Neutron Data Life Cycle

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

**Neutron Facility**
- Acquire Data
- Reduce Data
- Change Configuration = New Proposal

**Home Institution**
- Data Analysis
- KB-TB

Timescales of Months or longer

Acquire Data

Reduce Data

Data Analysis

Change Configuration = New Proposal

Publication

**Neutron Facility**
- Acquire Data
  - <1 Gbs
- Reduce Data
  - <1 Gbs
- Change Configuration

**Home Institution**
- Data Analysis
  - KB-TB
- HPC Resource

Seconds / Minutes / Hours

Publication

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Acquire Data

Reduce Data

Data Analysis

Change Configuration

Publication

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Live View

HPC Resource
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.
- 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.
- Hours worth of data and simulation compiled in ~20GB data sets each.

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

Courtesy O. Delaire
Simulations during experiment future

- Other instruments it is minutes
  - Vision – Molecular Spectroscopy and Density Functional Theory
- But the user only wants to see kB of reduced data

The vibrational modes (H: cyan, C: grey, S: yellow, I: purple):

Courtesy A. Ramirez-Cuesta
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
Data Management

- Neutron Data
- Proposal Info
- Other Facilities
- Simulation

Event NeXus

Automated Processing

Experimental Logbooks

High-performance Scalable Storage

Access, Citation & Data reuse

PbTe experiment (INS)

PbTe calculation (DFT)

Analysis & Derived data

DataCite DOE Research Data

PbTe experiment (INS)

PbTe calculation (DFT)
Improving Acquisition

- 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

[Diagram showing the flow of data and services]