



# Inelastic Subproject Report

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Scope of Science in WBS 10

Tasks and goals of the inelastic subproject

Risks and Challenges

# WBS 10: Science Scope for Inelastic Scattering

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Neutron scattering research measures:

- arrangements of nuclei or spins, and
  - **dynamics of their motion (broad scope for inelastic).**
- 1) spin correlations in magnets, superconductors, and materials close to metal-insulator transitions
  - 2) vibrational excitations in solids and their relationship to phase diagrams and equations of state of materials
  - 3) vibrational spectra of molecules or individual atoms such as hydrogen
  - 4) diffusional motions and relaxation processes studied by quasielastic scattering



# Inelastic Reduction Software

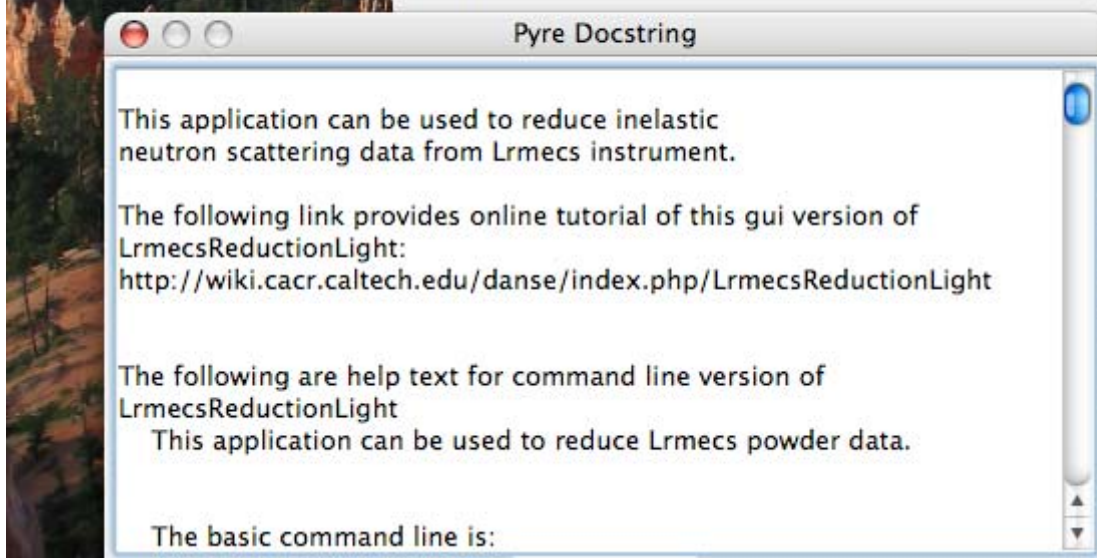
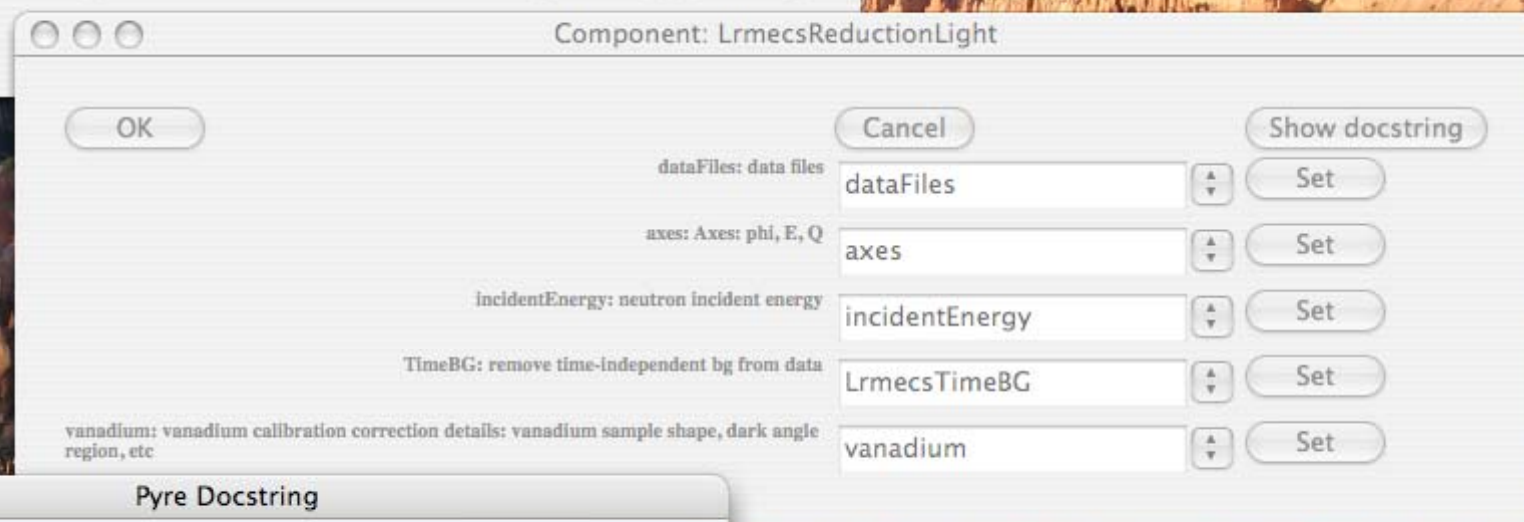
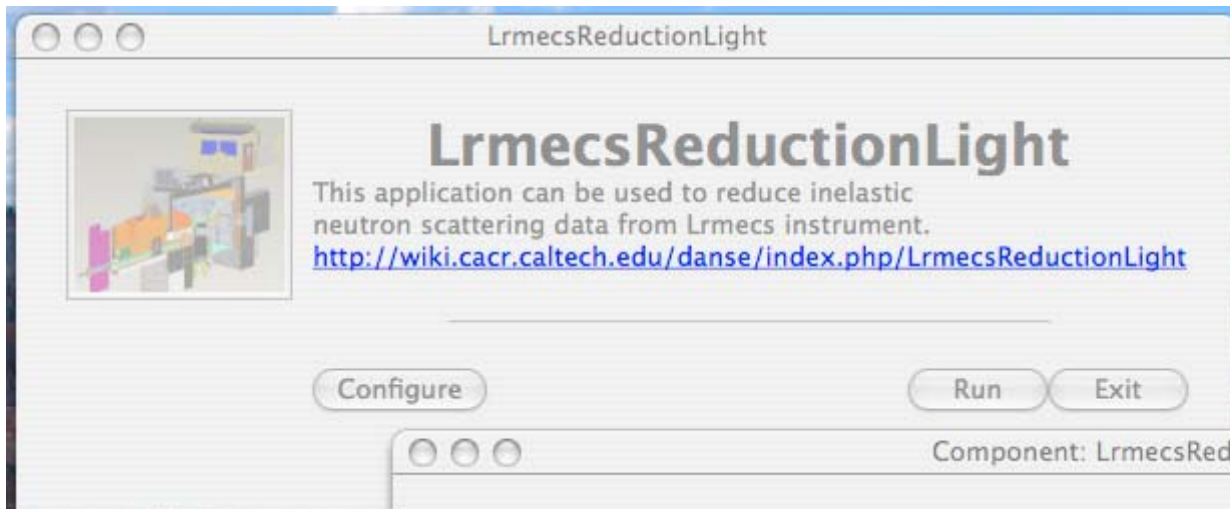
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## Release 1.1

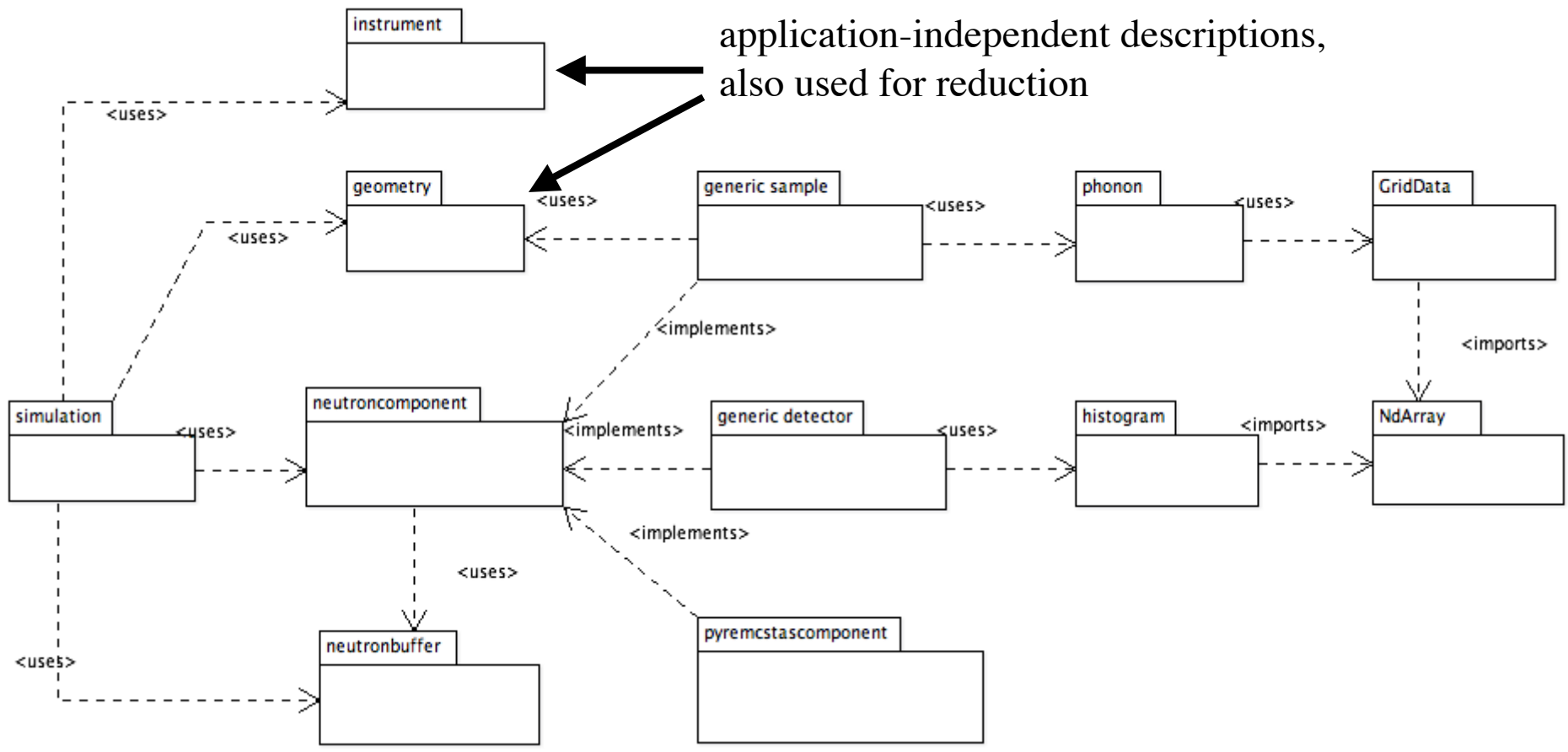
- Out now. Build of 10,094 files (!)
- New: detector visualization tools
- New: multiphonon plus multiple scattering correction
- Modular components - reduction framework
- Presented at ARCS/SEQUOIA IDT meeting last week
  - The group wanted more python command line access

## Release 1.2 plans

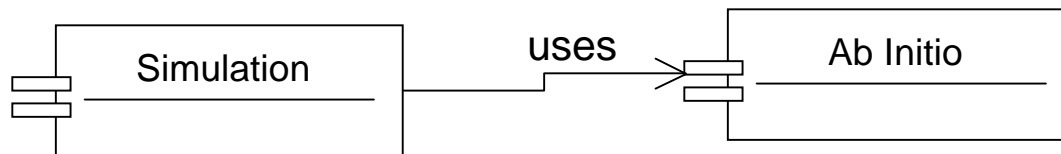
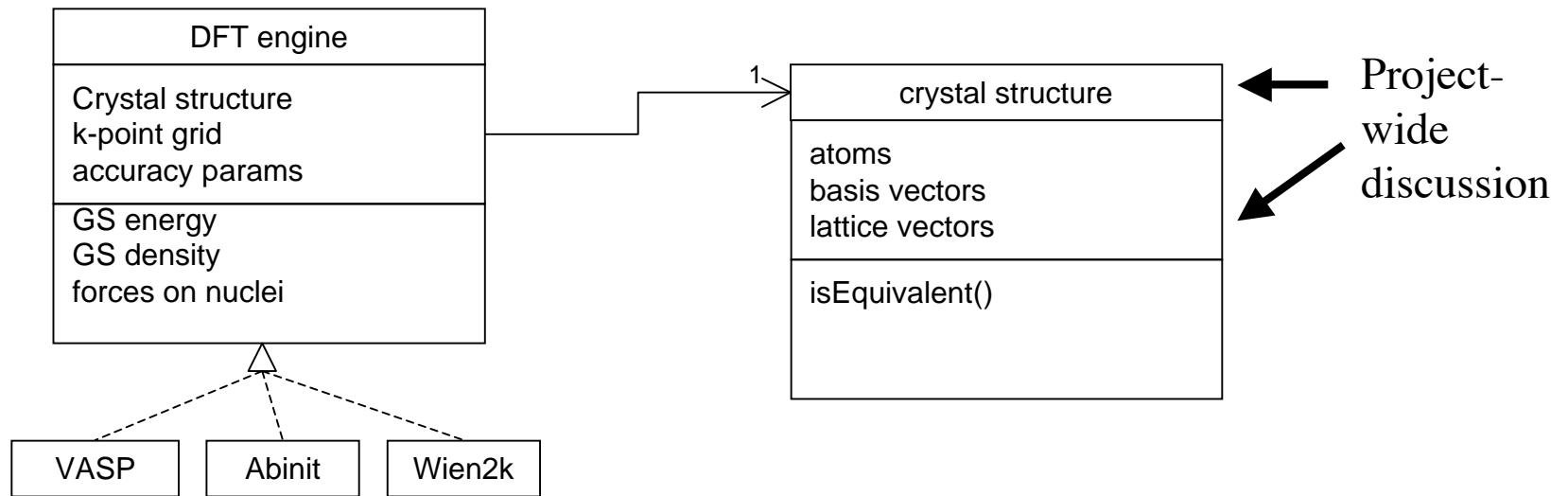
- More user documentation for direct python function calls
- ARCS itself (need data to try it out)
- September 2007 release



# Simulation Framework (package diagram with dependencies)

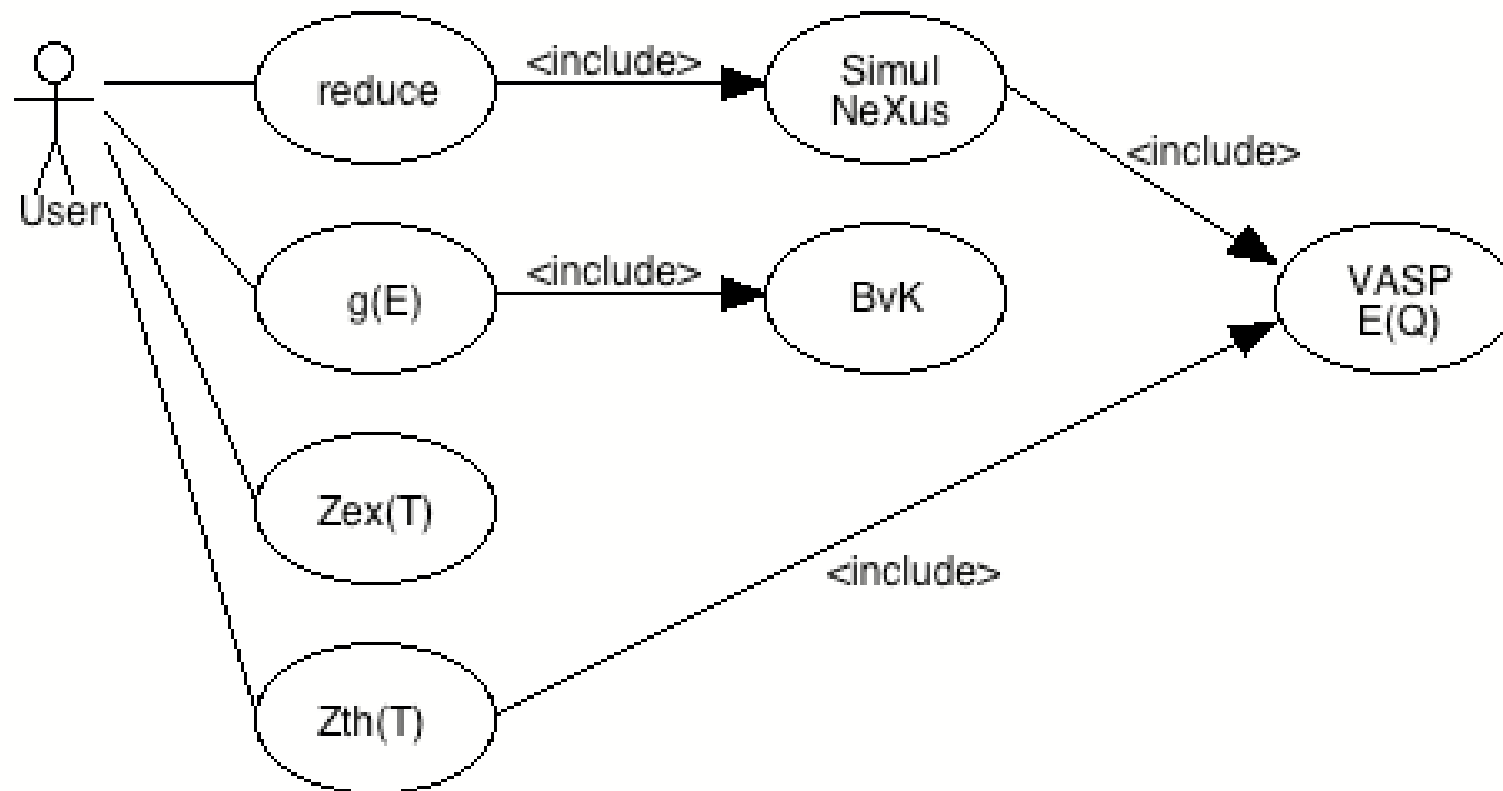


# Ab-Initio: Two features for 2007

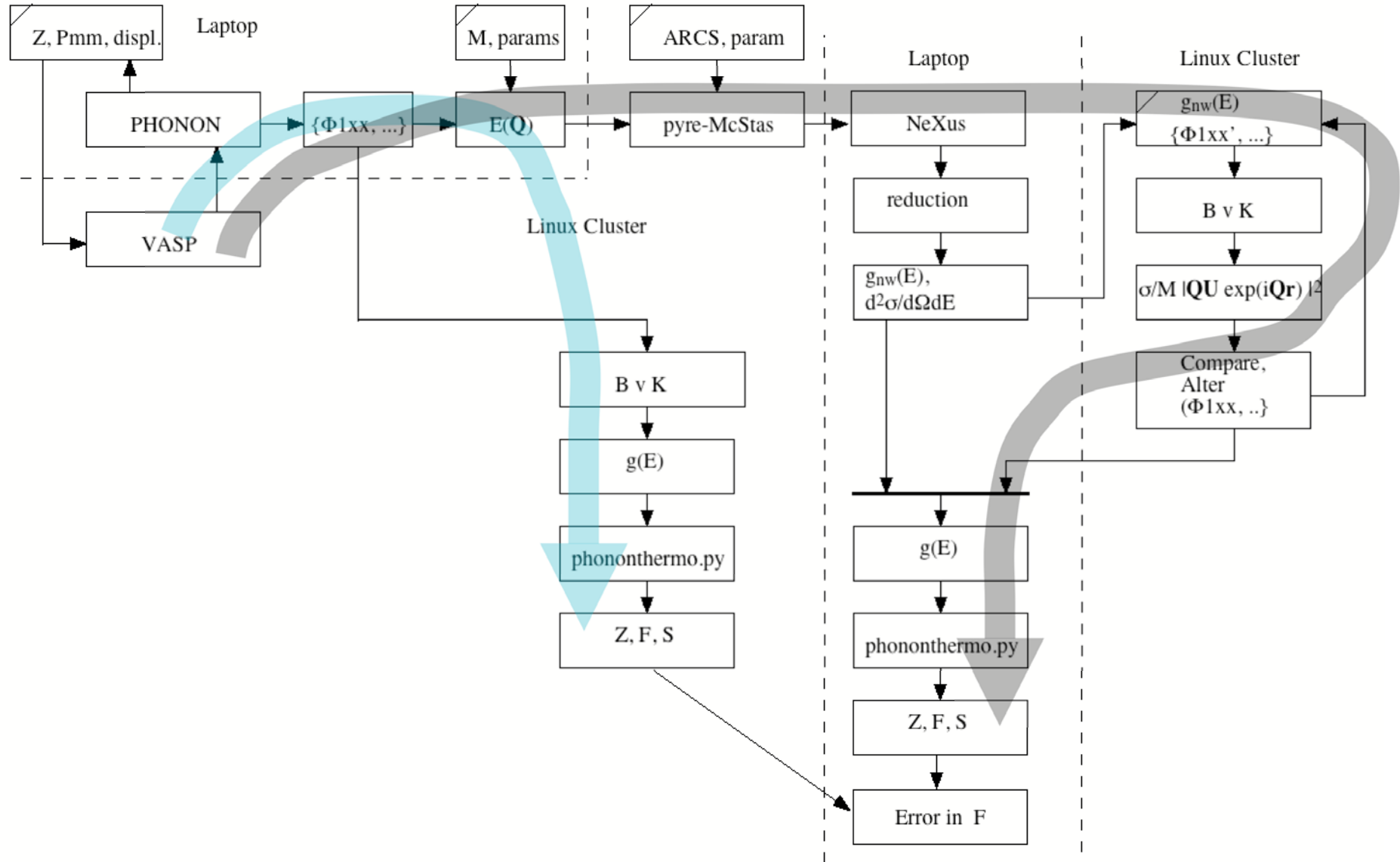


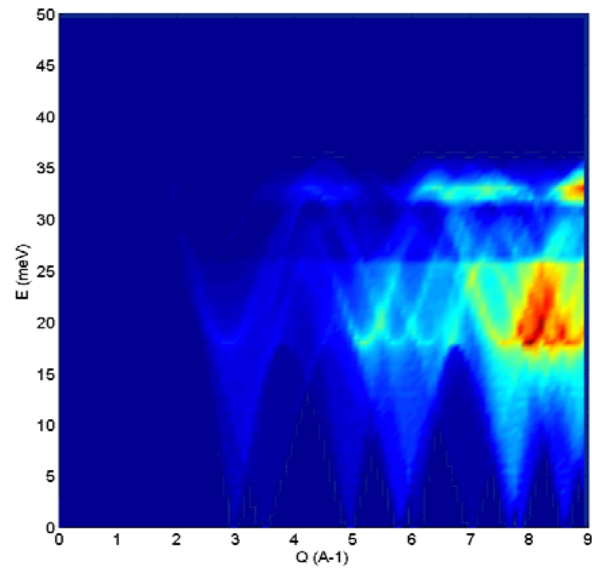
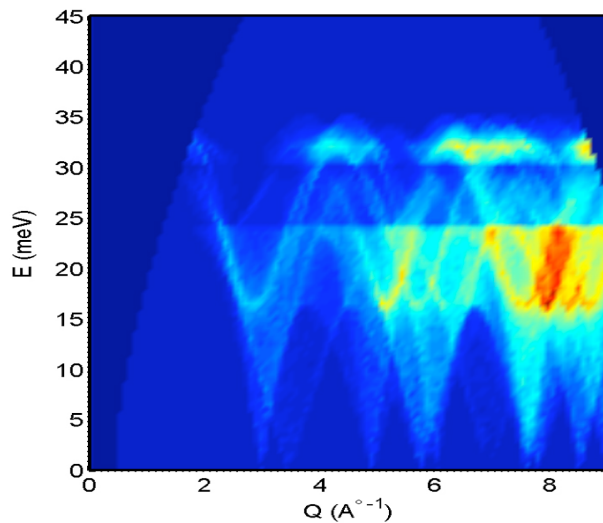
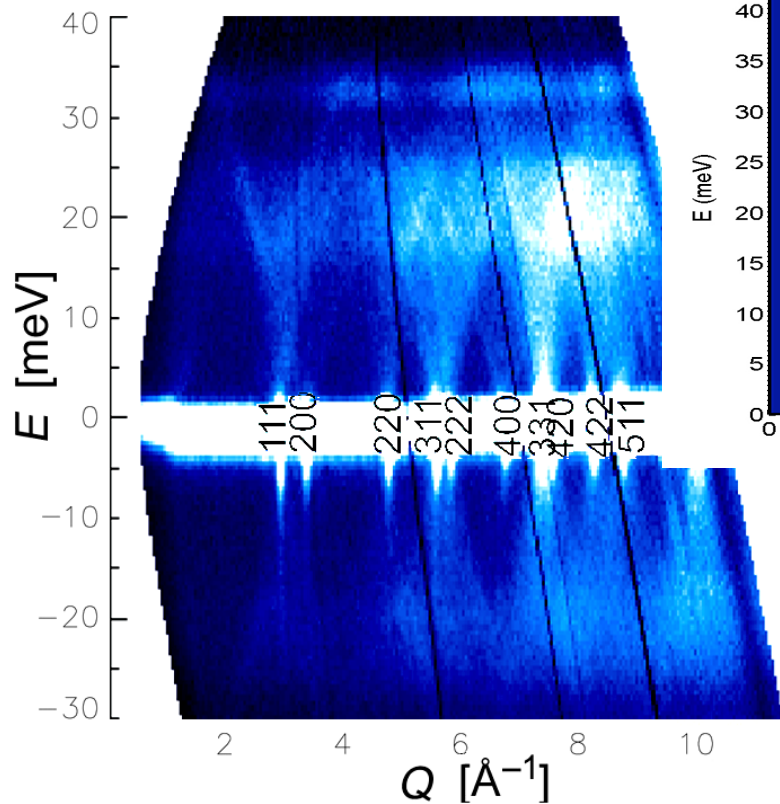
# Error Bars in Thermodynamic Quantities

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# Error Bars in Thermodynamic Quantities





Experiment (Pharos)

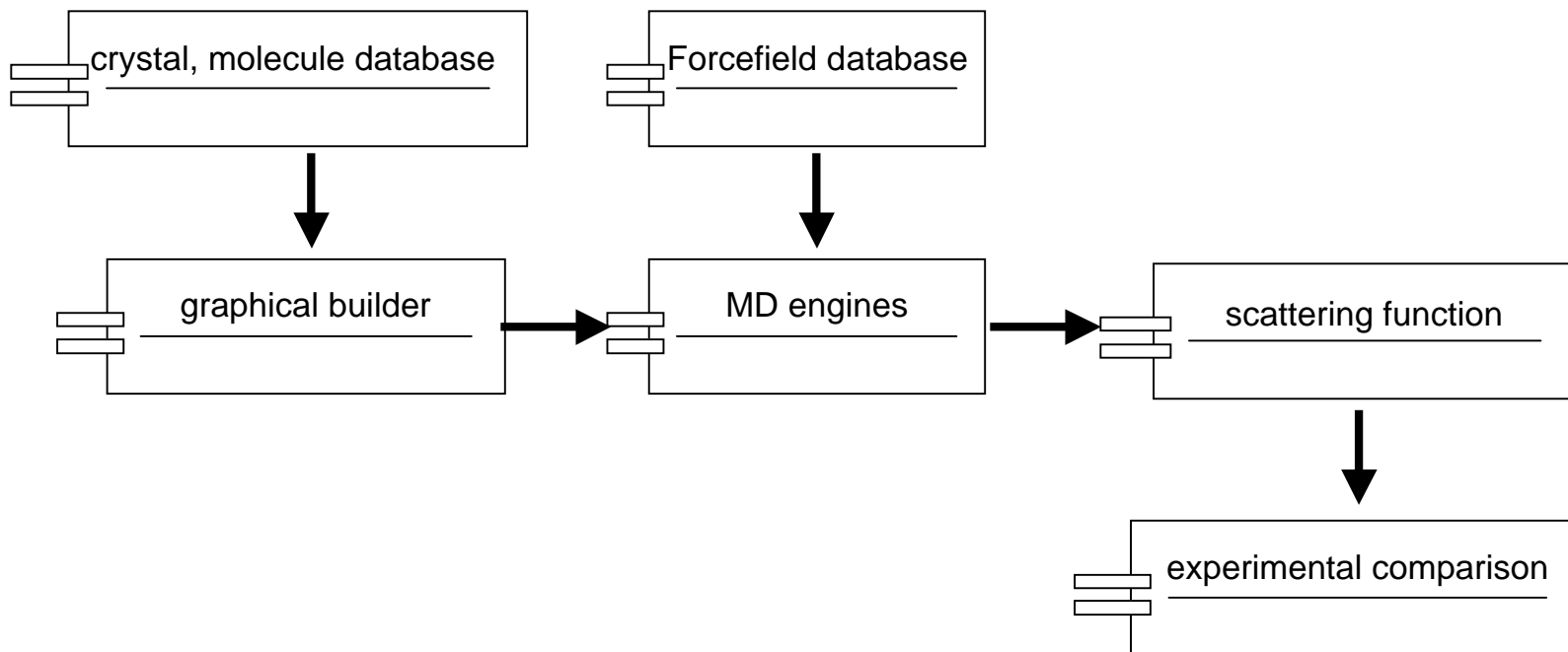
Bv-K Model (Brockhouse)

VASP (mag Ni)

Prototype results

# Chemical Physics (increments in 2007, more 2008)

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# Plans for 2008

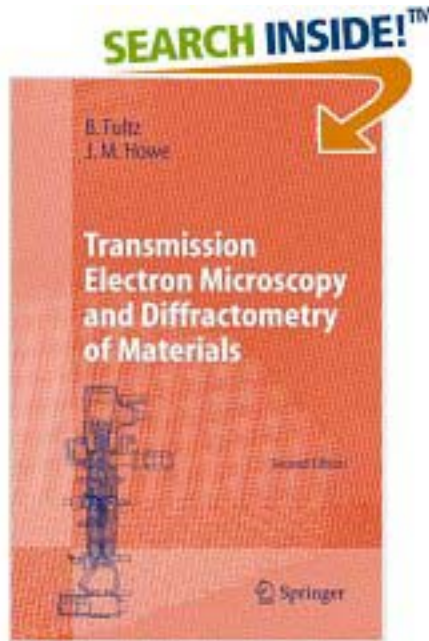
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- Chemical Physics
- Magnetic scattering (magnon models)
- Monte Carlo Instrument Simulation
- Advanced Data Reduction
  - Single crystals using UB matrix
  - Fits to dispersive information
  - Separation of phonons and magnons by Q-dependence
  - Neutron weight correction (prototypes in use now)
  - SEQUOIA, CNCS (TBA)
  - Possibility of processing event mode streams?

# Education and Outreach

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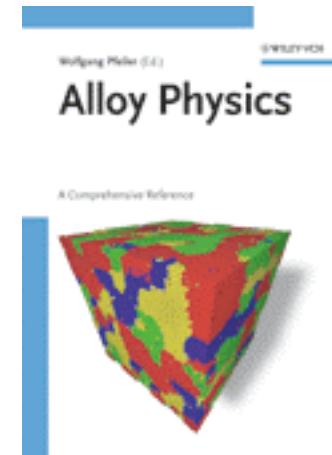


2

Inelastic Neutron Scattering  
with the ARCS Spectrometer

ARCS Software Release 0.1.0a

3



- Students

- J. Munoz, U. Texas El Paso, underrepresented minority student
- J. Ernhardt, Caltech undergrad underrepresented minority student
- Eliot Setzer, Caltech CS undergraduate
- M. Kresch, Chen Li, Caltech graduate students

# Inelastic Effort Today

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- Fully staffed
  - Mike McKerns (in his spare time)
  - Jiao Lin
  - Olivier Delaire
  - Brandon Keith
  - Max Kresch (grad student)
- Find science for everyone, consistent with project

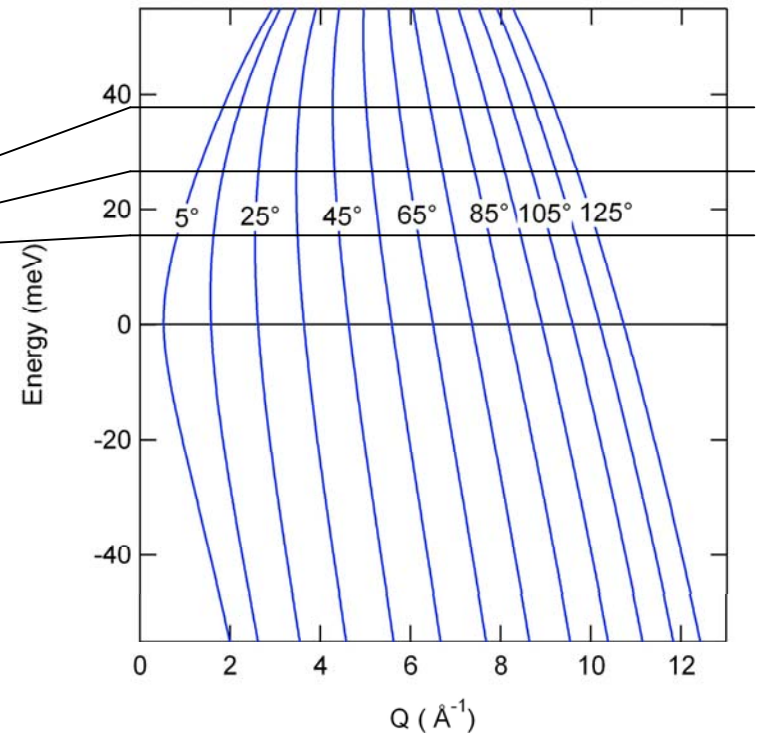
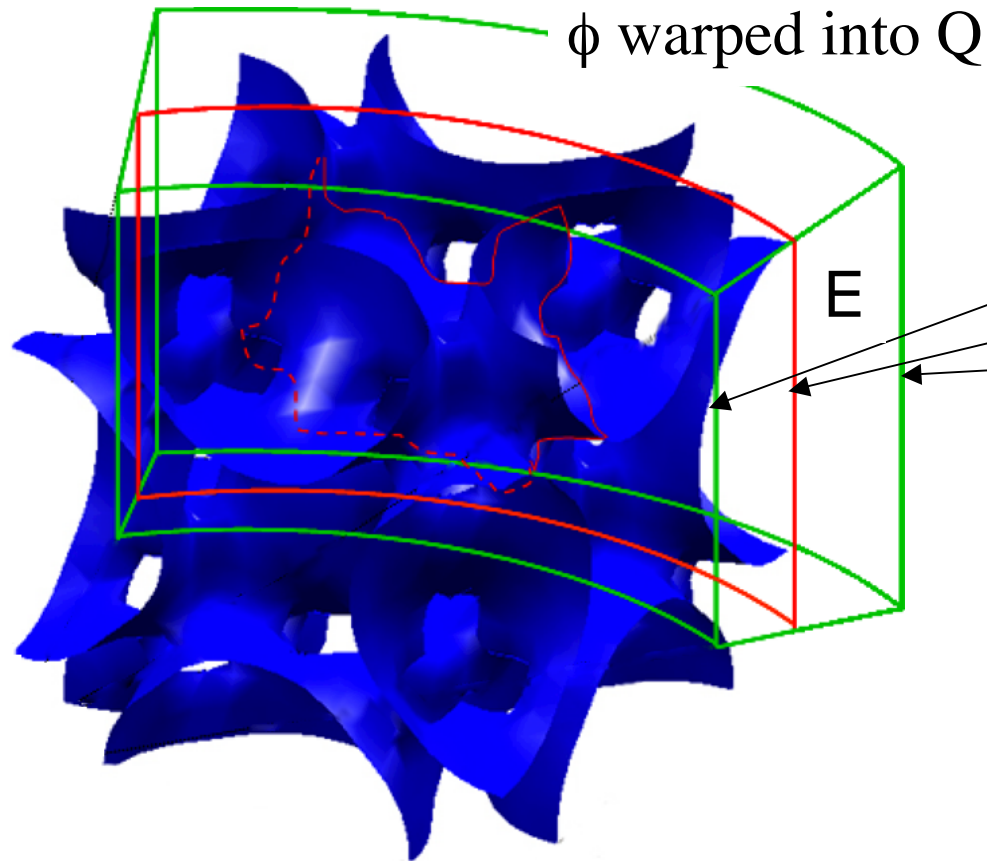
# Risks (and Opportunities)

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- Direction in magnetic scattering -- requires real science and beamtime.
- Direction with single crystals -- requires real science beamtime.
- Robustness of fitting dispersive information in noisy data -- ideas may change as source power increases at SNS.
- User science expertise needs to be high for some applications.
- Laptop computer performance and user expectations.
- How do we support users?

# Single Crystal Initiation: Momentum and Energy Conditions for Excitations

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# Reasons for Confidence and Optimism

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- Most of the big science packages have been tested.
- Prototypes have been tested for many of the 5-year deliverables.
- Team skills are international-class.

# Summary of WBS 10: Inelastic Scattering

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- 1) Scope for:
  - dynamics of small molecules
  - elementary excitations in solids
- 2) Reduction application is mature. Plans for Release 1.2.
- 3) Prototypes exist for some of the main deliverables, and parts of many others have been tried.
- 4) Staff in place for all scope.
- 5) Nearly all functionality can be tried out in 2008.