VNF: Virtual Neutron Facility
Context, capabilities, and lessons learned

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What is DANSE?

- Collection of software to perform neutron scattering analysis.
- Divided up into 5 subgroups--Diffraction, Engineering Diffraction, SANS, Reflectometry, Inelastic Scattering.
- 5 year project funded by the NSF, made especially to complement the SNS, 2011 is its last year
- http://danse.us

Current Releases:

Diffraction

- PDFgui: Profile Refinement of Atomic PDF
- SrRietveld: Rietveld Refinement of Powder Data
- SrFit prototype: Configurable Diffraction Fitting Application

Engineering Diffraction

- SCM: Self-Consistent Modeling (EPSC: Elasto-Plastic Self-Consistent)
- Real time Rietveld Analysis
- Vulcan Instrument & Microstructure Simulation

Current Releases:

Small-Angle Scattering

- SansView: 1D, 2D SANS modeling and data analysis software
- SliceView: 2D modeling prototype
- SimView: real-space simulation prototype
- PrView: P(r) inversion

Reflectometry

- GArefl: Genetic Algorithms Depth Profile Modeller
- KsRefl: Interactive Depth Profile Modeller
- DiRefl: Direct Inversion Depth Profile Modeller

Current Releases:

Inelastic Scattering

- DRCS: Data Reduction for Chopper Spectrometers
- VNF: Virtual Neutron Facility

DANSE Infrastructure and Central Services

- pyre Runtime Component Framework
- mystic: a global optimizer
- pathos: a framework for heterogeneous computing
- luban: a generic user interface builder

Laptop

Distributed Data Analysis for Neutron Scattering Experiments

Welcome

Scientific Software

Release Pages

FAQ

News, Discussion, Meetings

Project

Contact Us

Neutron scattering experiments reveal the structure and motions of atoms in molecules, materials and condensed matter. The hardware facilities and instrumentation for these measurements are major international scientific investments. DANSE is a five-year project to build software for interpreting data obtained in neutron scattering experiments.

About DANSE

To develop software for neutron scattering research, DANSE is organized around five scientific subfields. Each subproject is a small team led by a scientist who has identified new opportunities for computing in neutron scattering science. The five subfields are 1) Diffraction, 2) Engineering Diffraction, 3) Small-Angle Scattering, 4) Reflectometry, 5) Inelastic Scattering. The five subfields require different types of data analysis, owing in part to the different physical phenomena under investigation. They also have historical differences in user expectations -- the choice between ease-of-use and configurable features has reached a different balance in the biology and physics communities, for example. The DANSE project manager coordinates common components and algorithms, software quality standards, and development processes. A central services group provides a common runtime framework for interoperability of software components.

Annual releases of software occur by April of each calendar year, driven in part by the review requirements of the NSF award for DANSE. The released products are unique to each subfield, but a common theme is how they allow users to calculate how materials scatter neutrons. For example, Monte Carlo simulations of neutron instruments have been extended to include simulations of material characteristics, enabling new types of neutron scattering science to be done on the computer.

All work derived from DANSE software should acknowledge DANSE with the following statement: "This work benefitted from DANSE software developed under NSF award DMR-0520547." For more detail, see the DANSE license.

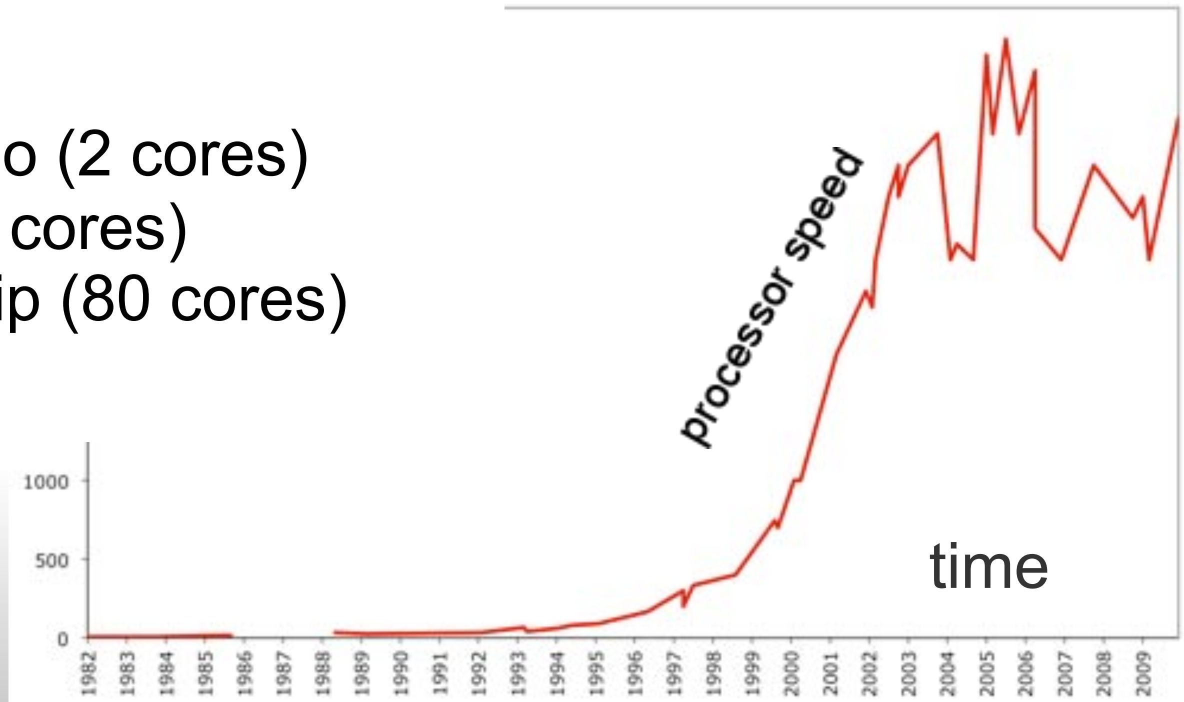
DANSE Resources and Where to Find Them

Descriptions and Highlights
Software Repositories
Developer's Trac Pages
Wiki Site
Activity in the Project
Development Practices
Mailing Lists
Questions
License

Prologue

- Processor speed, and now multicore capabilities, are increasing exponentially

- Intel case study:
  - 2006: Core 2 Duo (2 cores)
  - 2008: Core i7 (4 cores)
  - 2011: Polaris chip (80 cores)

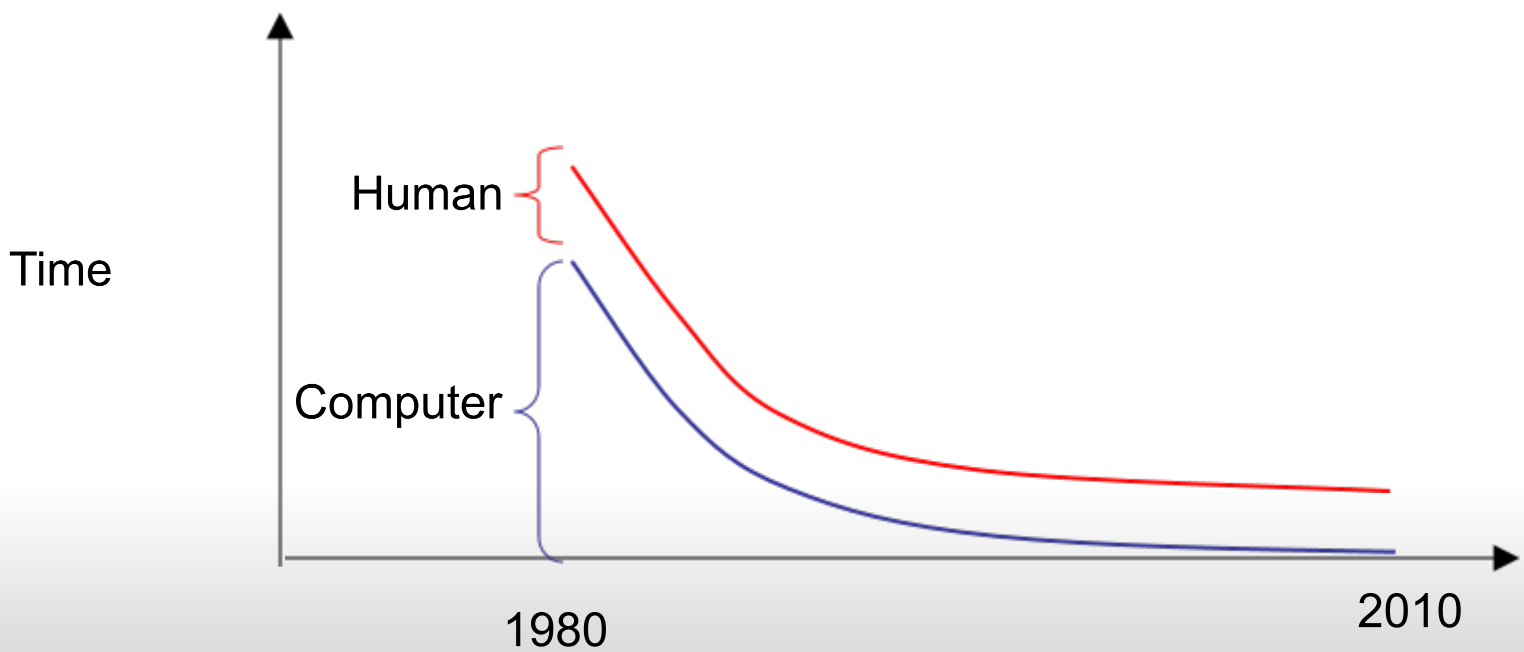


More processors-->More complex, realistic materials

- High-end physics simulations are finally possible, even on commodity desktops
- VNF is an attempt to not only analyze neutron scattering data, but ***predict*** it
- Accuracy of prediction scales with number of processors
- According to Intel, in several years, 80 cores will become 100s of cores
- Average desktop will be today's supercomputer

Prologue II

Time needed to complete a high-end physics simulation



Easier simulation setup

- VNF is an attempt to take advantage of web formatting (css, javascript, more widgets) to construct more usable, connected, and convenient interfaces than desktop
- VNF catalogues all user's simulations (settings/ results), samples, instruments, virtual neutron experiments, etc. so they can be
  1. altered slightly and rerun
  2. shared with collaborators (similar to google docs)
  3. datamined
  4. connected to third party databases (materials, real neutron experiments, etc.)

The web is great...

- Web interface allows us to merge documentation and interface in seamless way--->overcome user intimidation with staging such calculations
- No installation necessary
- No software updates necessary
- No ssh'ing, scp'ing
- No file conversion
- All workflows automated with wizards
- Extensible scripting API allows VNF use as library

Specialized for neutrons

- Anyone can run simulations, but VNF has **specialized algorithms** to back out:
  - Scattering functions from dynamics
    - S(Q,E), EISF, multiphonon scattering
  - Structural functions from equilibrium structures
    - S(Q), PDF
  - McVINE: Online, enhanced remake of McSTAS
  - Related material properties (DOS, RDF, MSD, VACF, Diffusion constant, etc.)

Physics engines & dbs...

- Integration with third-party databases:
  - Crystallography Open Database (116179 entries)
  - NIST Neutron database
  - SNS Orbiter data system
- Forcefield phonons/md/spinwaves
  - GULP*, MMTK*, BvK*, (Lammps*), (McPhase)
  - Database of forcefields / forceconstants
- Ab Initio phonons/md
  - Quantum Espresso*, (Vasp*)
  - Convergence tools to speed up calculations
- Scattering functions from dynamics
  - Parnasis*: capabilities of aClimax and nMoldyn

* = runs on multiple processors   () = in progress

Fitting capabilities

1. AtomSim-->Can fit forcefields/forceconstants to:

- S(Q,E) spectra (beta version of GULP)
- bulk moduli
- Young's modulus
- Poisson's ratios
- shear moduli
- static dielectric constants
- high frequency dielectric constants
- refractive indices
- piezoelectric constants
- phonon frequencies
- non-analytic correction for gamma point modes
- phonon densities of states
- projected phonon densities of states
- phonon dispersion curves

Fitting capabilities

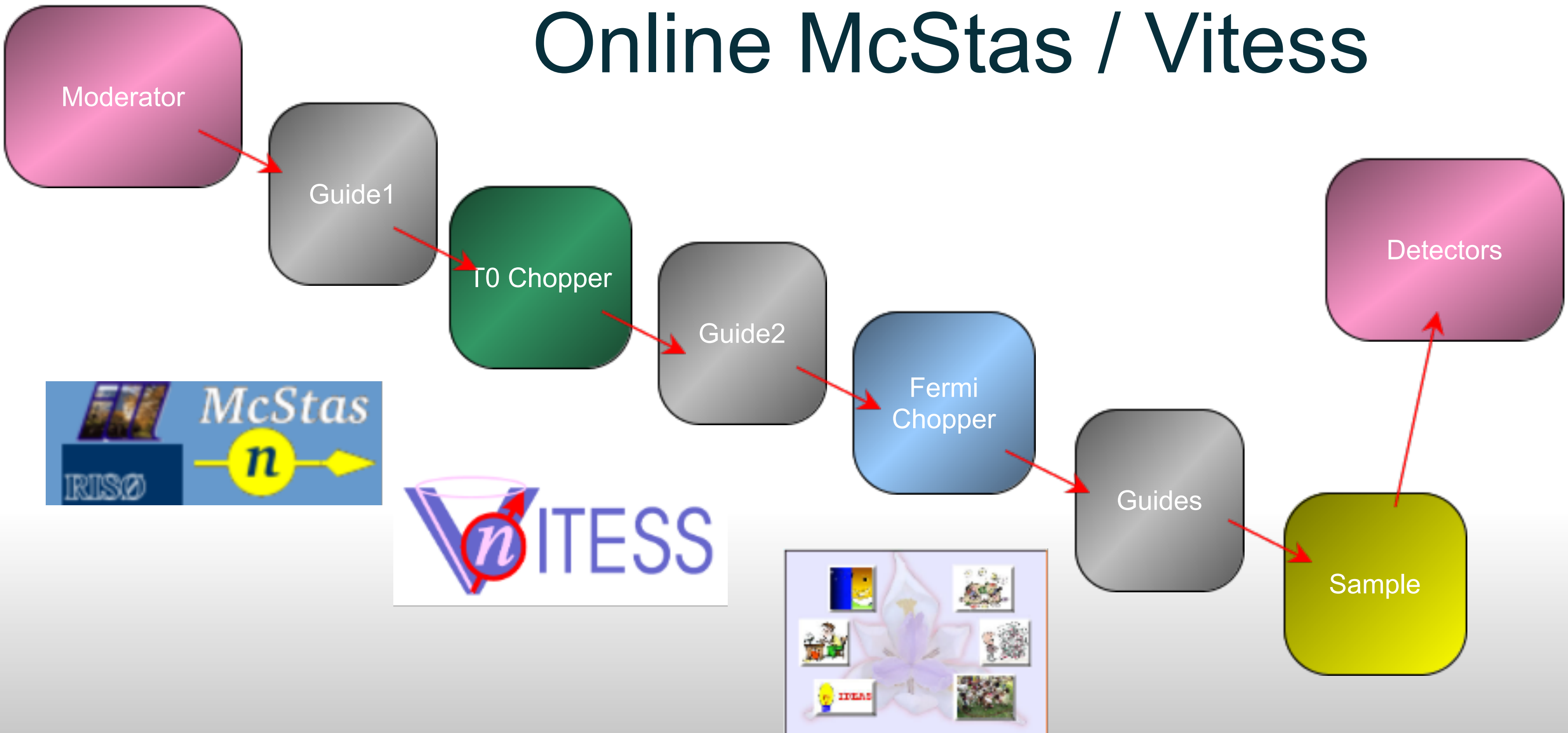
- zero point vibrational energies
- entropy (constant volume)
- heat capacity (constant volume)
- Helmholtz free energy
- electrostatic potential
- electric field
- electric field gradients
- Born effective charges
- frequency dependent dielectric constant tensor
- reflectivity

AtomSim: Web-deployed atomistic dynamics simulator (Keith et al.), J. Appl. Cryst., accepted

2. Mystic--Only available with scripting interface
3. Other subprojects: Pdfgui, Pdffit, Sansview, Prview...

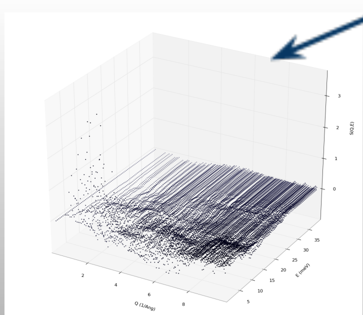
Instrument simulation...

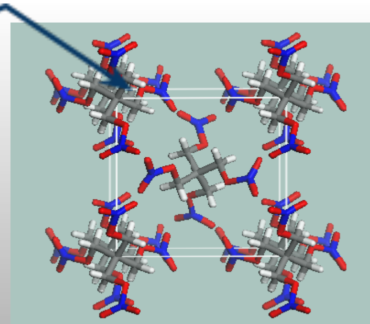
- McVINE: Enhanced Online McStas / Vitess

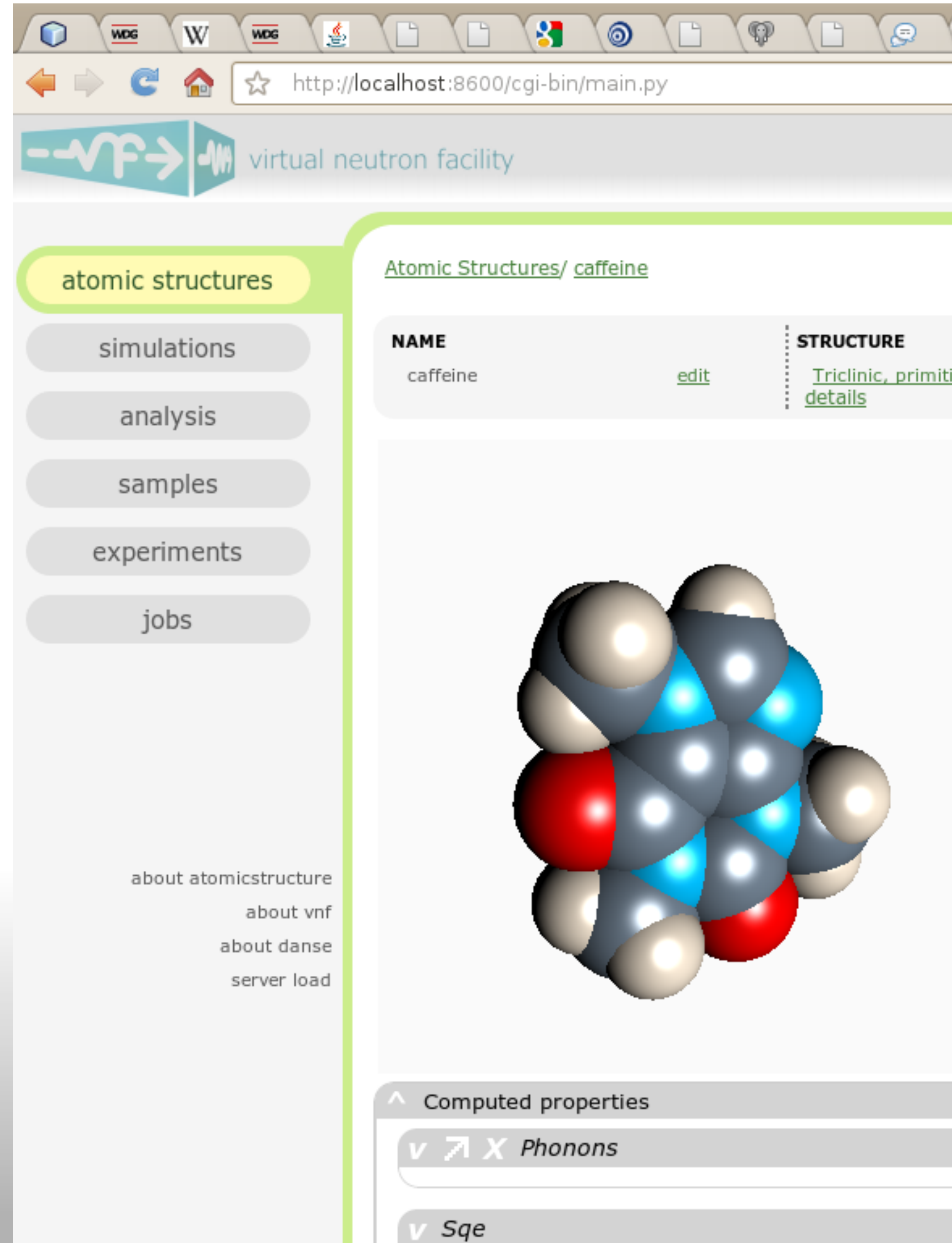


Visualization

- Jmol and O3D viewer/plotter for 3D
- Flot and Matplotlib static images for 2D
- Linking 3D animation of dynamics with 2D SQE







Making libraries easy_install-able from PyPI...

- plotlib - Inelastic
- parnasis - Inelastic
- matter - Inelastic
- qecalc - Inelastic
- mystic - Central Serv.
- pathos - Central Serv.
- pyina - Central Serv.
- dill - Central Serv.
- pox - Central Serv.
- pdffit - Diffraction
- pdfgui - Diffraction
- srrietveld - Diffraction
- diffpy - Diffraction
- drchops - Central Serv.
- luban - Central Serv.
- qecalc - Inelastic
- pyIDL - Inelastic
- pygrace - Inelastic
- histogram - Inelastic
- cy-scm - Eng. Diffraction
- others....

Testing...

- Buildbot tests after each svn check-in
  - Python unit tests
  - Automated html tests through capturing user workflows with Selenium
- Users are testing science...
  - Starting to fly in users every two months to Caltech to stress test it with actual science
  - Capture major user workflows
  - Help users understand VNF

Typical Workflow...

(1) create material (upload, import from db, etc.)

(2) calculate dynamics or structure

(3) calculate scattering functions

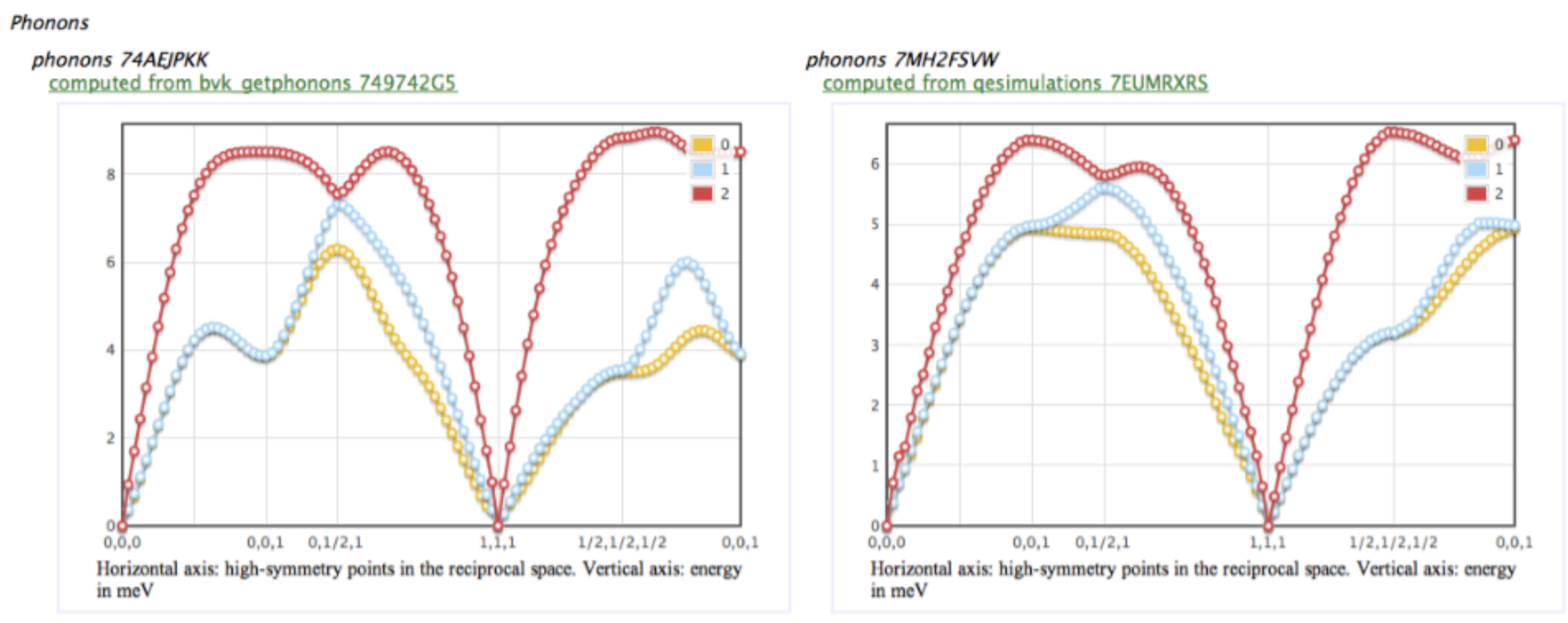
(4) run through virtual neutron instrument

(5) visualize

(6) compare or fit to experiment

(2)

Pb Phonons--Forcefield vs Ab Initio

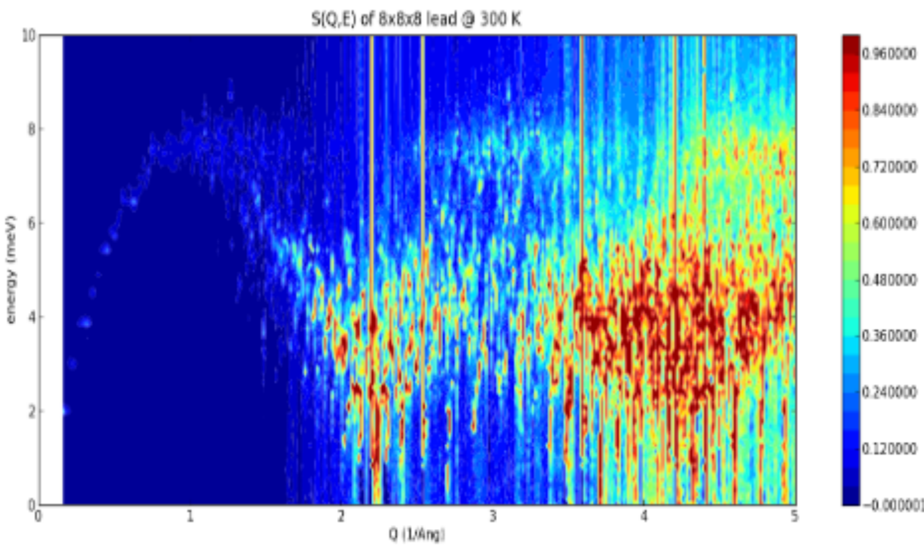


BvK model

Quantum Espresso

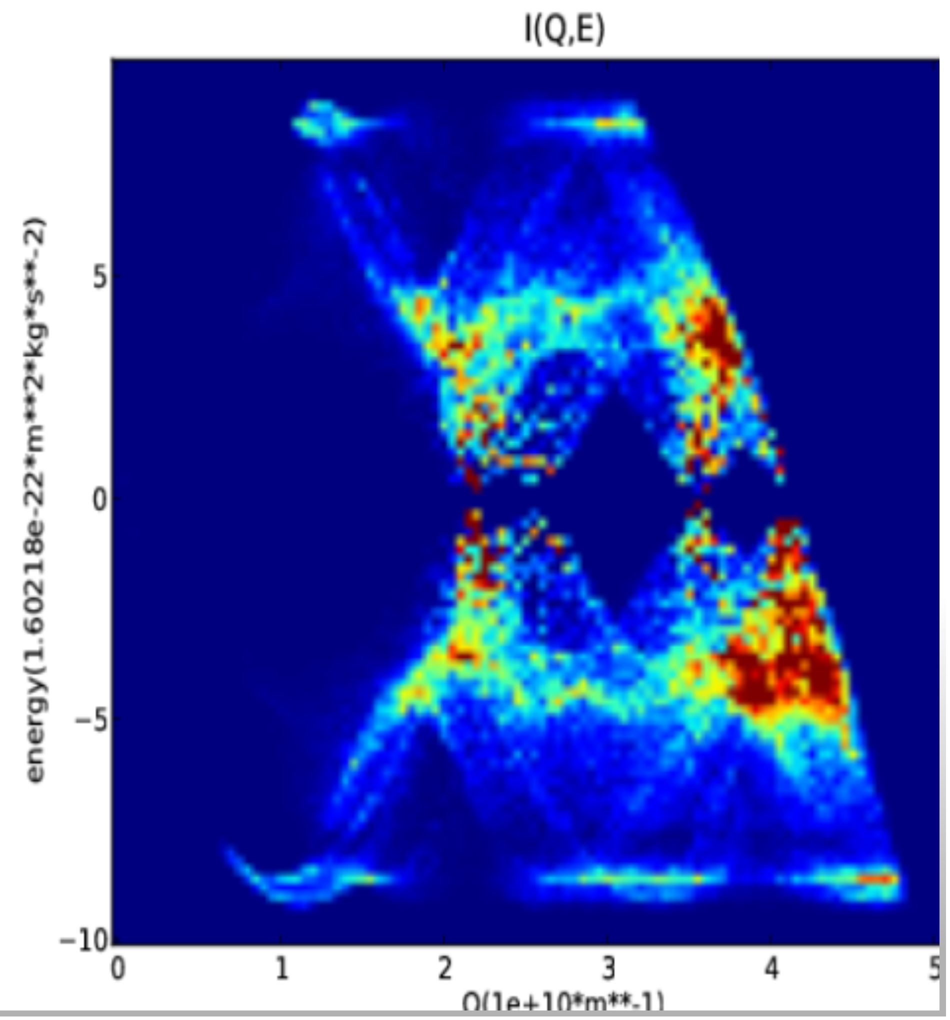
(3)

MD S(Q,E)



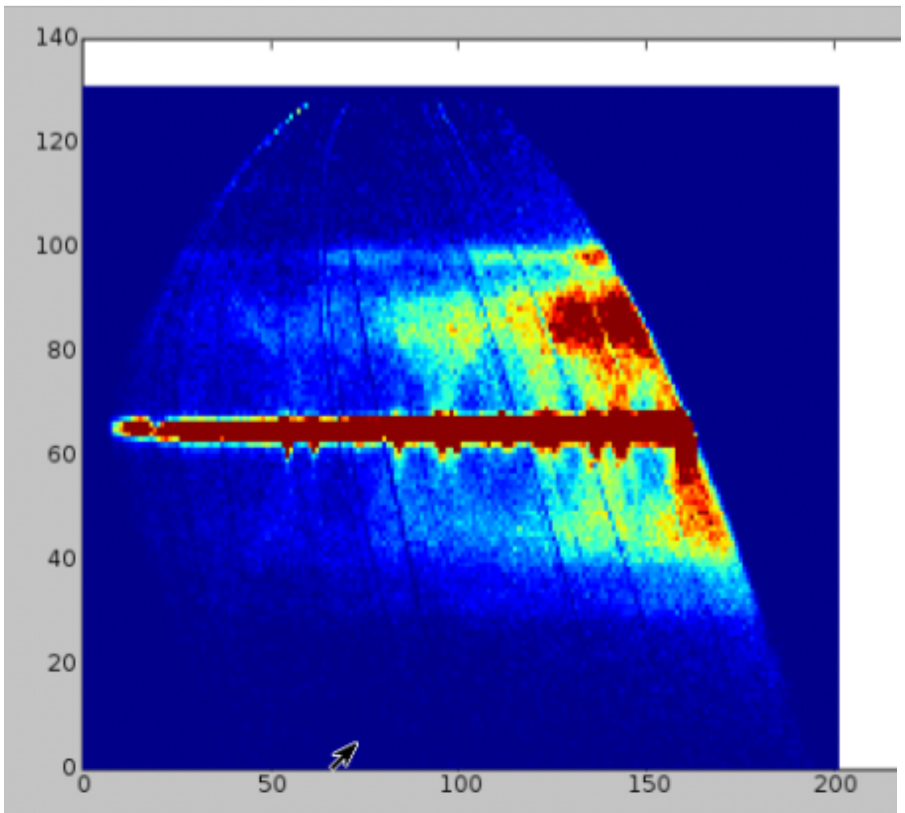
(4)

Phonon S(Q,E)

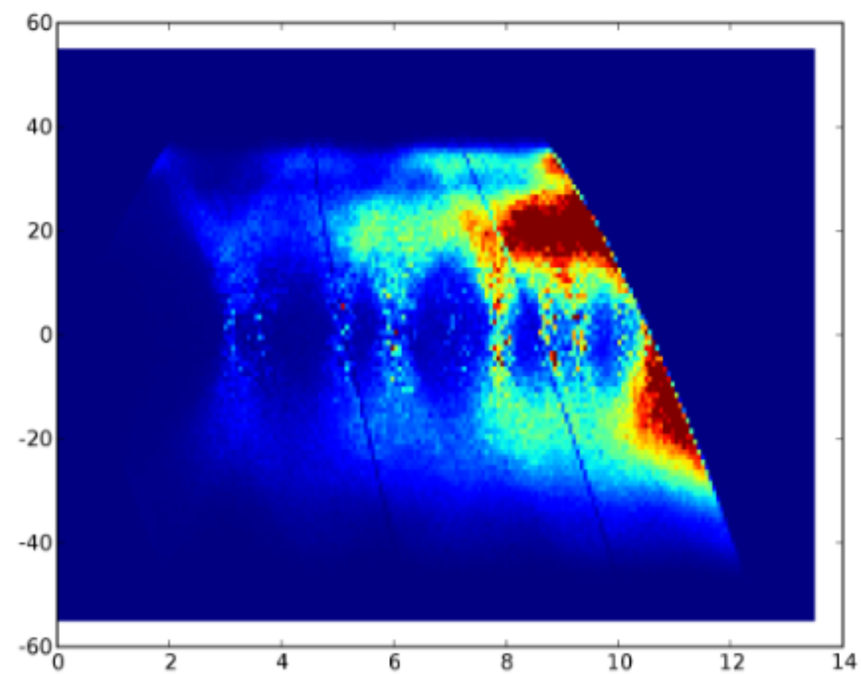


(6)

Experiment:
Ni at PHAROS



Forcefield
Simulation



Development status

- DANSE is in the final stage of "Term paper evolution":
  - Spent a lot of effort accumulating quality material
  - Our scope is large
  - "mad dash to finish term paper" is underway
    - make interface easier to understand
    - no bugs
- Need **harsh criticism**, *probing* questions, & lots of healthy skepticism

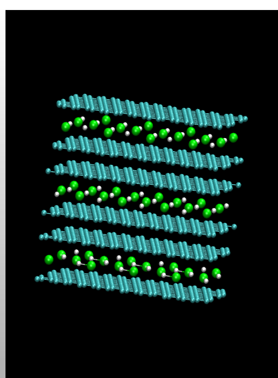
Lessons learned

- Avoid **NIH** ("**Not Invented Here**"): a term used to describe persistent social, corporate or institutional culture that avoids using or buying already existing products, research or knowledge because of their external origins. http://en.wikipedia.org/wiki/Not_Invented_Here
- Have framework documentation ready **before** the project starts (not in 3rd year).
- Developers should have been meeting with instrument scientists every week...
- Web is a great platform...use javascript libraries

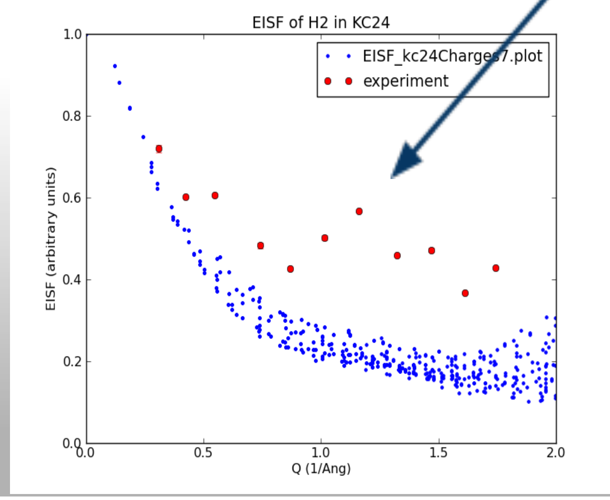
Lessons learned

- Compared to real experiments, virtual experiments are:
  - faster
  - cheaper
- As number of cores increase, virtual experiments are becoming:
  - "more accurate" than real experiments

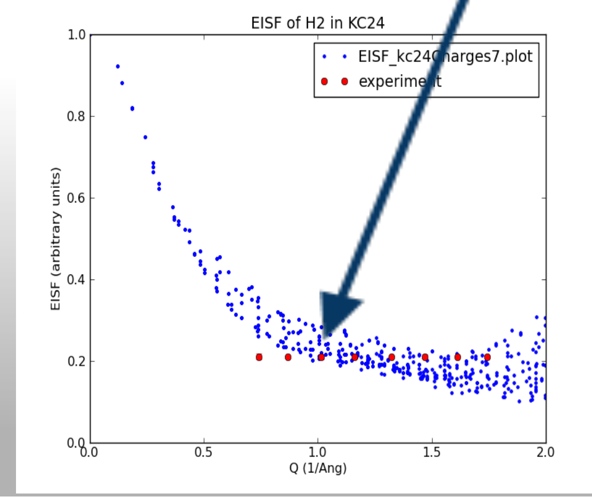
hydrogen dynamics



old experiment



new experiment

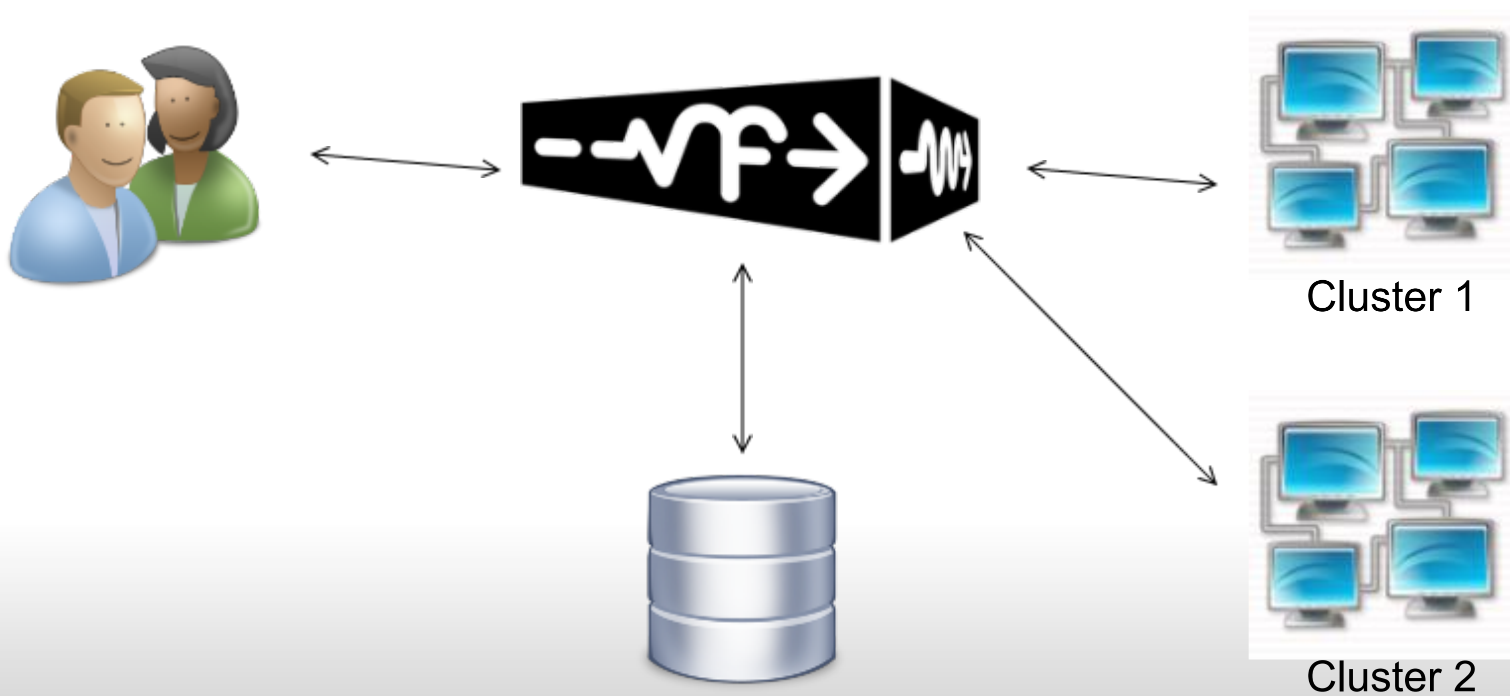


Future work

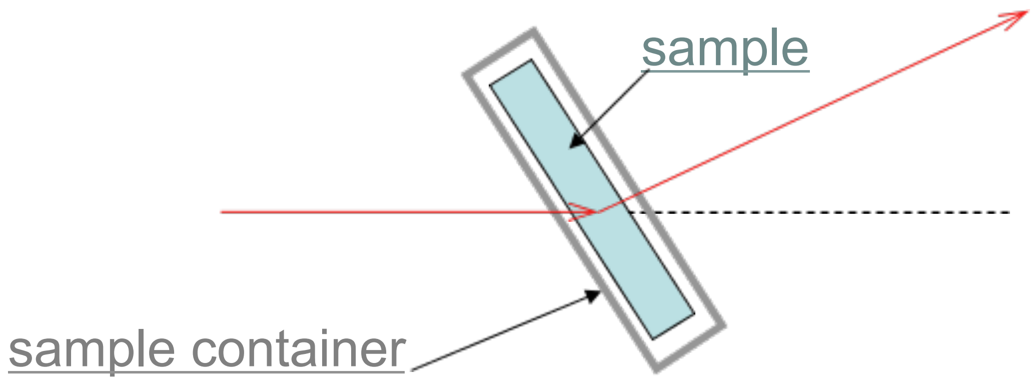
- Coarse-grained simulation of:
  - polymers (SANS)
  - membranes (Refl & SANS)
  - phase-field textured models (Refl & Engineering Diffraction)
- Integrate forward-algorithms for spectra
- Connect to more experimental databases
- Systematically compute neutron spectra of all materials in databases
- Workflow: users **look up** spectrum in VNF, **propose** experiment to confirm it, and **publish**

Thank you

- https://vnf.caltech.edu


Cluster 1
Cluster 2

MCViNE: what is a sample?



- Multiple scatterers with different shapes
- Various scattering-mechanisms (phonon/magnon/…) and variable forms (crystal/powder/…) for a scatterer
- Multiple scatterings inside and among scatterers
- Instruments: ARCS, VULCAN, Ideal Inelastic instruments

MCViNE

- A python-based framework allow interoperation of neutron components of various origins
- A sample simulation framework
  - Separation of geometry and physics
  - Arbitrary complex geometrical shape
  - Arbitrary combination of scattering physics
  - Xml file easy to read and understand