Scientific Discovery in Neutron Scattering Data

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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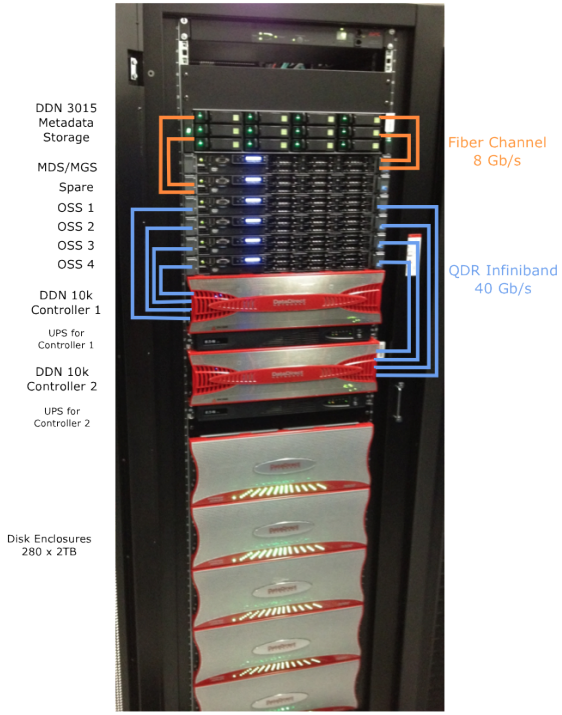
Analysis – “data on disk is useless”

- Data on disk is “useless” – analyzed data leads to scientific discovery

- Users should analyze the data,… but SNS will help
  - Download/transfer data
  - Access to computer resources
  - Access to “standard” analysis packages
  - Access to software development tools
  - Develop “new” analysis packages
  - Assimilate/curate (user) analysis packages
  - Help/collaboration using analysis packages

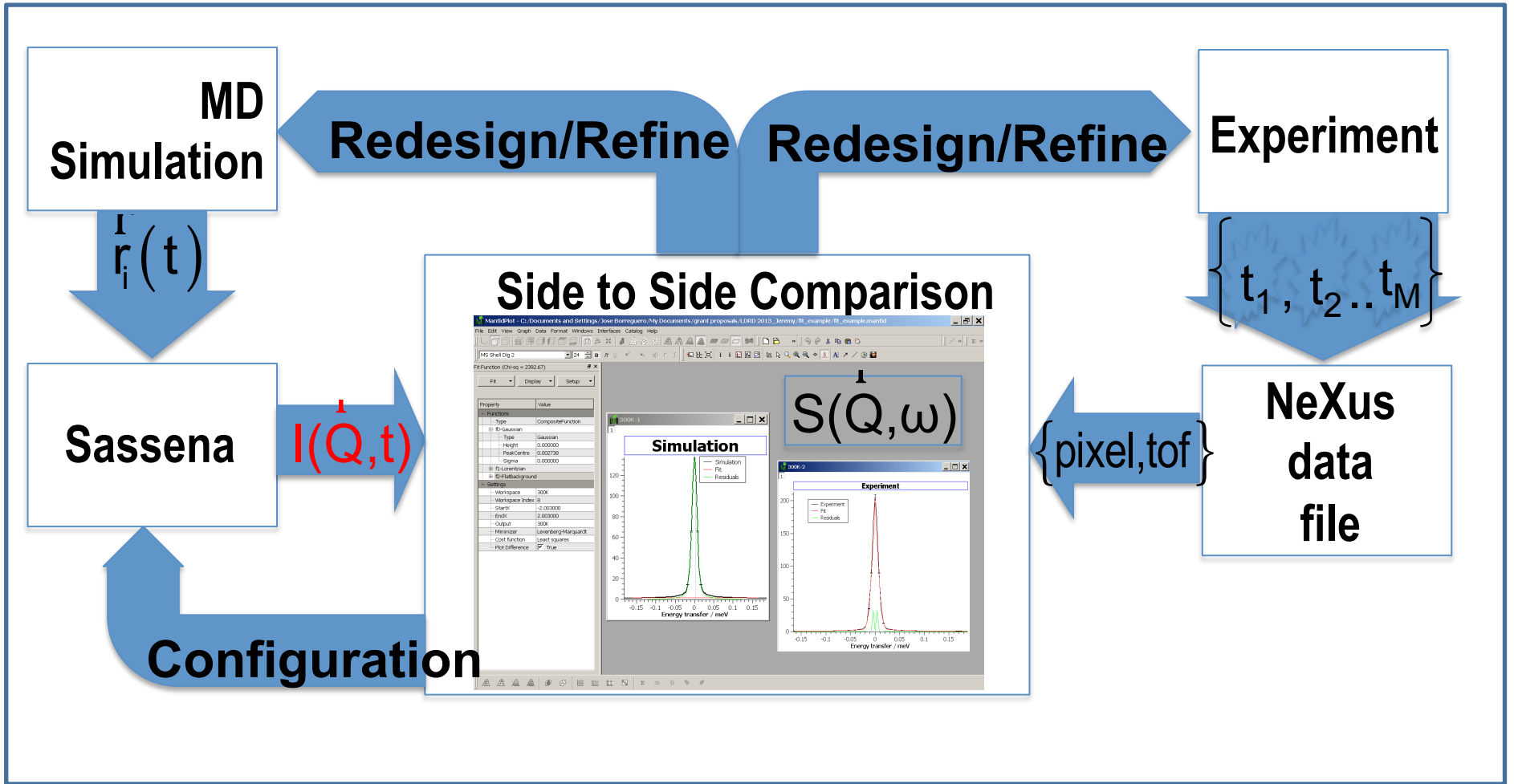
(Analysis = modeling/simulation/fitting/statistics)



- MANTID, DANSE software: Virtual Neutron Facility (VNF), SANSview, PDFgui
- Compilers/Languages – (Intel) FORTRAN/C++, Python, IDL, Matlab, Paraview
- Materials Studio, Amber, NAMD, Gromacs
- NERSC (VASP, LAMMPS,…)

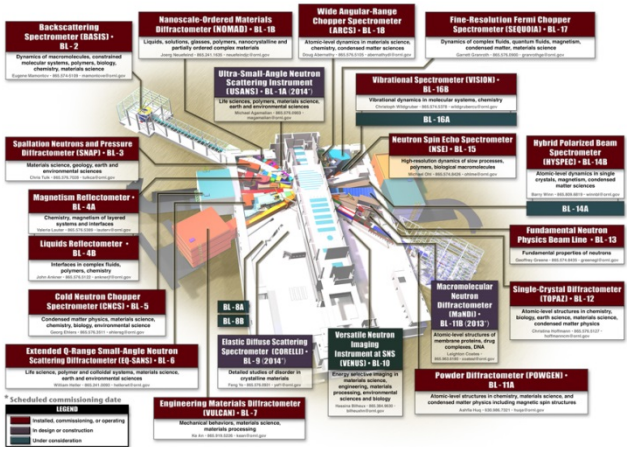
Center for Accelerating Materials Modeling

- BES Proposal Call in *Predictive Theory and Modeling*
- Partnership between Neutron Sciences and Computational Sciences
- Bring materials modeling/simulation directly into the chain for neutron scattering data analysis



Validation, Refinement & SNS

- SNS + HFIR collect a lot of materials spectra – if we can validate/refine simulation models against SNS/HFIR data then models "predict" measured atomistic properties. (Same for – APS, ALS, NSLS-I/II, LCLS, SSRL)
- Need a framework that (i) runs simulations, (ii) computes neutron spectra + does corrections, (iii) refines against experimental data.
- *Don't re-invent computational wheel* – use existing software tools and concentrate on applying them
- Flexible framework – can *plug-in* more advanced simulations later on.
- Started with classical MD & quasi-elastic scattering + 2 projects to advance the simulation types.



camm.sns.gov →

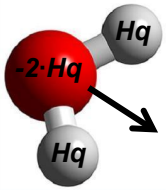
chadwick

hopper (NERSC)

titan (OLCF)

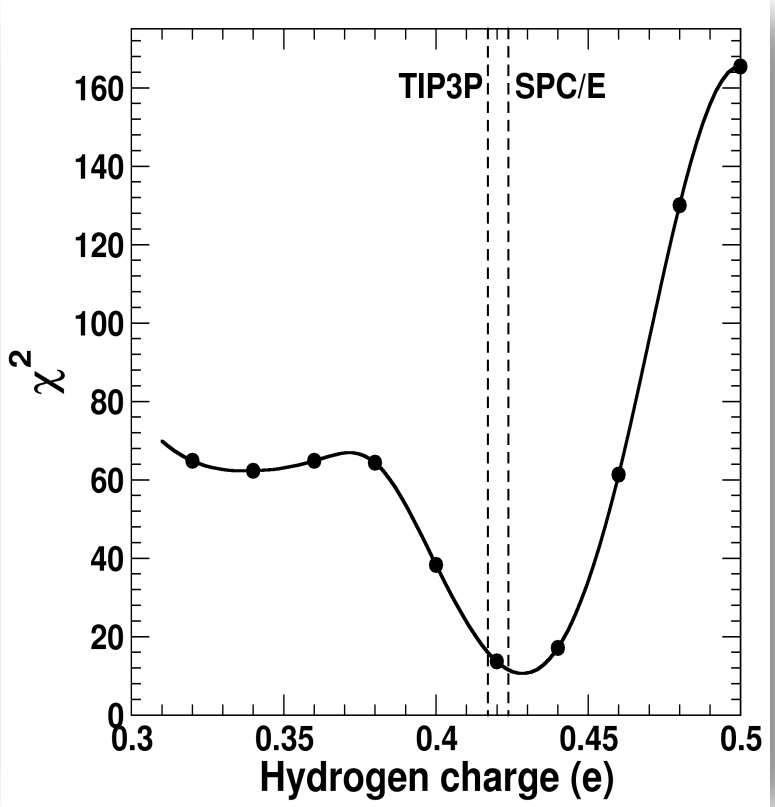
Modeling LiCl data from BASIS at SNS

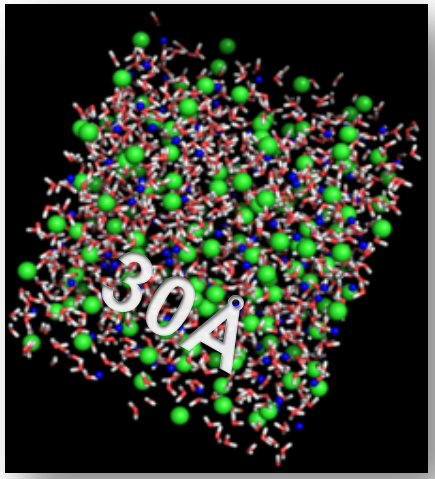
- NAMD simulations
- 154 Li+ Cl- pairs
- 1128 water molecules
- Total of 150ns production
- S(Q,ω) obtained with Sassena + Mantid



- Standard Hydrogen charge values:
  - *Hq=0.417 (*TIP3P)
  - *Hq=0.424* (SPC/E)
- We vary *Hq* from 0.32 to 0.50

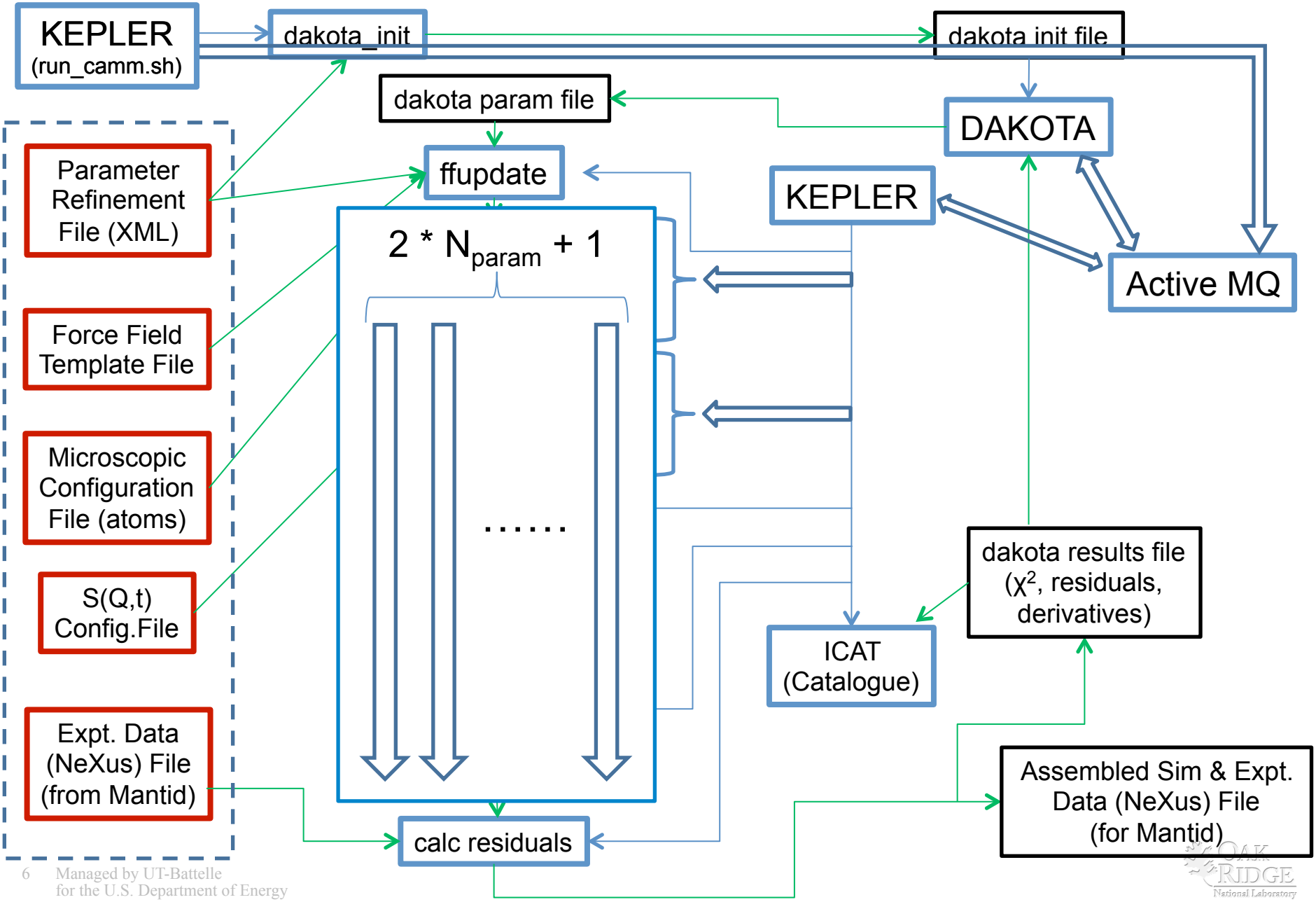
$\vec{p}$





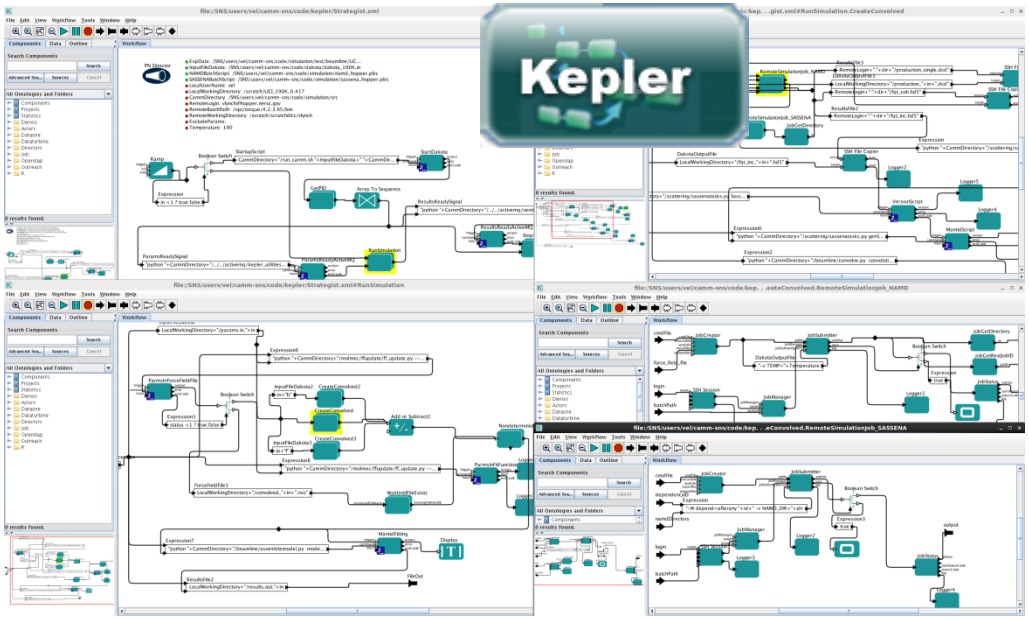
Li Cl in water

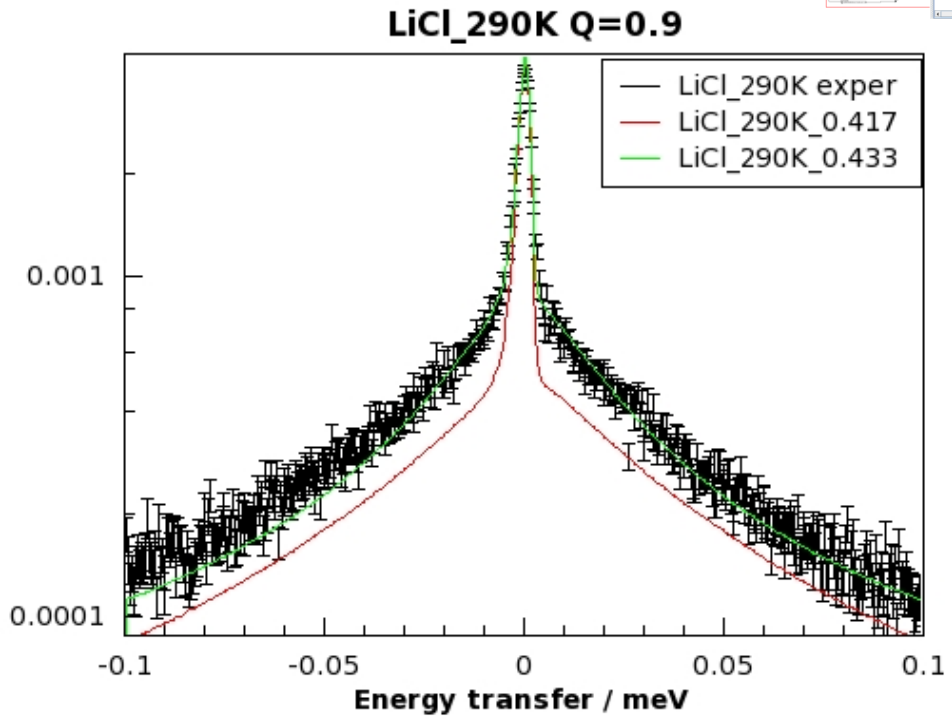
CAMM Refinement Workflow



Modeling LiCl data with workflow

- Kepler workflow submits simulations to Hopper
- Dakota optimizes model parameters
- Process automated with Kepler GUI for input



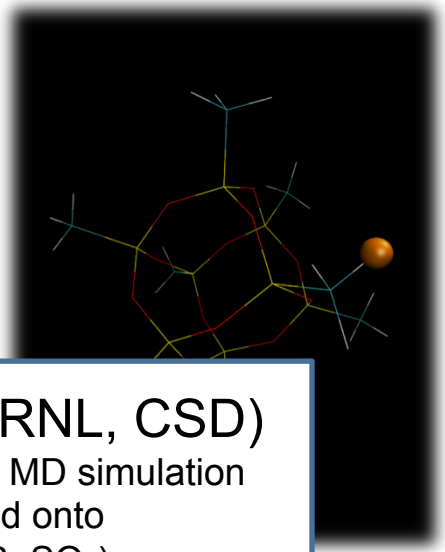


<<<<< Best data captured at function evaluation 2
Confidence Interval for c0 is [7.7181005978e-01, 7.9133911535e-01]
Confidence Interval for b0 is [3.5683719031e-05, 4.1095168905e-05]
Confidence Interval for e0.0 is [4.7649690032e-02, 5.0604743707e-02]
Confidence Interval for e0.1 is [3.8658107943e-02, 4.0925369124e-02]
Confidence Interval for e0.2 is [3.2393364793e-02, 3.4198221349e-02]
Confidence Interval for eshift is [2.2784599458e-04, 2.7276832227e-04]
Confidence Interval for FF1 is [4.3254547020e-01, 4.3403369489e-01]

Testing with friendly users

Jose Borreguero

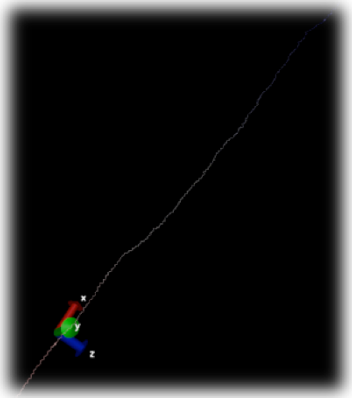
- Mike Crawford (Dupont) & Niina Jalarvo (Julich)
  BASIS experiment / MD simulation studies of Methyl rotations in methyl-Polyhedral oligomeric silsesquioxanes (POSS)



Jonathan Nickels (UTK)

Complementary CNCS experiment / MD simulation studies of the Boson peak in *Poly-L-Glutamic acid* (polyE) homopolymers

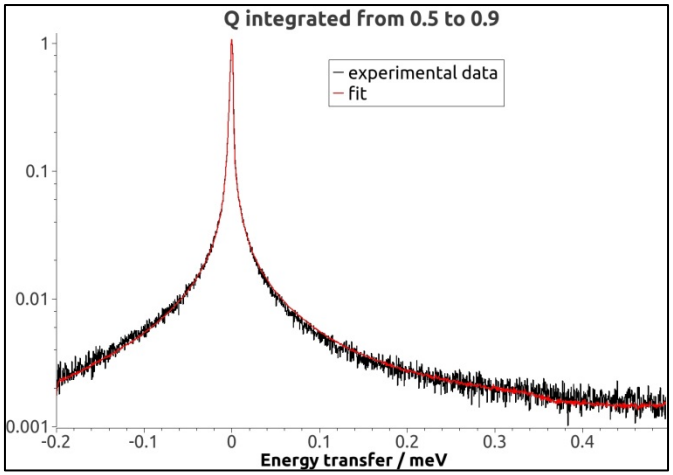
- The Boson peak is a collective excitation in the 2-5 meV range, often observed in soft-matter materials.
- polyE displays a Boson peak that shifts in energy upon changes in the environment.
- Quasi-elastic data collected at CNCS beamline.



One of the preparation steps in the simulation involves the collapse of the homopolymer chain from an initial stretched conformation

Andrew Stack (ORNL, CSD)

Complementary BASIS / MD simulation studies of water adsorbed onto nanoparticles of barite ($BaSO_4$)

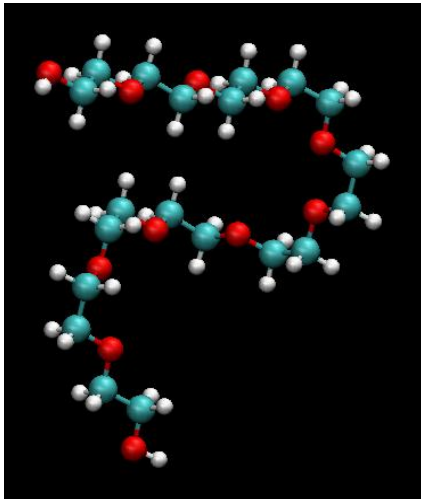


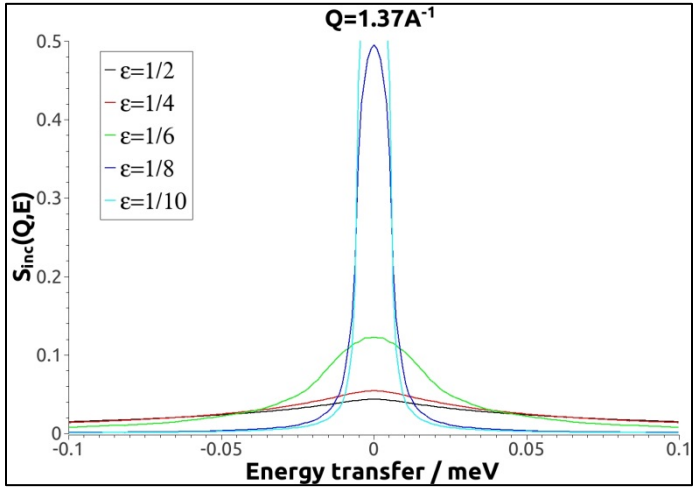
Coarse grained modeling of polymer electrolytes

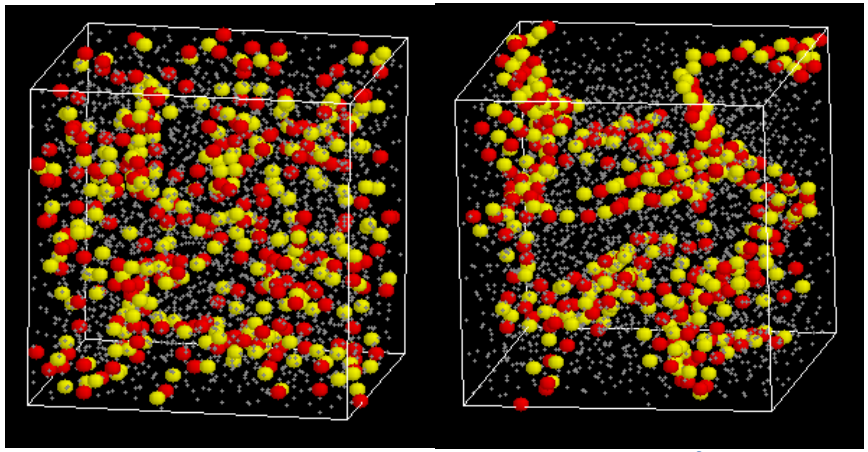
Bobby Sumpter & Monojoy Goswami

- Previous simulations were atomistic, here we'd like to examine how far we can go with coarse-grained simulations
- Modification of the S(Q,E) calculation to include b_{eff} $F(Q)$ as the scattering factor for the "block"
- Polymer electrolyte batteries have poor ionic conductivity so interested in simulating ionic hopping and comparing to quasi-elastic neutron scattering
- Also doing full atom simulation for comparison

Polyethylene Oxide - Acrylic Acid (+ LiCl)





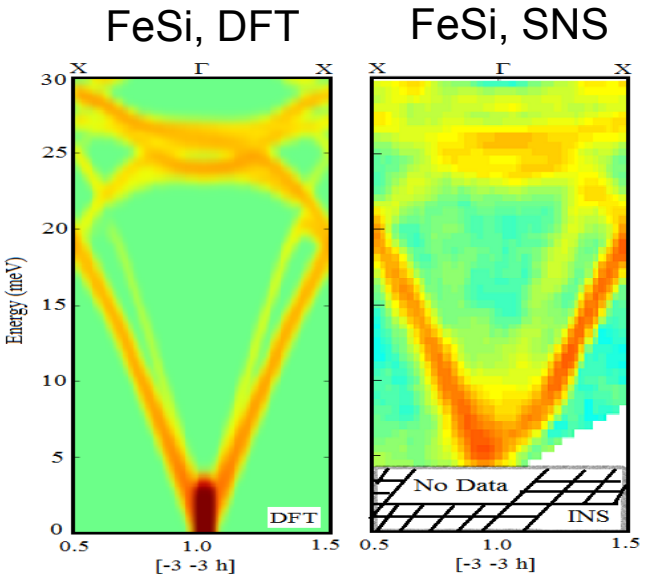


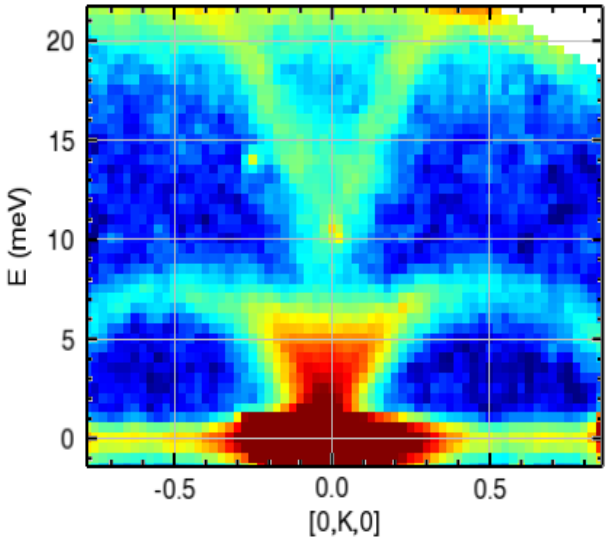
$\xi_B = 1/\varepsilon$

First-principles modeling of phonon spectra

Olivier Delaire, Jiawang Hong, Jennifer Niedziela & Vickie Lynch

- Leverage first-principles simulations to simulate phonons in ferroelectrics and thermoelectrics.
- Fitting of parameterized models to correct possible deficiencies of DFT.
- Enable quantitative assessment of non-harmonic behavior in measured phonons.
- Perform large-scale ab-initio molecular dynamics to capture phonon temperature dependence, and anharmonic effects (phonon scattering rates).
- Within CAMM, provide expertise for modeling of phonon data in important energy materials.



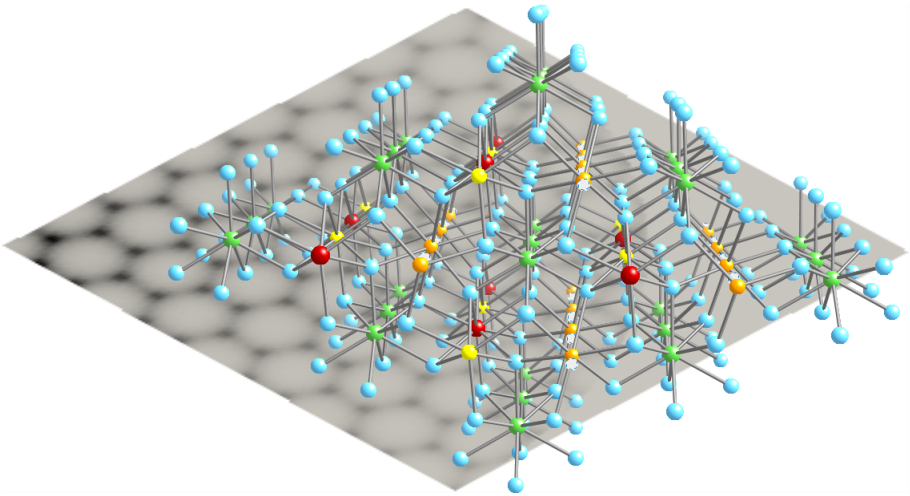


$K(Ta,Nb)O_3$ phonon S(**Q**,E), HYSPEC at SNS

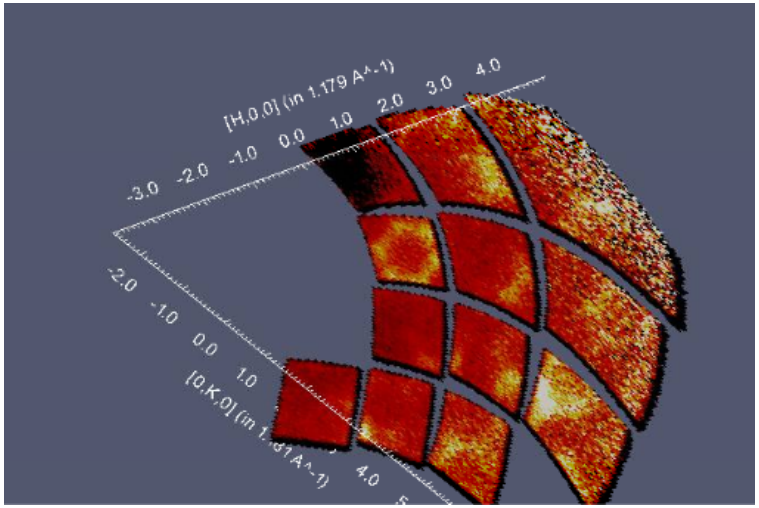
Modeling diffuse scattering

Tara Michels-Clark, Christina Hoffmann & Vickie Lynch

- Diffuse X-Ray and neutron data of β NaLaF4 have been measured
- Local disorder structure was modeled with ZODS on the high performance computer, Hopper.
- ZODS (Zurich Oak Ridge Disorder optimizes the structure specific model parameters derived from the disentanglement of the structural disorder elements indicated in the governing structure.
- Requires large scale computational resources for differential evolution optimizations of model parameters.
- Extracts quantitative structural information from a crystalline material's diffuse diffraction pattern



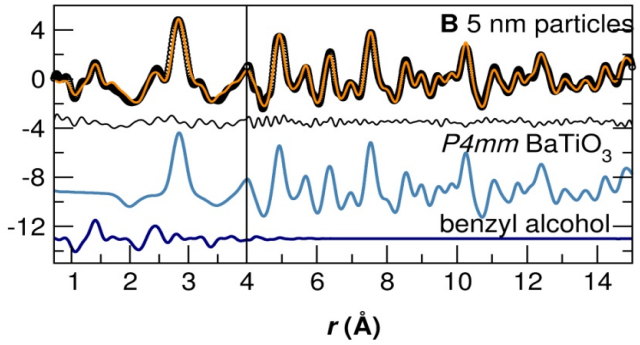
The super cell of β NaLaF4 illustrates occupational structural disorder
http://web2011.acscomp.org/awards/brochureimagecontest



Neutron 100K diffuse diffraction of the H,K,4.5 layer of β NaLaF4

Interfacing with other initiatives

- CAMM framework – how to “standardize” I/O for useful exchange of force fields etc.?
- What other modeling & simulation codes/science areas should we integrate into the framework? (… should be measurable with neutrons)
- Inclusion of other probes/techniques?
- Data Pilot Project – APS/MSD/MCS & SNS – *Advanced Structural Characterization Using Experimental Data from Multiple Facilities*
- Partnership proposals 11ID-B (APS) & NOMAD (SNS) – nanoscale disorder (PDF)
  Future: 11ID-D (APS) & Corelli (SNS) – single crystal diffuse scattering
- Joint data catalogue, co-refinement software, user interface & single sign-on



Summary

- Transforming the data landscape at SNS:
  - Leveraging NERSC computational resources
  - CAMM – Integrating modeling and simulation into data analysis
  - Closing the loop with computational steering