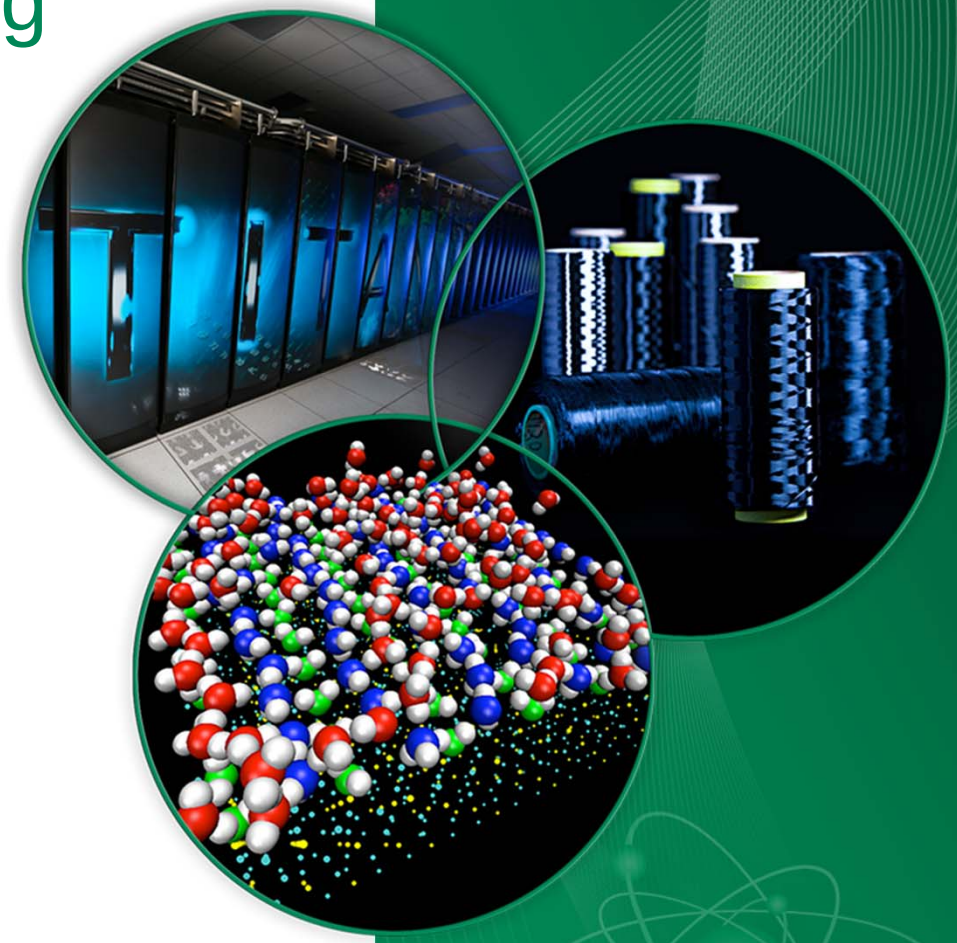
Neutron scattering Data: Analysis, Visualization, and Simulation



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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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Neutron Data Life Cycle

Feedback

DAS
- Neutron events
- Events from sample environment
- Other triggers

Reduction
- Corrected reduced data (histograms, S(Q,E), ..)
- Merging, reconstruction of data
- Instrument/technique dependent
- Need for 'real' time reduction

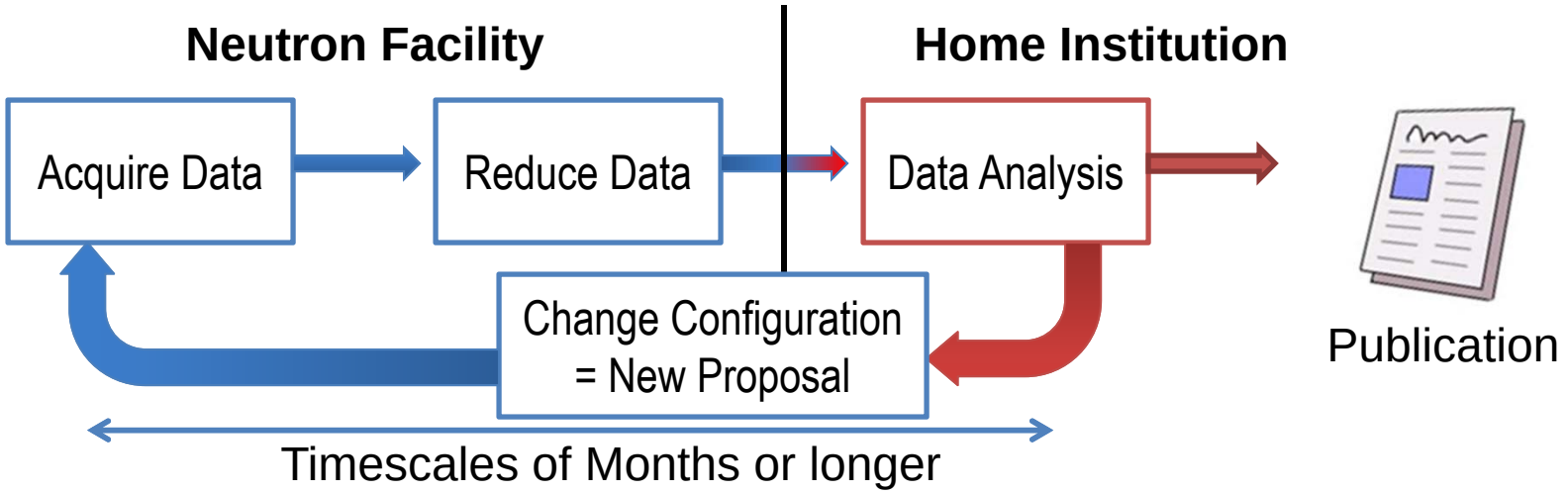
Analysis
- Multi dimensional fitting
- Advanced visualization
- Comparison to simulation / feedback
- Field dependent, large variety of approaches

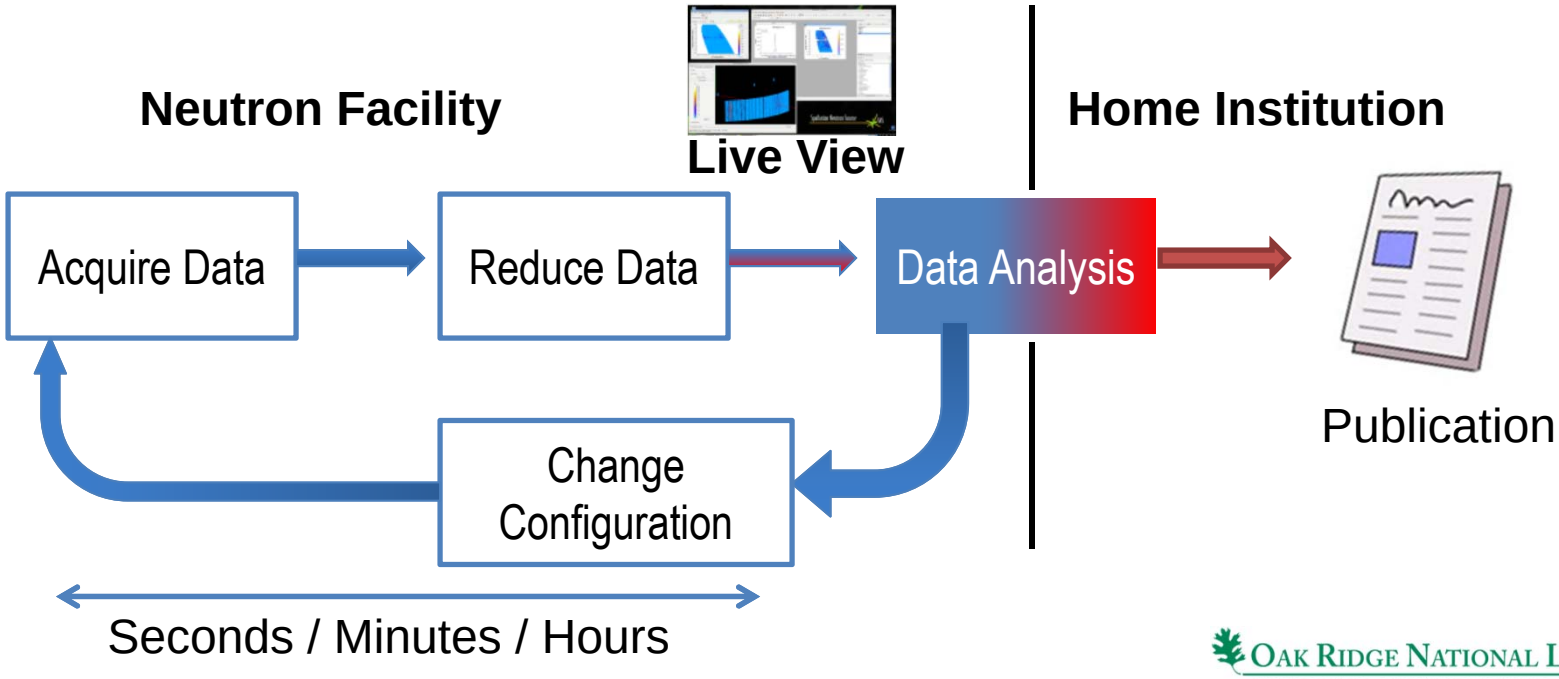
Simulation Modeling
- Multitude of techniques (DFT, MD, ..)
- Advanced simulation of experiments
- 'Refinement' using experimental data
- Multiple experiments / probes

User Facility

- Variety of experiments, topics, methods and 'computer literacy' of users are significant challenge.

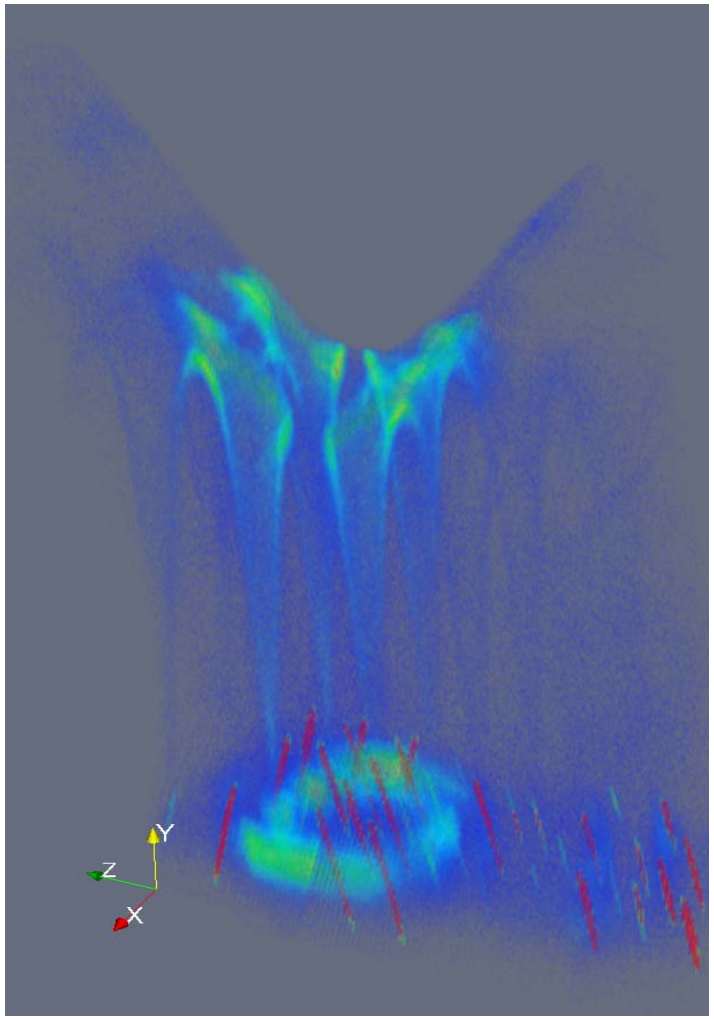
Improving Productivity = Changing the Workflow



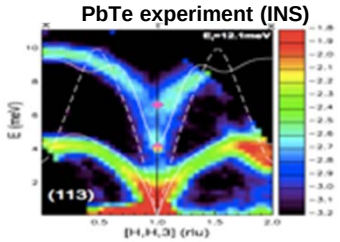


Data Requirements

- Raw event data up to 5 million events per second
- Reduced data sets are dependent on instrument but up to 20 GB. Usually 2 to 5 are analyzed together.
- Data needs to be “live” and readily accessible over WAN for about 5 years
- Commonly visualization is the biggest resource user.



Data Management



Neutron Data

Event NeXus

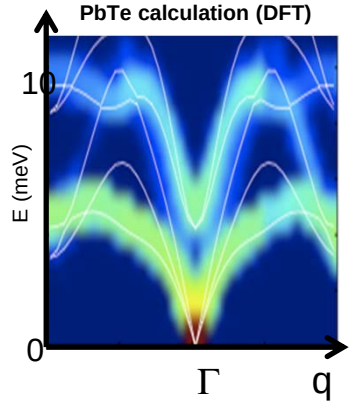
Automated Processing

Experimental Logbooks

Proposal Info

Other Facilities

Simulation



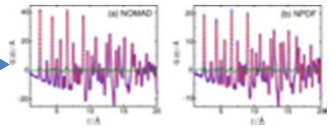
ICAT

High-performance Scalable Storage

Access, Citation & Data reuse

osti.gov

MANTID



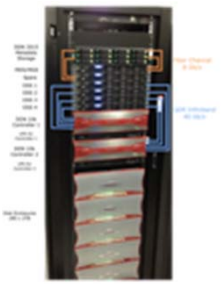
Analysis & Derived data

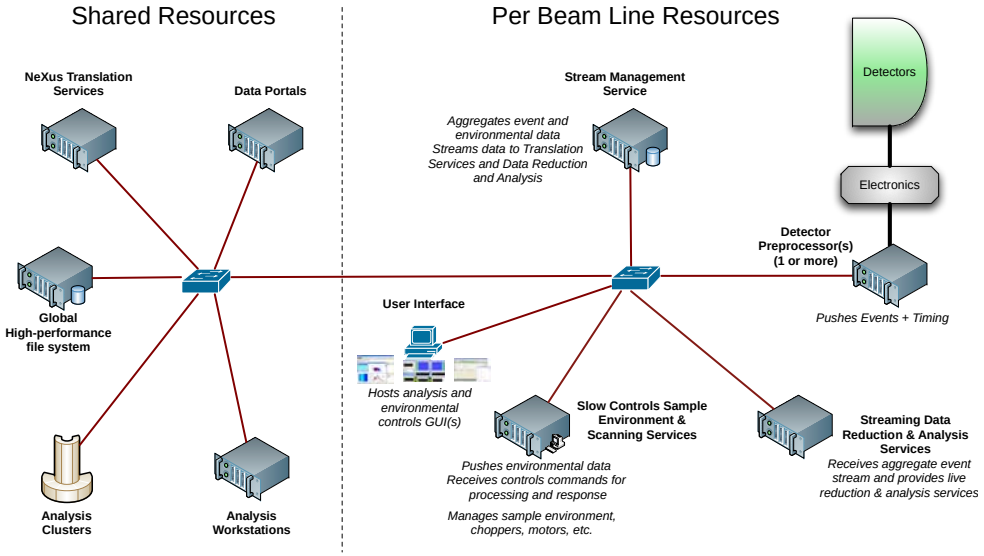
Improving Acquisition

Accelerating Data Acquisition, Reduction, and Analysis at the SNS

- Accelerating Data Acquisition, Reduction, and Analysis at SNS

- We stream data (neutron and SE) from the DAS to a publish subscribe system
  - *Stream Management Service (SMS)*
- We re-configure the data translation (file creation) to read the data stream from SMS and create the files while the run is taking place… end of run = close file [file appears "instantly"]
  - *Streaming Translation Service (STS)*
- We modify MANTID (data reduction) to read from the data stream live from SMS
  - *Streaming Reduction Service (SRS)*
- Files are created on an HPC infrastructure for subsequent parallel analysis and data reduction

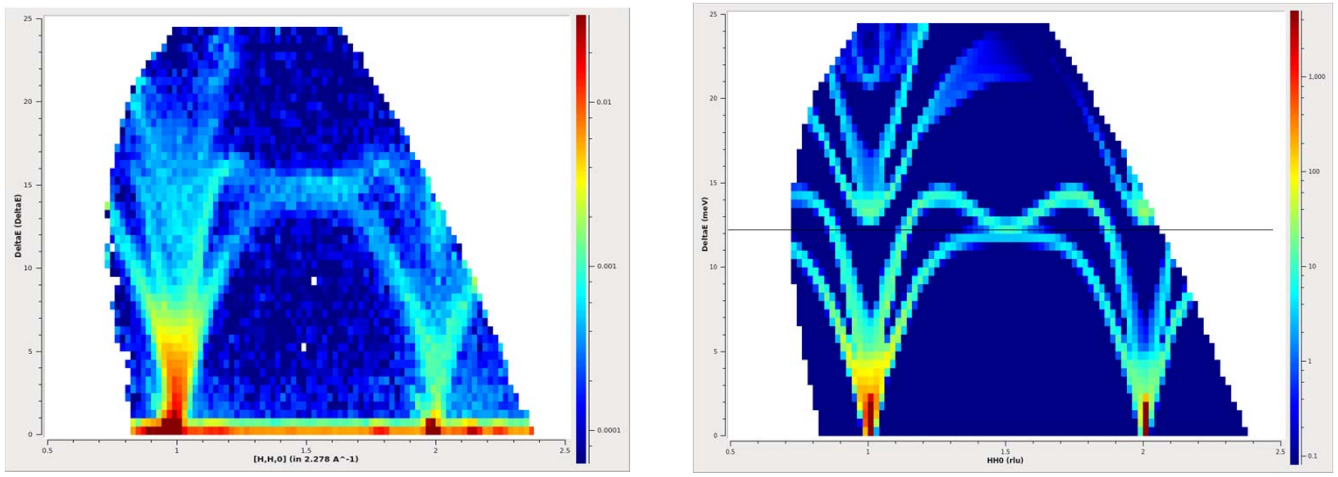




Concurrent Simulations and Experiment

- Ab-initio molecular dynamics (AIMD) simulations on the EOS cluster and experiment on $SrTiO_3$ on the HYSPEC instrument at the SNS.
- Used dedicated 23,000 computing cores on EOS (a Cray XC30 cluster).
- Large AIMD calculations capture the anharmonic renormalization (stabilization) of phonon dispersions and achieve good agreement with the experiments.
- Parameters in the simulations were adjusted based on observed scattering intensity.
- The simulations also helped refine the range of crystal orientations collected.
- Volume datasets from HYSPEC measurements and SimPhonies simulations were visualized side-by-side with MANTID SliceView

HYSPEC

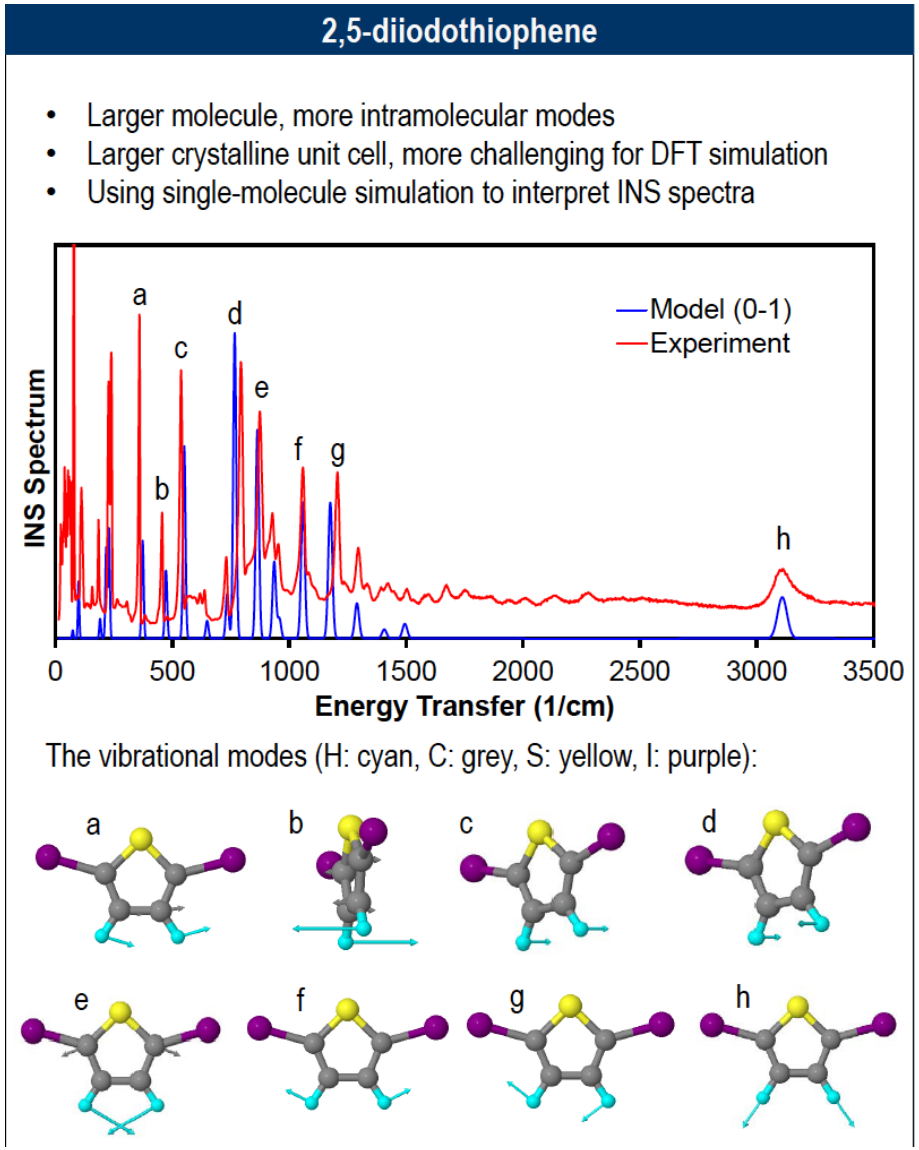


EOS

S(Q,E) from experiment (left) and simulation (right) along [HH1] direction.

Simulations during experiment future

- The time scale for the previous example is hours
- Other instruments it is minutes
  - Vision – Molecular Spectroscopy and Density Functional Theory



BES Data Pilot Project – Coupling SNS and APS

- Understanding the properties of disordered materials based on analyzing the diffuse scattering from powder and single crystal diffraction data
- PDF analysis of total scattering data collected on NOMAD (and later CORELLI) at the Spallation Neutron Source (SNS) and on 11ID-B and D at the Advanced Photon Source (APS)
- Allow researchers to
  - Derive features from large numbers of large data files
  - Search for experimental data of interest based on derived features
  - Analyze selected subsets of data