Accelerating Scientific Discovery at the Spallation Neutron Source

Stuart Campbell

Neutron Data Analysis & Visualization Division
Developing and applying the world’s best tools for neutron scattering

High Flux Isotope Reactor:
Intense steady-state neutron flux and a high-brightness cold neutron source

Spallation Neutron Source:
World’s most powerful accelerator-based neutron source

Biology and Soft Matter
Chemical and Engineering Materials
Neutron Data Analysis and Visualization
Quantum Condensed Matter
Spallation Neutron Source at Oak Ridge National Laboratory

The world’s most intense pulsed, accelerator-based neutron source

**Backscattering Spectrometer (RASiS) - BL-2**
Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science
Eugene Mamontov - 865.574.0108 - mamontov@ornl.gov

**Nanoscale-Ordered Materials Diffractometer (NOMADi) - BL-1B**
Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials
Joerg Neuhaeusl - 865.241.1838 - neuhaeusl@ornl.gov

**Wide Angular-Range Chopper Spectrometer (ARCS) - BL-18**
Atomic-level dynamics in materials science, chemistry, condensed matter science
Doug Abernathy - 865.617.5824 - abernathyd@ornl.gov

**Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) - BL-17**
Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science
Garrett Granroth - 865.805.0631 - granrothg@ornl.gov

**Ultra-Small-Angle Neutron Scattering Instrument (USANS) - BL-1A (2014)**
Life sciences, polymers, materials science, earth and environmental sciences
Michael Agarwall - 865.382.6387 - magarwall@ornl.gov

**Vibrational Spectrometer (VISION) - BL-16B**
Vibrational dynamics in molecular systems, chemistry
Christopher Wisteieder - 865.576.1781 - wisteiederc@ornl.gov

**Neutron Spin Echo Spectrometer (NSE) - BL-15**
High-resolution dynamics of slow processes, polymers, biological macromolecules
Michael Ohl - 865.574.8429 - ohlim@ornl.gov

**Hybrid Polarized Beam Spectrometer (HYSPEC) - BL-14B**
Atomic-level dynamics in single crystals, magnetism, condensed matter science
Barry Winn - 865.805.6819 - winnbb@ornl.gov

**Fundamental Neutron Physics Beam Line - BL-13**
Fundamental properties of neutrons
Geoffrey Green - 865.576.0023 - greenge@ornl.gov

**Cold Neutron Chopper Spectrometer (CNCs) - BL-5**
Condensed matter physics, materials science, chemistry, biology, environmental science
Georg Ehlers - 865.241.0030 - ehlersg@ornl.gov

**Spallation Neutrons and Pressure Diffractometer (SNAP) - BL-3**
Materials science, geology, earth and environmental sciences
Chris Tuck - 865.574.0184 - tuckc@ornl.gov

**Magnetism Reflectometer - BL-4A**
Chemistry, magnetism of layered systems and interfaces
Valeria Lavine - 865.387.6389 - lavinev@ornl.gov

**Liquids Reflectometer - BL-4B**
Interfaces in complex fluids, polymers, chemistry
John Anker - 865.387.6385 - ankerj@ornl.gov

**Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) - BL-6**
Life science, polymer and colloidal systems, materials science, earth and environmental sciences
William Heller - 865.241.0093 - hellerw@ornl.gov

**Elastic Diffuse Scattering Spectrometer (CORELLi) - BL-9 (2014)**
Detailed studies of disorder in crystalline materials
Fei Ye - 865.576.0091 - yeilf@ornl.gov

**Versatile Neutron Imaging Instrument at SNS (VENUS) - BL-10**
Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology
Hassine Biloucoux - 865.384.9630 - biloucouxh@ornl.gov

**Elasmch Neutron Diffraclorator (MaNDi) - BL-11B**
Atomic-level structures of membrane proteins, drug complexes, DNA
Leighton Cote - 865.954.4551 - cotele@ornl.gov

**Powder Diffractometer (POWGEN) - BL-11A**
Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures
Aashla Hsiao - 865.805.7321 - hsiaoa@ornl.gov

**Engineering Materials Diffractometer (VULCAN) - BL-7**
Mechanical behaviors, materials science, materials processing
Ke An - 865.919.0226 - keaan@ornl.gov

*Scheduled commissioning date

**Legend**
- Red: Operating instrument in user program
- Green: In commissioning or operating development beamline
- Blue: In design or construction
- Gray: Under consideration

**U.S. Department of Energy Office of Science**
**Oak Ridge National Laboratory**
**Neutron Sciences**
# SNS Data Life Cycle

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<th>Analysis</th>
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<td>Corrected reduced data (histograms, $S(Q,E)$, ..)</td>
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<td>Events from sample environment</td>
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<td>Advanced visualization</td>
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<td>Instrument/technique dependent</td>
<td>Comparison to simulation / feedback</td>
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<td>Need for ‘real’ time reduction</td>
<td>Field dependent, large variety of approaches</td>
<td>Multiple experiments / probes</td>
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**User Facility**

Variety of experiments, topics, methods and ‘computer literacy’ of users are significant challenges.
Improving Productivity = Changing the Workflow

Neutron Facility

Acquire Data → Reduce Data → Change Configuration = New Proposal

Home Institution

Data Analysis → Publication

Timescales of Months or longer

Neutron Facility

Acquire Data → Reduce Data → Change Configuration

Home Institution

Data Analysis → Publication

Live View

Seconds / Minutes / Hours
Our Mission... what do we aspire to do?

SNS is an experimental user facility

What should we aspire to... create a data infrastructure that gives users

- The ability to reduce, and analyze, the data as it is taken
- Data files created instantly after acquisition (no matter how big)
- The ability to reduce a data set post-acquisition in ~1 minute
- The resources for any user to do post-acquisition reduction, analysis, visualization, modeling from anywhere...

Surely everyone signs up to these... but how does one make it happen?
An Example Diffraction Experiment

Raw Data: up to $10^{12}$ events per second

**Acquisition**

Translated Data: Gigabytes to Terabytes

**Reduction**

Reduced Data: e.g. Powder Diffraction Pattern

**Analysis & Simulation**

Analysis: PDF, Rietveld, simulation, etc.

Feedback guiding changes to the experiment setup

Data captured and stored on multiple systems at the beamline

After completion of a “run” data is aggregated on a single system, translation begins

Once data is aggregated reduction begins using a workstation

Analysis and Simulation using mid-scale compute
Funded by Laboratory Directed Research & Development at ORNL

- 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
‘Live’ Reduction & Analysis

Optimal Experimental Design
Computational “Steering” (Decision Support System)
USERS watch their data live on SEQUOIA

- Users E. Kermarrec and D. Maharaj watch their live data from a double Perovskite
- Enabled by Adara and Mantid
- SEQUOIA Staff
  - A. I. Kolesnikov
  - L. Debeer-Schmitt
Center for Accelerating Materials Modeling

- 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)
- Bring materials modeling/simulation directly into the chain for neutron scattering data analysis
Validation, Refinement & SNS

- BES Proposal Call in *Predictive Theory and Modeling*

- Partnership between Neutron Sciences and Computational Sciences

- Funded by Materials Science and Engineering Division, Office of Basic Energy Sciences, U.S. Dept. of Energy

- 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 different simulations later on.

- Started with classical MD & quasi-elastic scattering + 2 projects to advance the simulation types.
Modeling LiCl data with workflow

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

![Graph showing LiCl_290K Q=0.9](image)

Confidence Interval for \( c_0 \) is [ 7.7181005978e-01, 7.913911535e-01 ]
Confidence Interval for \( b_0 \) is [ 3.5683719031e-05, 4.1095168905e-05 ]
Confidence Interval for \( e_{0.0} \) is [ 4.7649690032e-02, 5.0604743707e-02 ]
Confidence Interval for \( e_{0.1} \) is [ 3.8658107943e-02, 4.0925369124e-02 ]
Confidence Interval for \( e_{0.2} \) is [ 3.2393364793e-02, 3.4198221349e-02 ]
Confidence Interval for \( e_{\text{shift}} \) is [ 2.2784599458e-04, 2.7276832227e-04 ]
Confidence Interval for FF1 is [ 4.3254547020e-01, 4.3403369489e-01 ]
A VERY Recent Example

- Performed live simulations at the same time as the scattering experiment was being performed.
- Used HYSPEC instrument at SNS.
- Used OLCF’s EOS machine.
- OLCF scheduled jobs synchronized with the SNS experiment.
- The simulations helped refine the range of crystal orientations that were collected on HYSPEC.
A Neutron Sciences & Computing Partnership

- CADES provides core compute and data capabilities for SNS users
  - Center wide parallel file system, HPC compute & utility compute
  - Expertise in HPC, data analysis, visualization, and computer science

Chadwick (196 cores)
Fermi (512 cores)
OIC (256 cores)
Titan (300K cores + 18K GPUS)
Collaborating with Other Facilities

• Data Pilot Project – APS/MSD/MCS & SNS – “Advanced Structural Characterization Using Experimental Data from Multiple Facilities”
  ORNL: Th.Proffen, M.Hagen, G.Shipman
  ANL: R.Osborn, S.Rosenkranz, P.Chupas, I.Foster

• 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
Fitting it all together

**CAMM**
- Simulation
  - Calculate Scattering

**CADES**
- Change Configuration
  - Side by Side Analysis

**ADARA**
- Experiment
  - NeXus (HDF5) Data File

**Collaborations / Pilot Project**
- Other Probes
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Whitfield, Marie Yao + Many More…
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