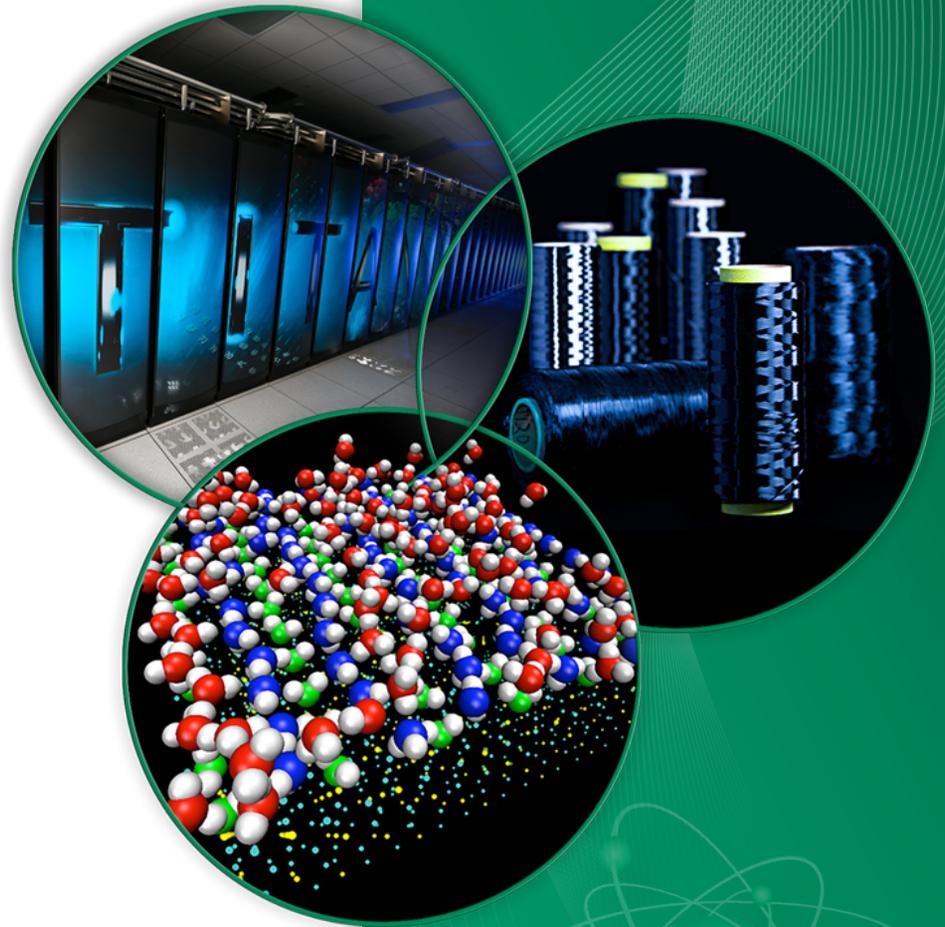
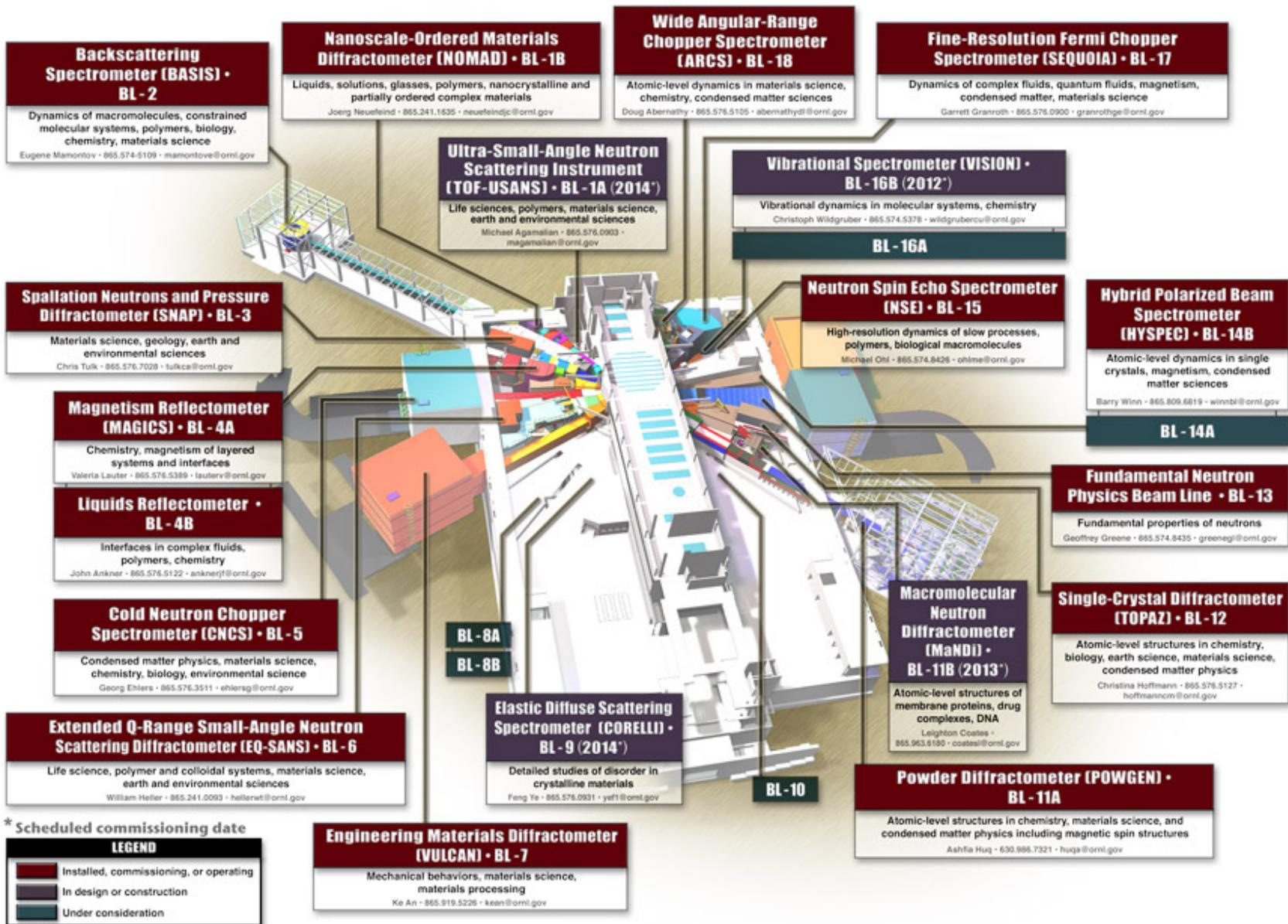


# Neutron scattering Data Networks for Analysis, Visualization, and Simulation

**Garrett E. Granroth**  
Scientific Data Analysis Group  
Lead

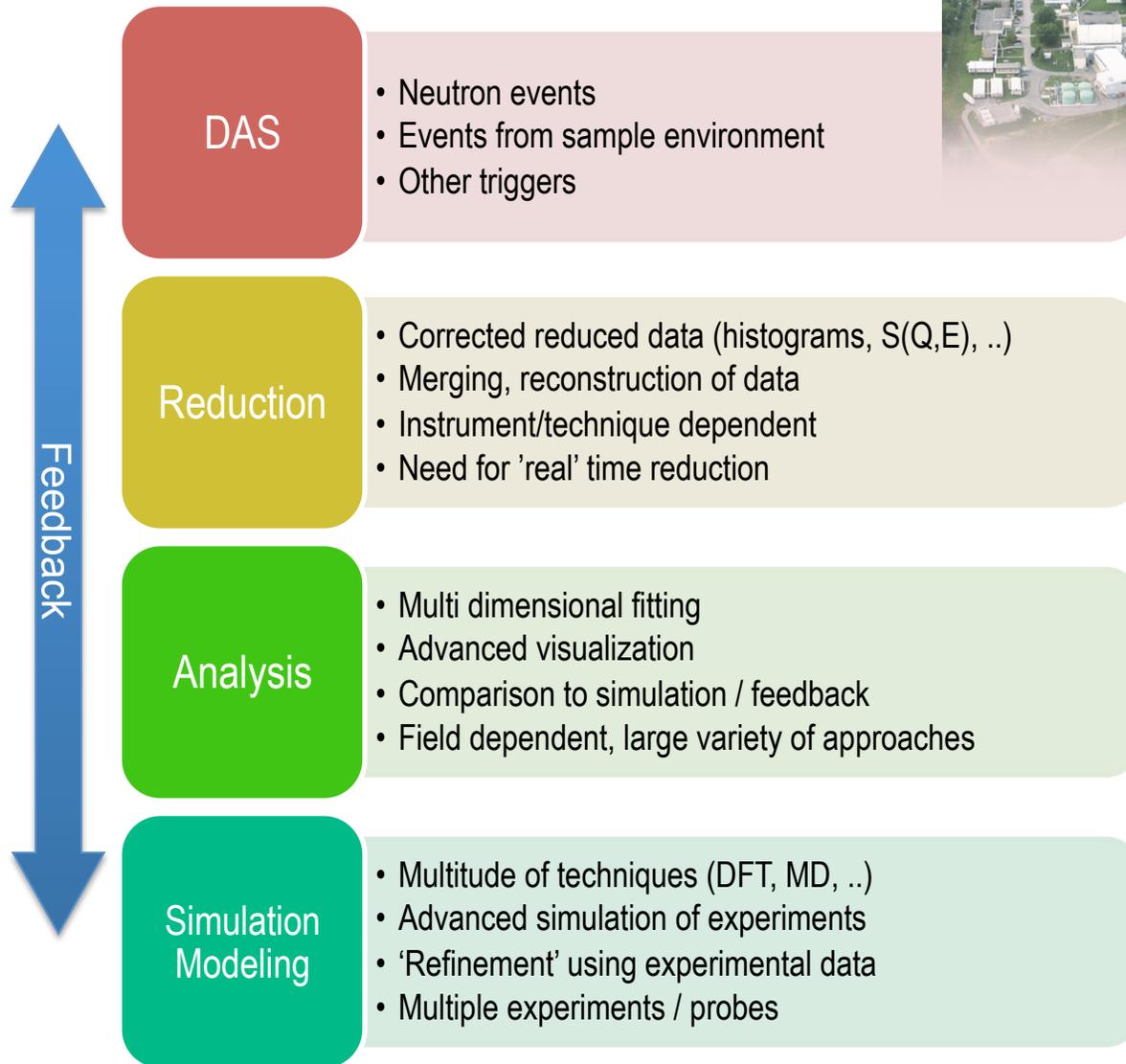
**August 6, 2014**





06-G00400P/gjm

# Neutron Data Life Cycle

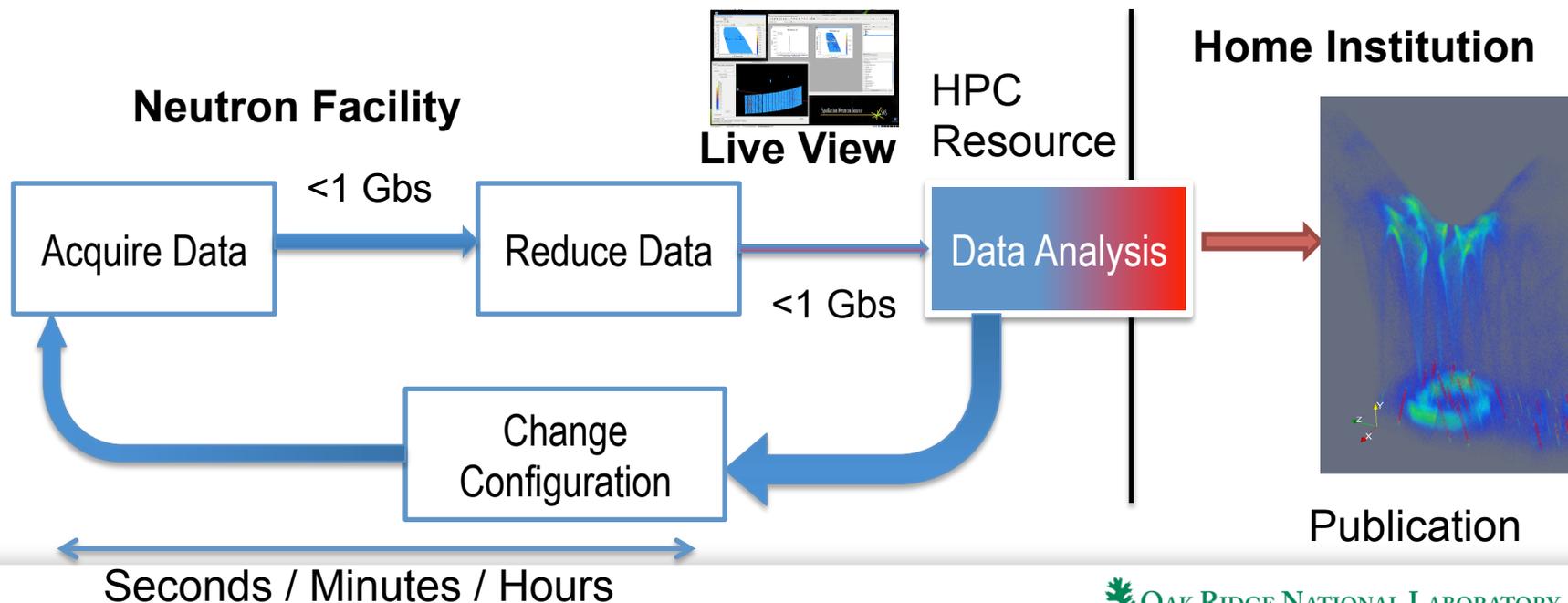
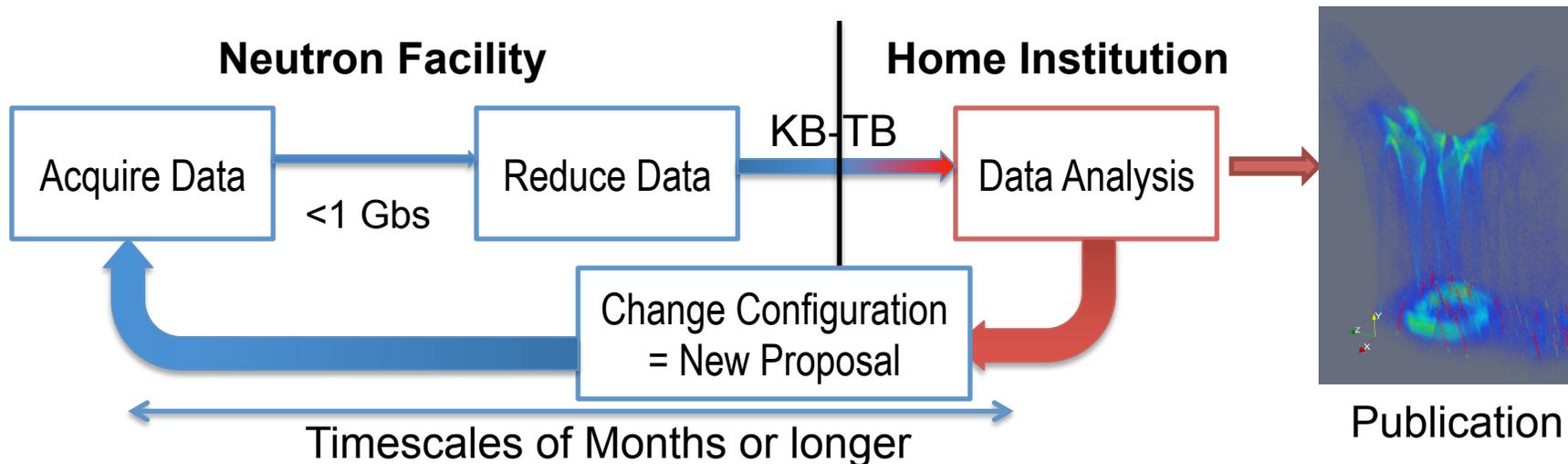


## User Facility

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



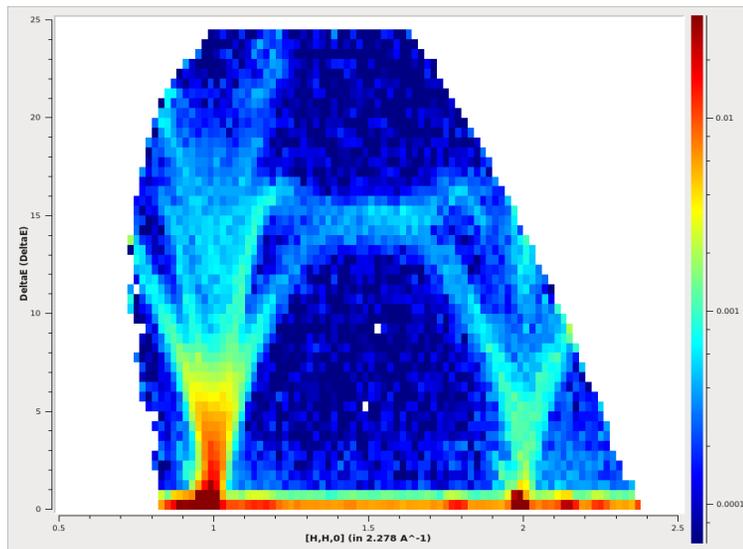
# Improving Productivity = Changing the Workflow



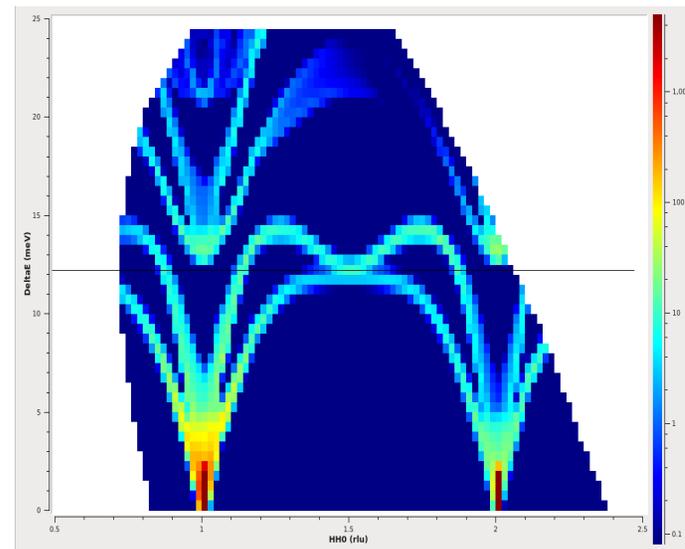
# Concurrent Simulations and Experiment

- Ab-initio molecular dynamics (AIMD) simulations on the EOS cluster and experiment on SrTiO<sub>3</sub> 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

HYSPEC



EOS

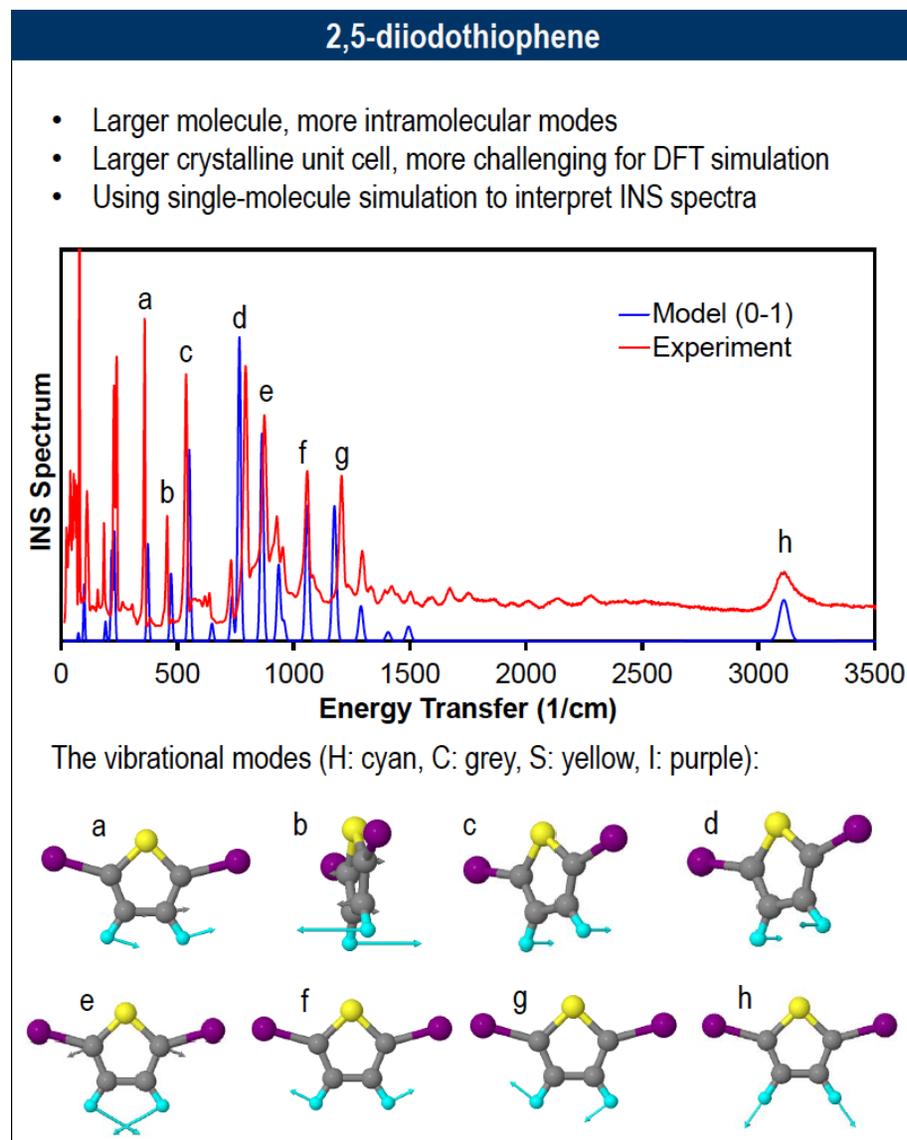


S(Q,E) from experiment (left) and simulation (right) along [HH1] direction. Courtesy O. Delaire

# Simulations during experiment future

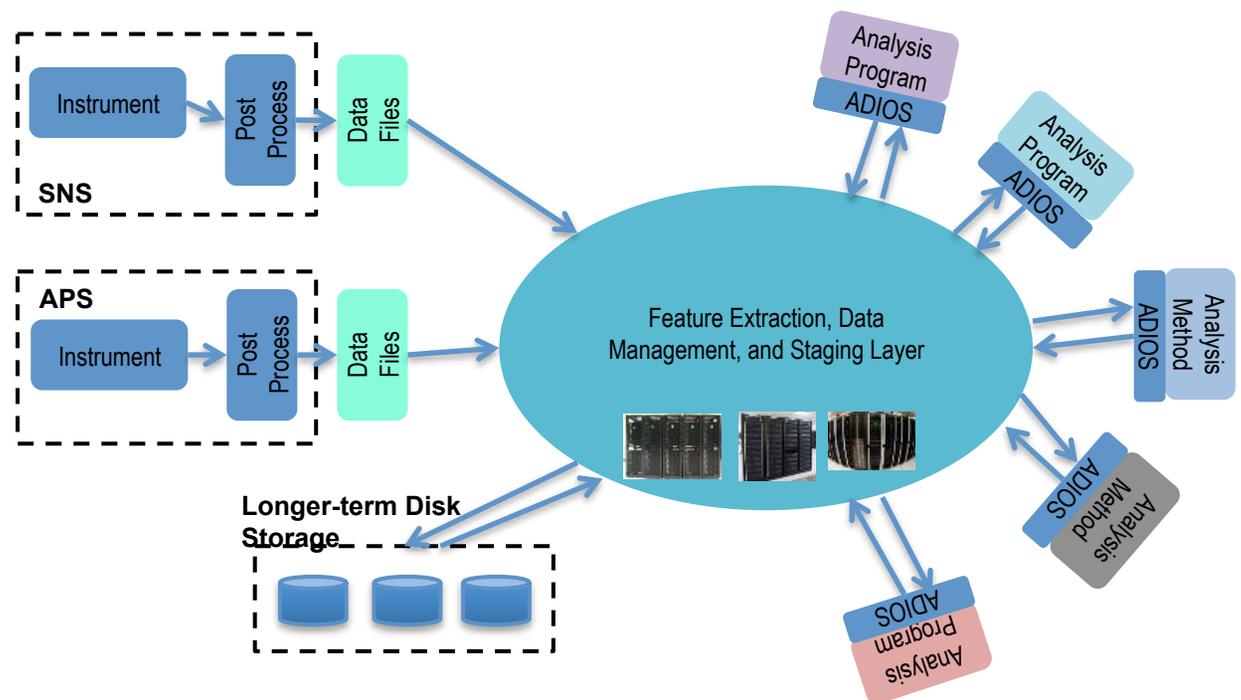
- Other instruments it is minutes
  - Vision – Molecular Spectroscopy and Density Functional Theory
- But the user only wants to see kB of reduced data

Courtesy A. Ramirez-Cuesta



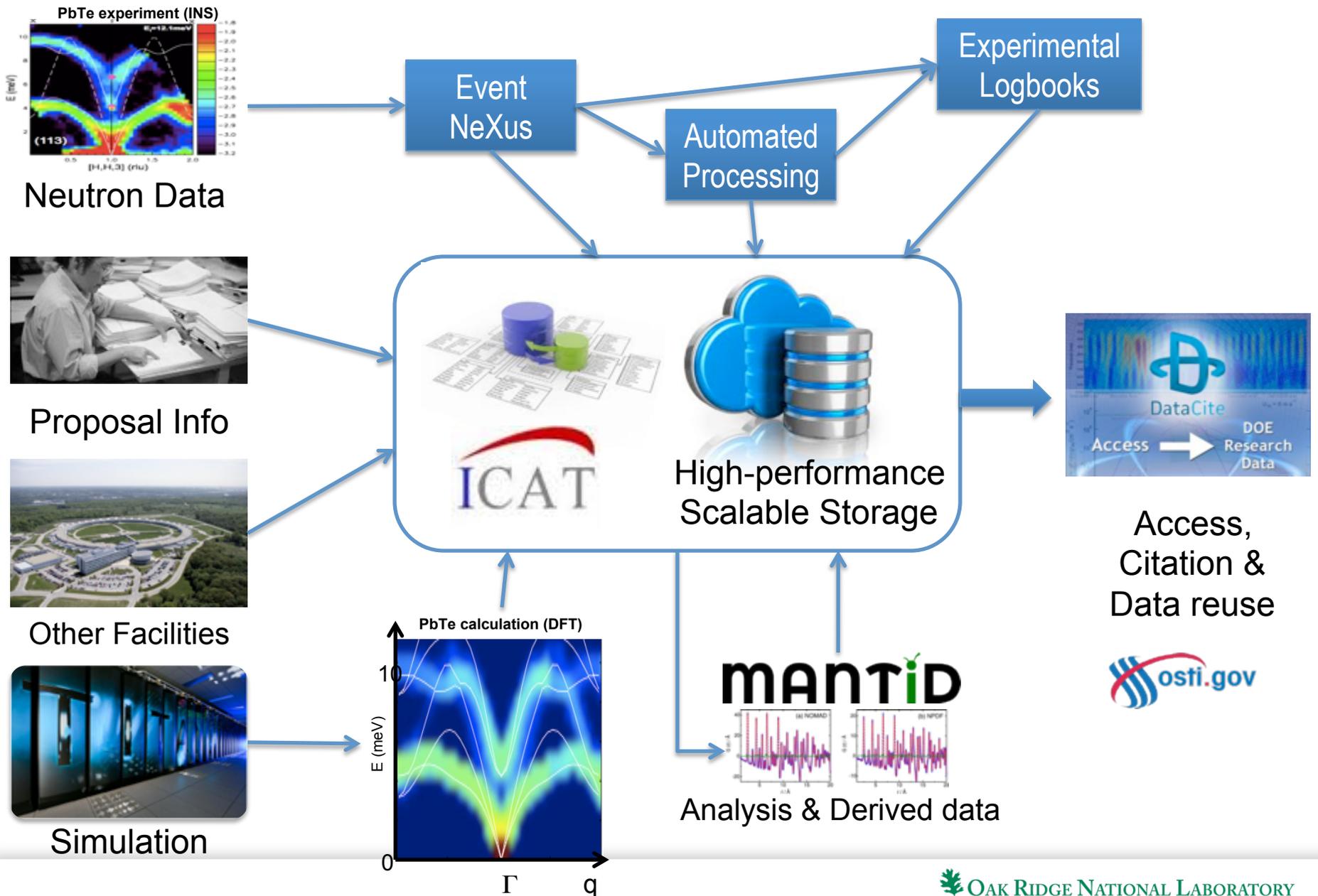
# BES Data Pilot Project – Coupling SNS and APS

- 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



# 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

