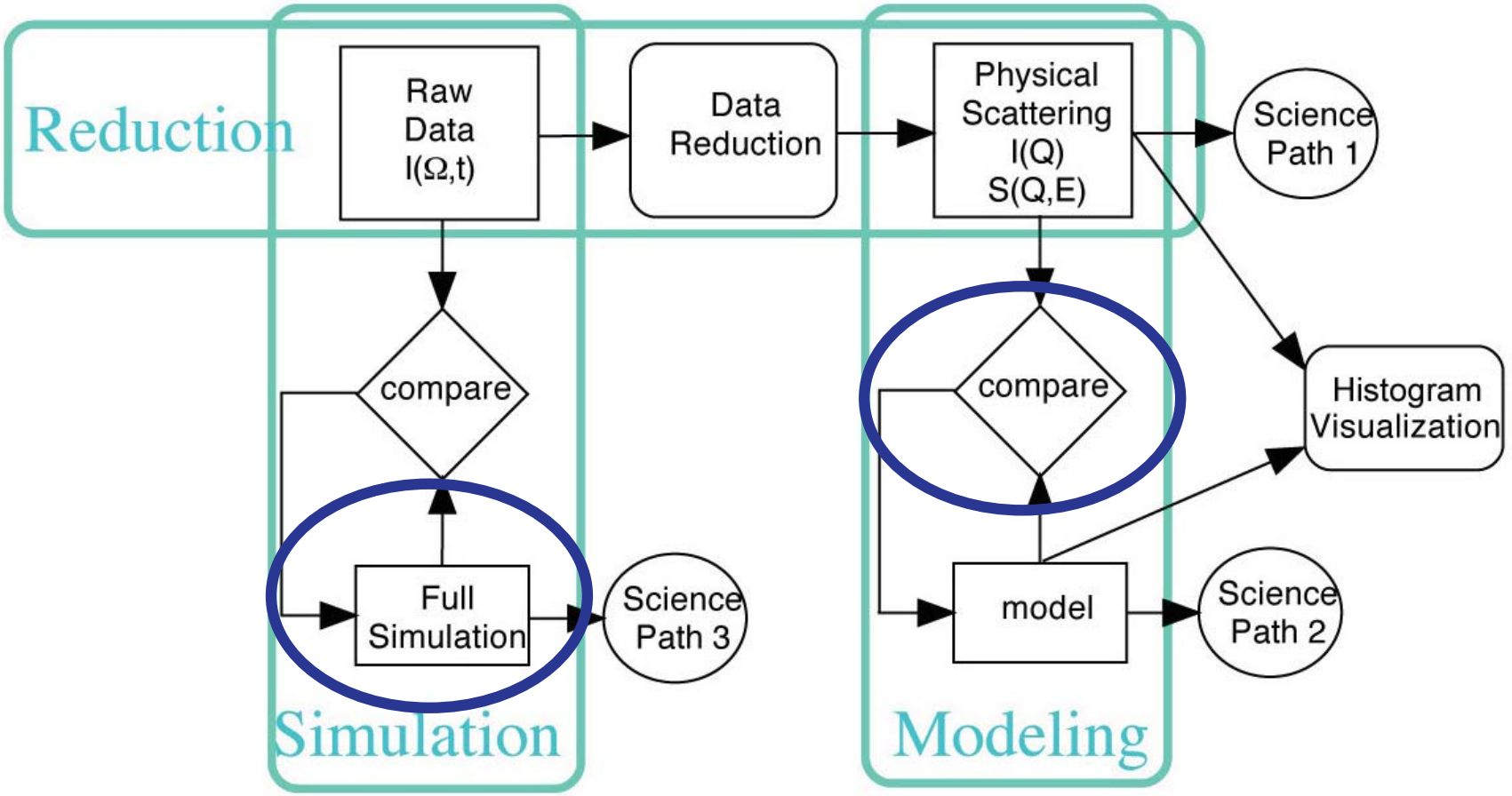
DANSE Overview

Brent Fultz, Caltech

- Scope of DANSE
- Project status (against new baseline)
- Subproject released products
- vnf, optimizers, web services
- Education and outreach
- Mid-term and long-term future


Reduction
Raw Data I(Ω,t)
Data Reduction
Physical Scattering I(Q) S(Q,E)
Science Path 1
compare
Histogram Visualization
Full Simulation
Science Path 3
model
Science Path 2
Simulation
Modeling

“vnf” “PARK”

DANSE focus is higher-level analysis tools

Approximately, the responsibilities of DANSE and SNS meet at S(Q,E) or I(Q)

SNS Data and Reduction } S(Q,E) { DANSE Analysis Modeling

Role of DANSE

Experiment

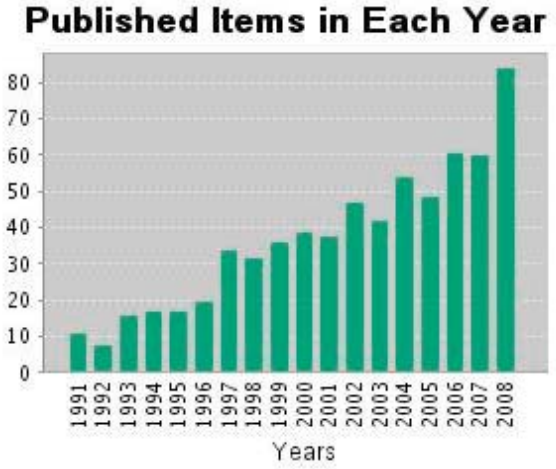
Not needed if interpretations are obvious

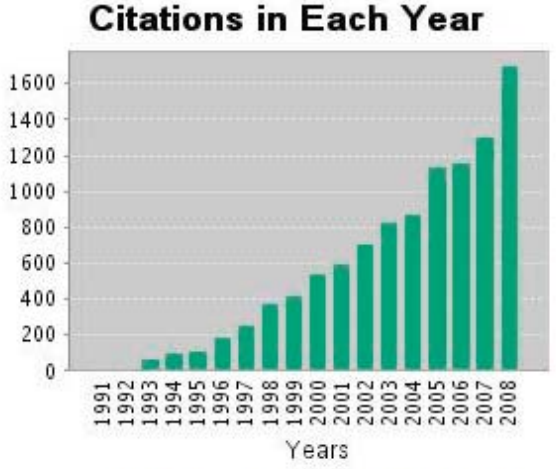
Computational Comparisons Reveal Relationships Between Different Data and Concepts

Theory

Not needed if not codified

690 records. Topic=(ab-initio AND scattering AND neutron)





Average Citations per Item [?] : 16.21

Field: Institution Name	Record Count	% of 690	Bar Chart
INST MAX VON LAUE PAUL LANGEVIN	60	8.6957 %	
RUTHERFORD APPLETON LAB	50	7.2464 %	
ARGONNE NATL LAB	19	2.7536 %	
MAX PLANCK INST FESTKORPERFORSCH	18	2.6087 %	
POLISH ACAD SCI	18	2.6087 %	
JOINT INST NUCL RES	17	2.4638 %	
RUSSIAN ACAD SCI	17	2.4638 %	
CNRS	16	2.3188 %	
UNIV PARIS 06	16	2.3188 %	
CEA SACLAY	13	1.8841 %	
LOS ALAMOS NATL LAB	13	1.8841 %	
UNIV MONTPELLIER 2	13	1.8841 %	
UNIV OXFORD	12	1.7391 %	
UNIV REGENSBURG	12	1.7391 %	
FORSCHUNGSZENTRUM KARLSRUHE	11	1.5942 %	

Field: Source Title	Record Count	% of 690	Bar Chart
PHYSICAL REVIEW B	113	16.3768 %	
JOURNAL OF CHEMICAL PHYSICS	62	8.9855 %	
JOURNAL OF PHYSICS-CONDENSED MATTER	44	6.3768 %	
JOURNAL OF PHYSICAL CHEMISTRY A	26	3.7681 %	
JOURNAL OF PHYSICAL CHEMISTRY B	25	3.6232 %	
CHEMICAL PHYSICS	24	3.4783 %	
JOURNAL OF MOLECULAR STRUCTURE	17	2.4638 %	
PHYSICAL REVIEW LETTERS	17	2.4638 %	
JOURNAL OF NON-CRYSTALLINE SOLIDS	13	1.8841 %	
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	13	1.8841 %	
PHYSICAL CHEMISTRY CHEMICAL PHYSICS	12	1.7391 %	
JOURNAL OF ALLOYS AND COMPOUNDS	10	1.4493 %	
JOURNAL OF PHYSICAL CHEMISTRY	10	1.4493 %	
MACROMOLECULES	10	1.4493 %	

Second Year Review, May 2008.

- On time, on budget, likely to produce something of value. But what is it?

  The major products of DANSE are released. They vary in maturity, but they now show the scope.

- Rebaselining is critical.

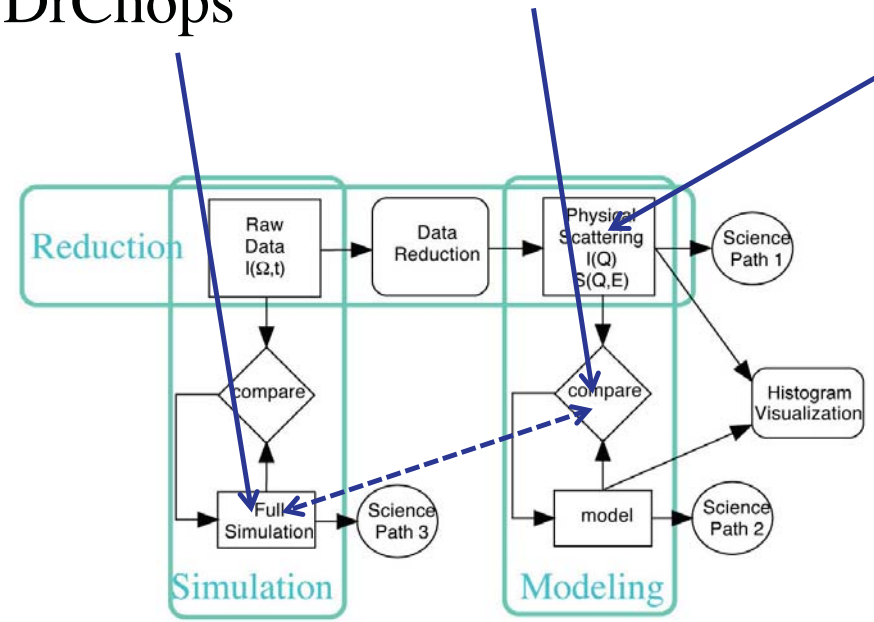
  Done (Oct 08). We are reporting against a new baseline.

- Who will maintain, enhance, and upgrade DANSE software after the project terminates?

  Internal discussions are frequent. Time for Community Involvement. Scope should be higher than DANSE.

A Simple Taxonomy of Packages

"vnf"	"PARK"	"Laptop Modeling"
McVine	SrRietveld, SrFit	PDFGui
Pseudopotential	CySCM, CyFEM	CySCM
Local basis DFT	GaRefl, KsRefl	Sliceview
Molecular dynamics	BvK	GaRefl
DrChops		DrChops



Please inquire to Mike McKerns
or Brent Fultz for access to
information contained on this slide.

Cost performance is good on average.
Schedule performance suffered from lack of personnel.
Quality feedback from present release.

SNS – DANSE Interactions

- All subgroups visited the SNS in 2008 (some more than once)
  - discuss science
  - awareness of software needs by instrument scientists
  - expectations and timescales are important to synchronize

- May 09 workshops at SNS on user authentication, inelastic scattering (and some work on data reduction).

- SNS personnel are regulars at DANSE meetings.

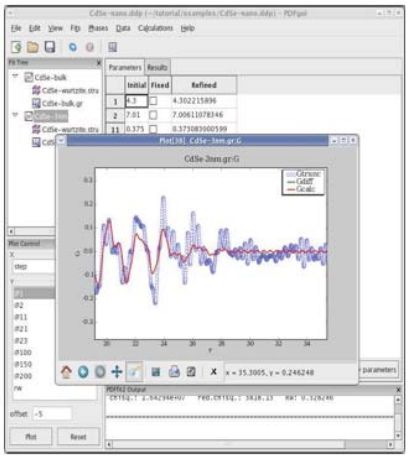
Diffraction: Local Structure by Real-Space Refinement

PDFfit --> PDFfit2

- least-squares refinements
- rewritten in C++/Python

PDFgui

- powerful visualization tools
- structure model manipulation
- wizards for series data

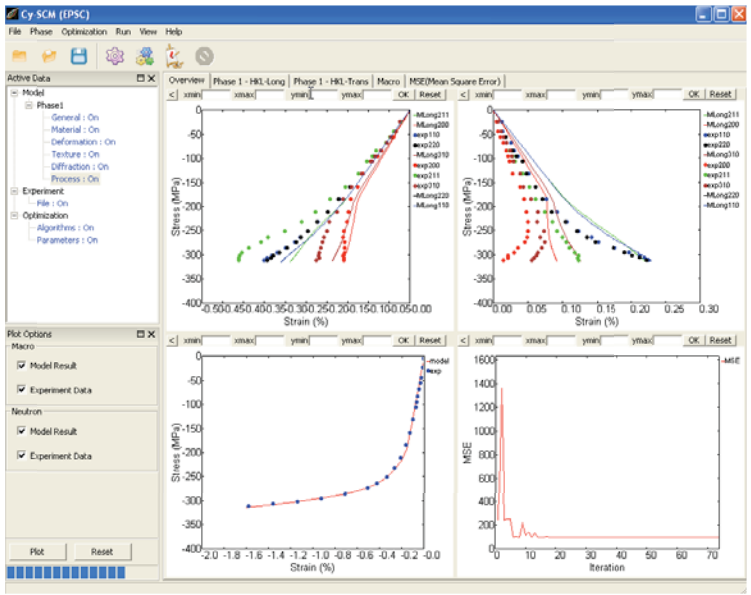


SrFit

- couple PDF fits with other refinements
- plug-in modular refinement engines
- multiprocessor computing for POWGEN3
- high-level scripts

Engineering Diffraction: Mechanics Models

Optimize stress-strain constitutive response of strained, multiphase alloys to fit lattice parameters.



- Cy-SCM
  - couple elastic-plastic self-consistent model to optimizer
- Cy-FEA
  - couple ABAQUS's finite element analysis to optimizer

SANS: Models and Data Fitting

SansView

- Simultaneous constrained fits of 1D & 2D data
- Standard model & model-independent functions
- 2D averaging methods & data manipulation
- instrument & slit smearing, polydispersity, ODF

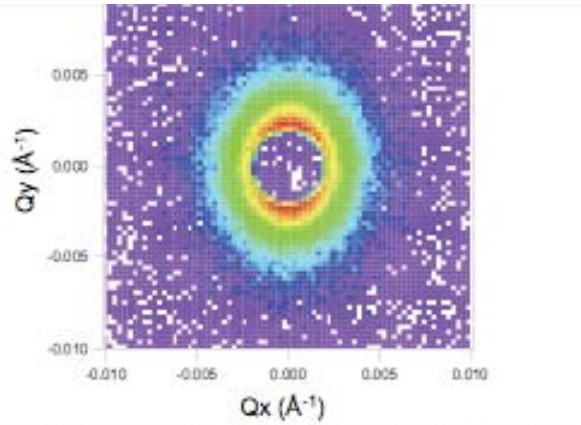


Figure 1. This data is part of a study of the structural origin of clot rheology, by D. Pozzo and L. Porcar.

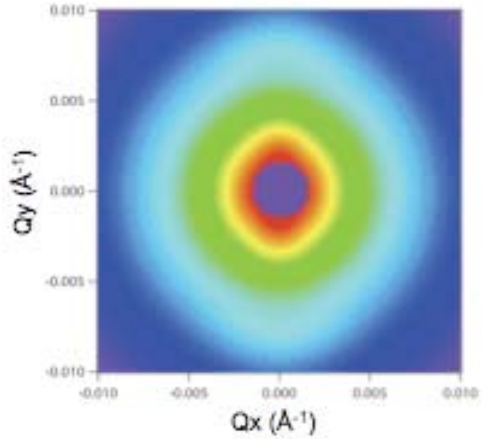
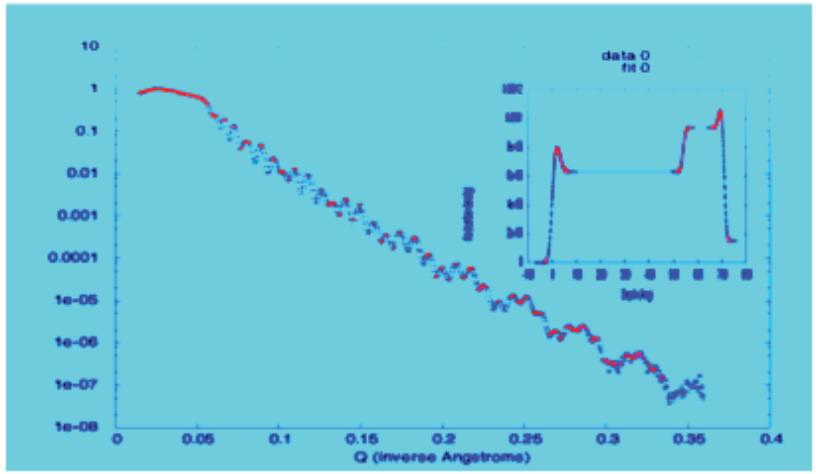


Figure 2. 2D simulation for a cylindrical model with angular dispersion.

Reflectometry: Model Fitting

Fitting biological samples with volume fractions in solvated proteins, and creating models for complex patterns of magnetism spanning multiple layers

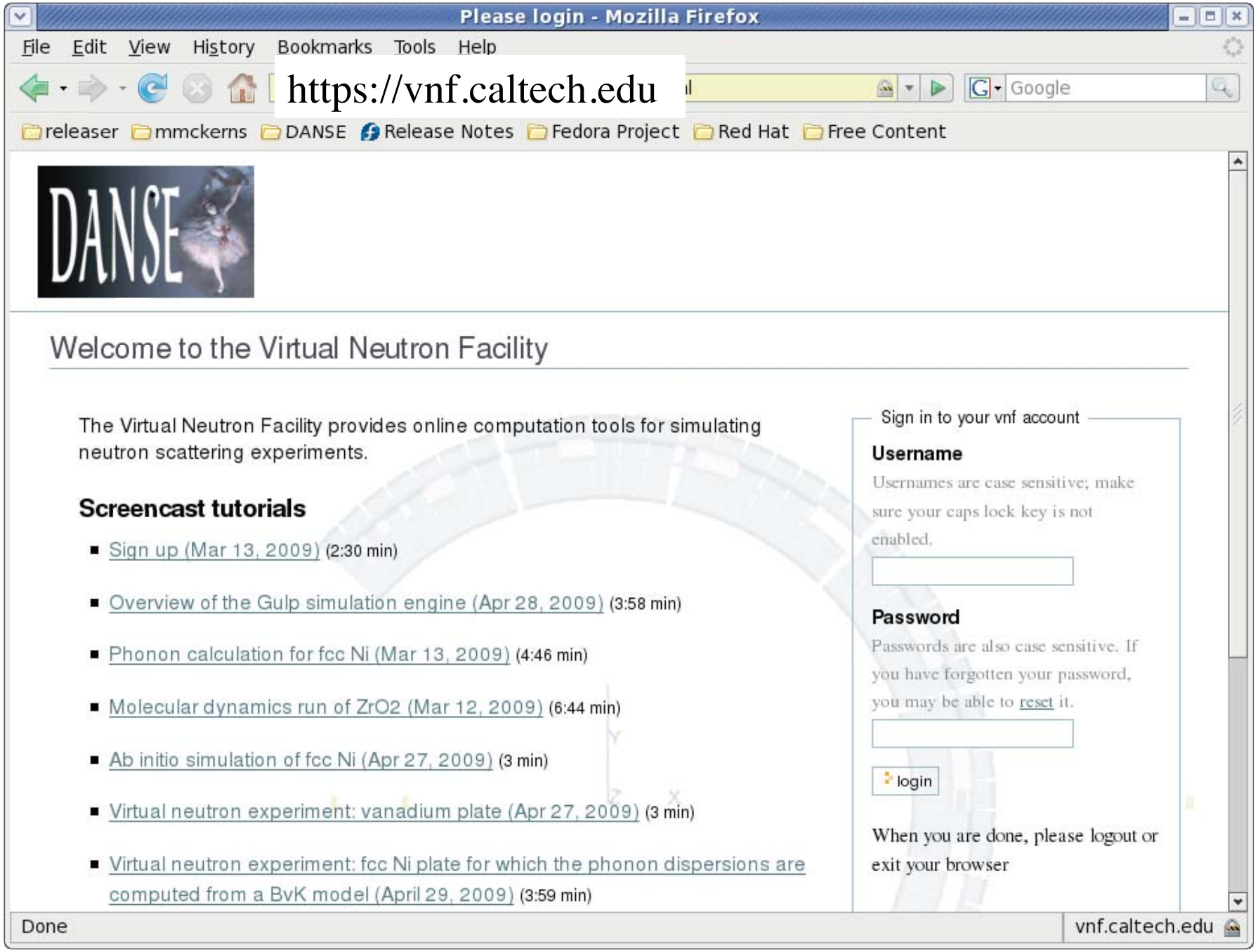
- GaRefl, KsRefl
  - interactive 1D model editor with dynamical updates of curve as parameters change
  - simultaneous fitting of x-ray and neutron data



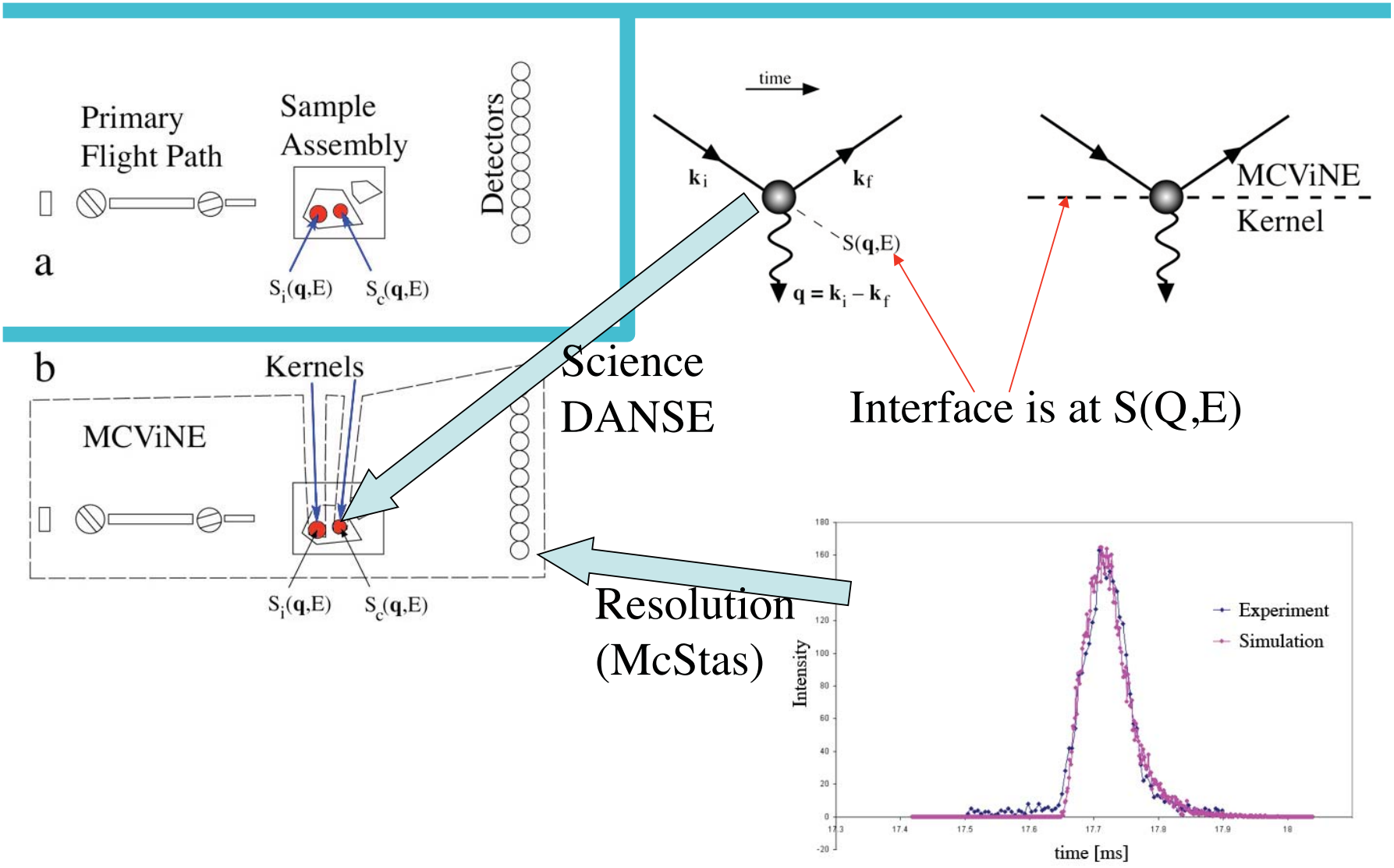
- 3D model editor
  - kinematical off-specular refinement of 3D structure

Why Web Service for Complex Computations?

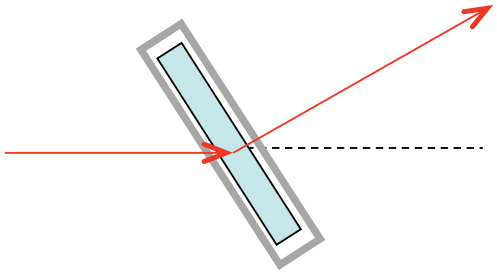
- Installation complexity
- Resource requirements
- Licenses
- Data management, data staging (user, local group, access to Open Crystallography Database)
- Computational provenance
- A natural environment for the DANSE Scientific Toolkit

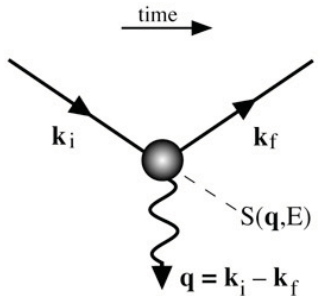

Please login - Mozilla Firefox
File Edit View History Bookmarks Tools Help
https://vnf.caltech.edu
Google
releaser mmckerns DANSE Release Notes Fedora Project Red Hat Free Content
DANSE
Welcome to the Virtual Neutron Facility
The Virtual Neutron Facility provides online computation tools for simulating neutron scattering experiments.
Screencast tutorials
Sign up (Mar 13, 2009) (2:30 min)
Overview of the Gulp simulation engine (Apr 28, 2009) (3:58 min)
Phonon calculation for fcc Ni (Mar 13, 2009) (4:46 min)
Molecular dynamics run of ZrO2 (Mar 12, 2009) (6:44 min)
Ab initio simulation of fcc Ni (Apr 27, 2009) (3 min)
Virtual neutron experiment: vanadium plate (Apr 27, 2009) (3 min)
Virtual neutron experiment: fcc Ni plate for which the phonon dispersions are computed from a BvK model (April 29, 2009) (3:59 min)
Sign in to your vnf account
Username
Usernames are case sensitive; make sure your caps lock key is not enabled.
Password
Passwords are also case sensitive. If you have forgotten your password, you may be able to reset it.
login
When you are done, please logout or exit your browser
Done
vnf.caltech.edu

MCViNE and Kernels



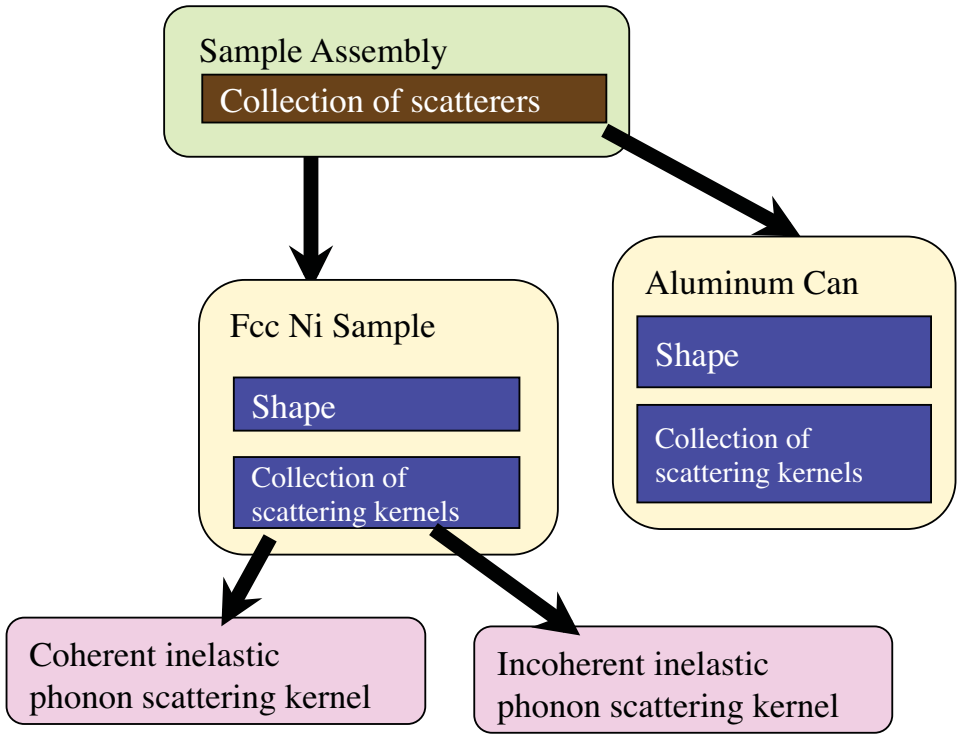
Inside the Sample





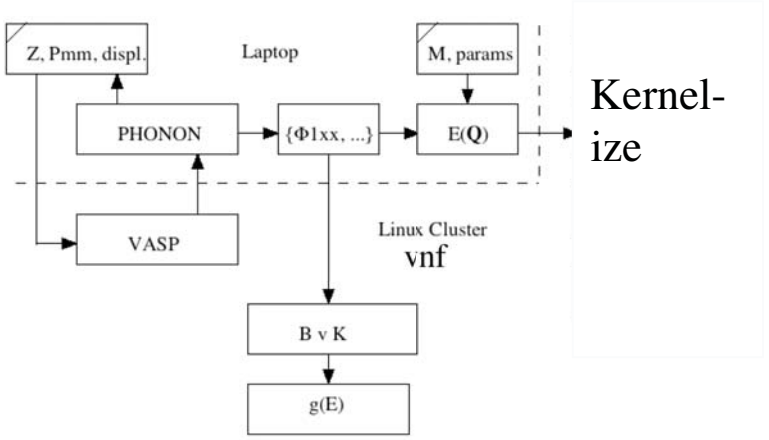
Scattering Kernel gives probability of deflection

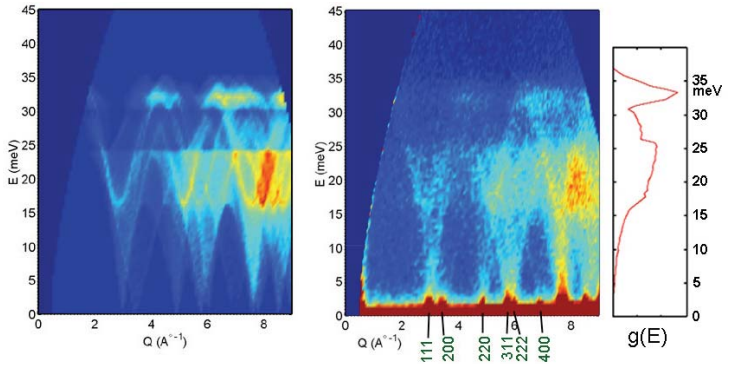
Sample Assembly gives shapes and coordinates of container and contents



Kernels Available Today

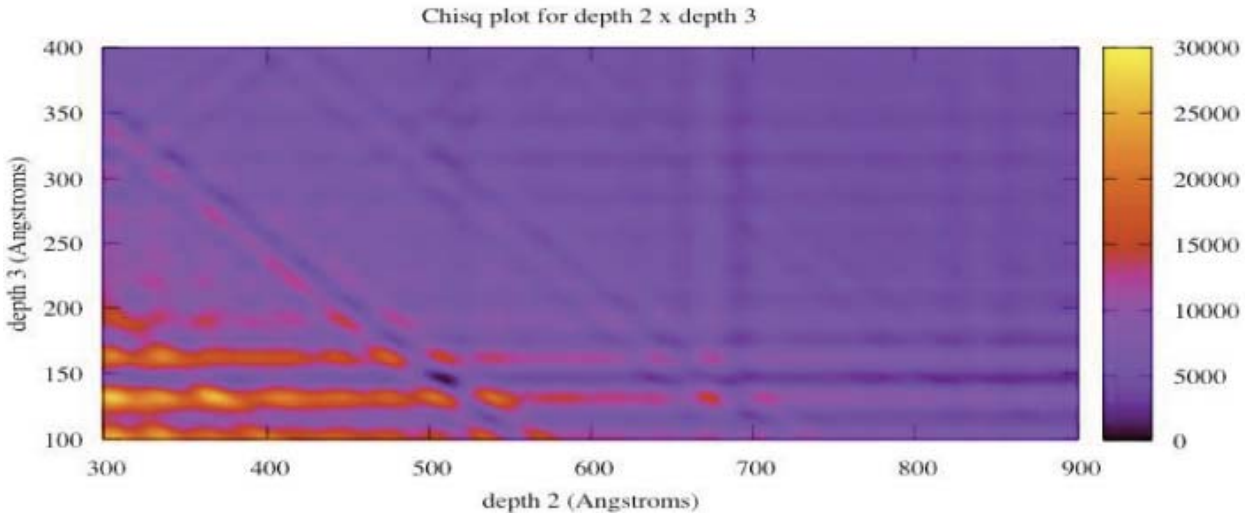
- Ab-initio (VASP + PHONON)
  - underway: QUANTUMESPRESSO
  - underway: FIREBALL
- Molecular Dynamics
  (GULP + nMOLDYN)
  - underway: MMTK
- BvK model E(Q) dispersions
- Diffraction kernels with simple rules to deflect neutrons.



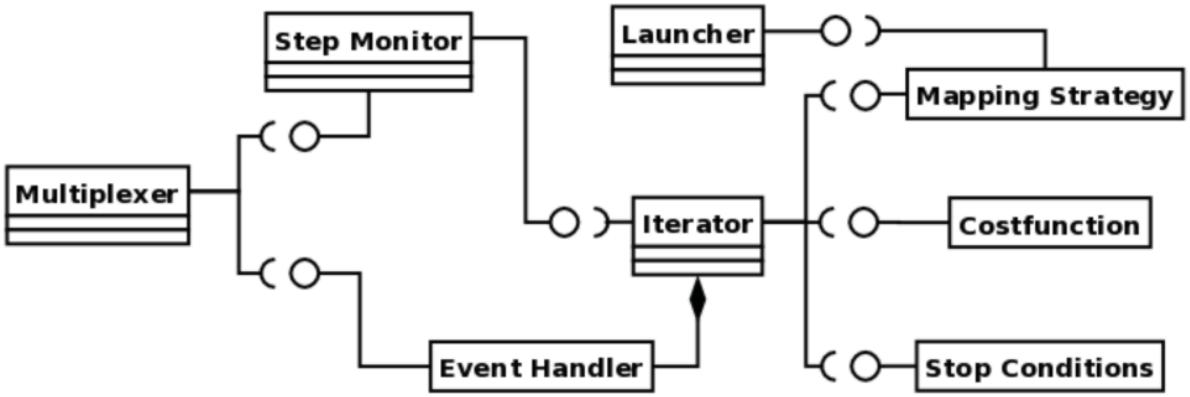


Optimization Framework (PARK)

- Optimization of parameters in models is used by all subgroups in flagship applications.
  - sometimes simple
  - often very complex, strategies difficult
  - developers planned for modularity
- Flexible optimization framework proved challenging.
- New framework allows further project integration in 2009.



Optimization Framework



- Iterators are built from Optimizers of SciPy or other packages.
- The Iterator acts on a Costfunction to provide the next set of values for evaluation.
- The workflow is directed by the Strategy.

Working With Users During Commisioning

- Release Site has focus on documentation, easy installation.
- Distribute work over multiprocessor resources at SNS, Teragrid, other systems at Caltech
- PARK and vnf to interoperate as services
- User feedback to help prioritize:
  - Work flow of web services
  - Tool development (for software developers)
  - Manuals, documentation, help

With modular software components, "What will scientists build to enable discovery?"

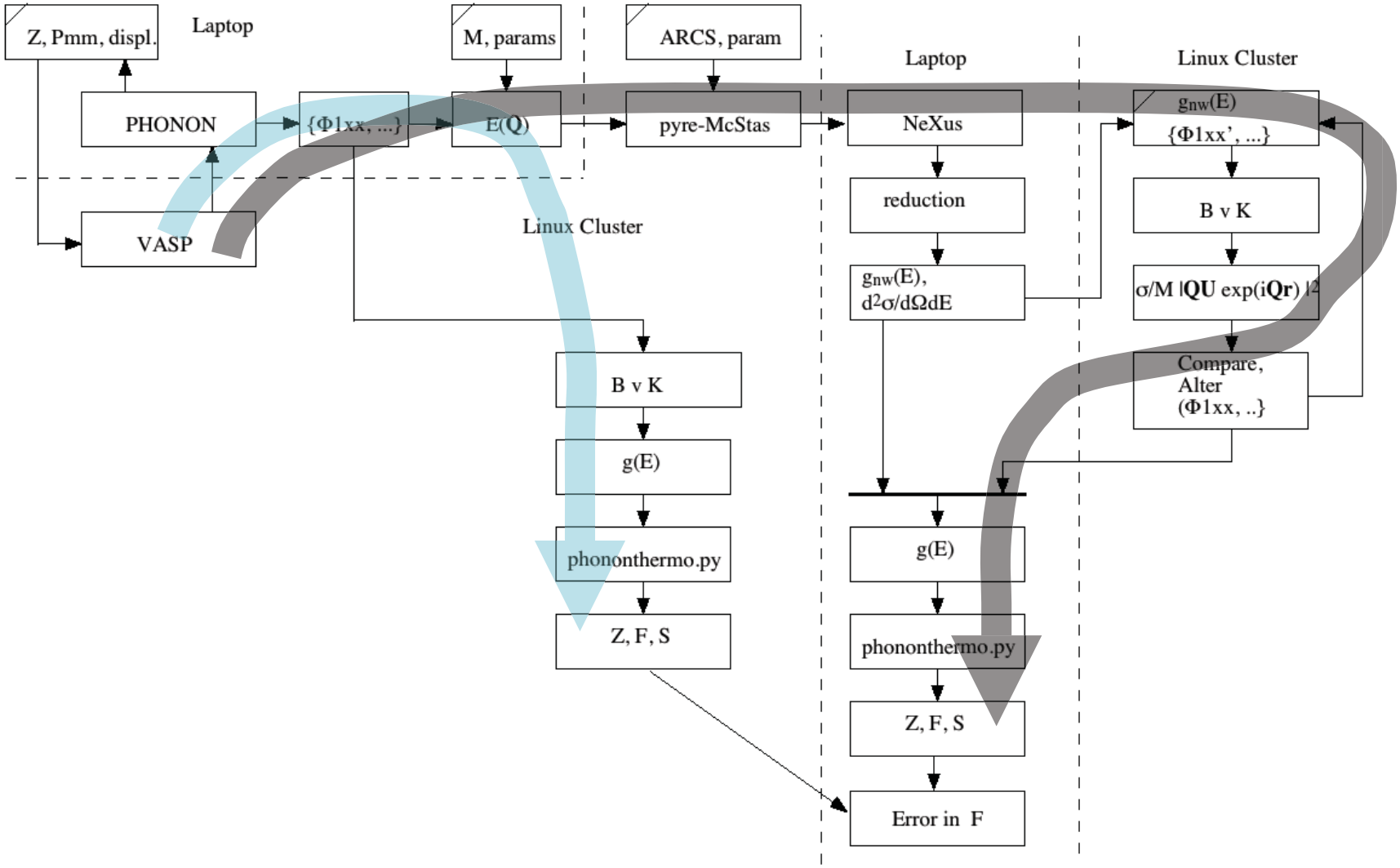
Depends on specific science.

Interoperability and flexibility enable creativity.

Goal: integrate tools across materials physics between diffraction and inelastic scattering.

Specific Study: PbTe structure and dynamics (integrate experimental results with underlying physics model)

Error Bars in Thermodynamic Quantities



Plan for Year 4

- Expand the DANSE Scientific Toolkit
  - more Virtual Instruments and Virtual Samples
  - more Materials Theory engines and Scattering Kernels
  - more Optimizers and Physical Models

- Integrate the Software Products (as appropriate)
  - integration of DANSE flagships with computing frameworks and services
  - deploy distributed computing services (test service interoperability)

- User Services and Feedback
  - More (friendly) users, but we need to work with them.
  - Match promises to development plan.
  - Be honest about capabilities and rough edges.
  - Expand computing resources for more users.

Diversity Strategic Plan

Emphasizes women in computational science.

Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

RISK WATCH LIST

1. User Expectations and Evaluation of Impact of DANSE
- Critical for any future plans
- How much user support can developers do?

2. Staffing Plan
- Scientist/software developers are hard to find.
- Hiring mistakes are very costly at this stage of the project.

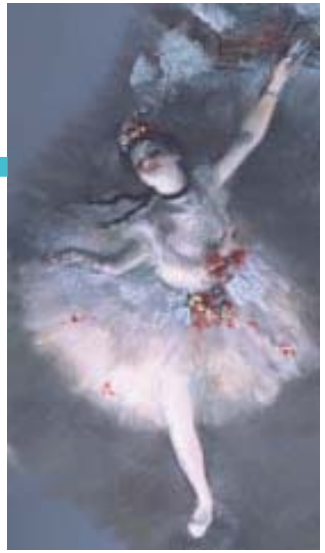
3. Schedule
- We do not have 5 years -- more like 4 if we are to get user acceptance of DANSE before the end of the project
- It is inappropriate to over-staff at this stage of the project.
- With present staff, we could end on time. If there are early departures in year 5, we may request a no-cost extension.

After DANSE Construction Ends in 2 Years

- "All that is human must retrograde if it does not advance."
  E. Gibbon.

- Three big issues to discuss now:
  - Maintenance of DANSE
  - User support
  - Future upgrades
- First examine the Big Picture of software in scattering science (Workshop to develop Roadmap)
- Future role for young computational scientist/developers.
- A community-based organization.

Summary



- Cost performance good. Schedule tracks hiring.
- Large release this year addresses scope and quality. Now acquiring usage information.
- Optimizer (PARK) and Simulation (vnf) tasks give project integration, interoperable tools, and new science capabilities.
- Toolkit for scientific creativity is being realized as a web service (the tree is there, we are adding leaves).
- Careful addition of users to the system.
- The future:

  - Computing opportunities in scattering are bigger than DANSE.

  - Start dialog now with users, facilities, NSF and DOE.

end