Toward “Real-Time” Analysis in Neutron Science

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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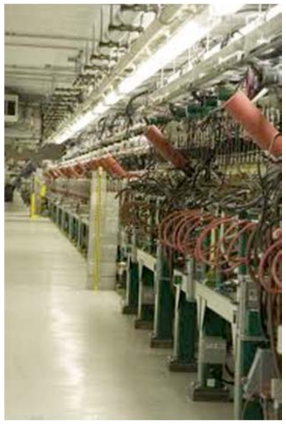
From Ion Source to Neutron Detectors

ION Source + Linac → H- → Proton Accumulator → H+ → Mercury Target → Neutrons! → Instrument Detectors

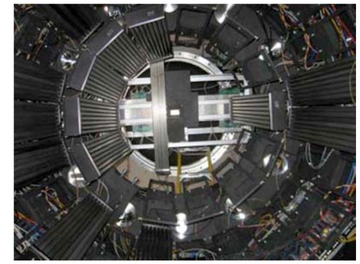


Ion source produces negatively charged hydrogen ions formed into a pulsed beam at 2.5 MeV

Linear accelerator accelerates the H- beam from 2.5 MeV to 1 GeV

H- pulse from linac is wrapped into a ring through a stripper foil, removing the electrons to produce protons H+. Protons are accumulated in the ring and then kicked out at 60 Hz

These pulsed, high-energy protons are directed to a mercury target, when a proton hits the target, 20 to 30 neutrons are released, moderated and directed to individual beam lines



Neutron detectors surrounding a sample environment detect collisions of neutrons with the detector. The TOF and angle of incidence of the neutron is calculated.

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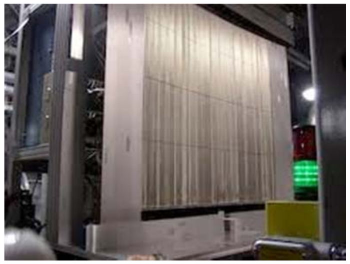
Many different types of instruments

- Inelastic Spectroscopy – ARCS, CNCS, SEQUOIA, HYSPEC
  - Resolves the change in kinetic energy when neutron/sample collisions are inelastic
  - Commonly used in condensed matter research to study atomic motion, magnetic and crystal field excitations
- Diffraction (Elastic) – POWGEN, NOMAD, VULCAN
  - Resolves the structure of a material
  - Use to study nanoscale structure and magnetic structure
- Small-angle neutron scattering (Elastic) – EQ-SANS, USANS
  - Uses small scattering angles to investigate the structure of materials at the mesoscopic scale
  - Use to study proteins, DNA, and other biological molecules; polymers, crystalline structures, etc.



SNS Data Life Cycle

Acquisition

- 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

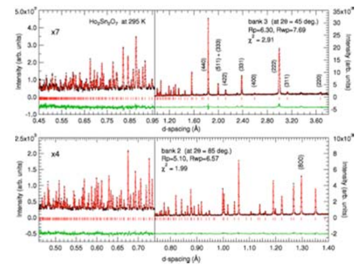
Simulation Modeling

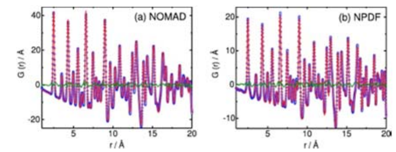
- Multitude of techniques (DFT, MD, ..)
- Advanced simulation of experiments
- ‘Refinement’ using experimental data
- Multiple experiments / probes

User Facility

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

Example: NOMAD Diffractometer





Raw Data: up to 10^12 events per second

Acquisition →

Translated Data: Gigabytes to Terabytes

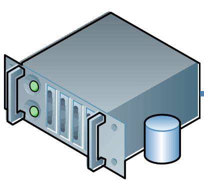
Reduction →

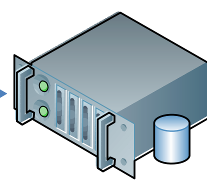
Reduced Data: e.g. Powder Diffraction Pattern

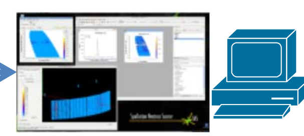
Analysis & Simulation →

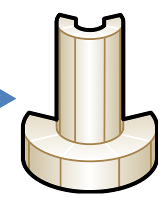
Analysis: PDF, MD simulation, etc.

Feedback guiding changes to the experiment setup









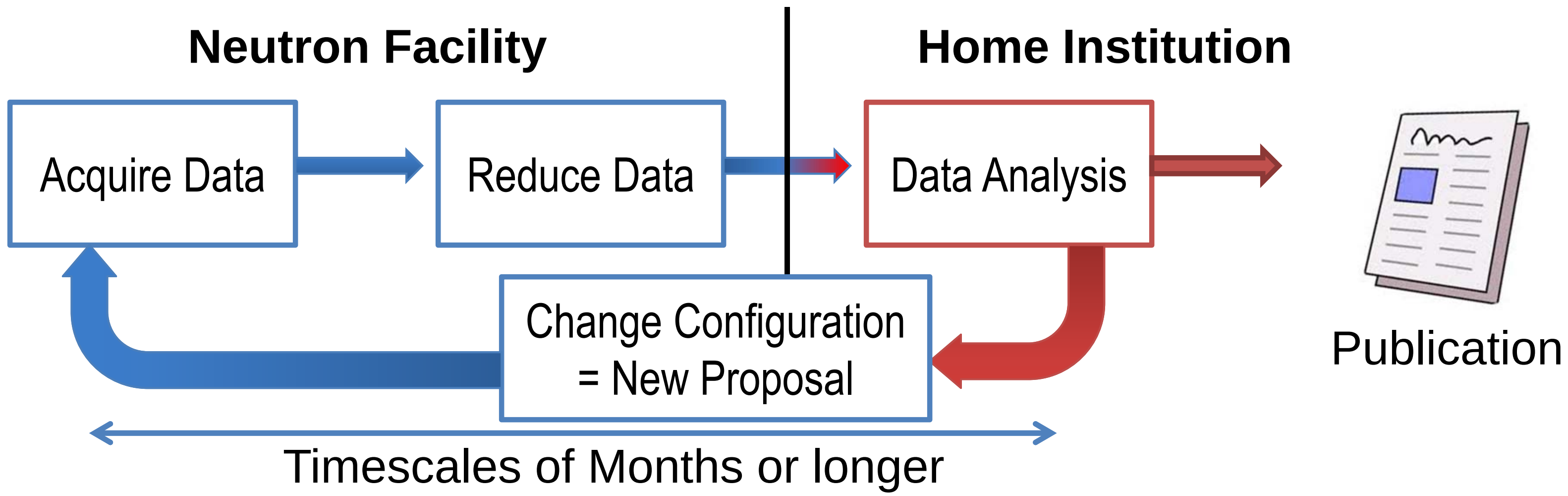
Data captured and stored on multiple systems at the beamline

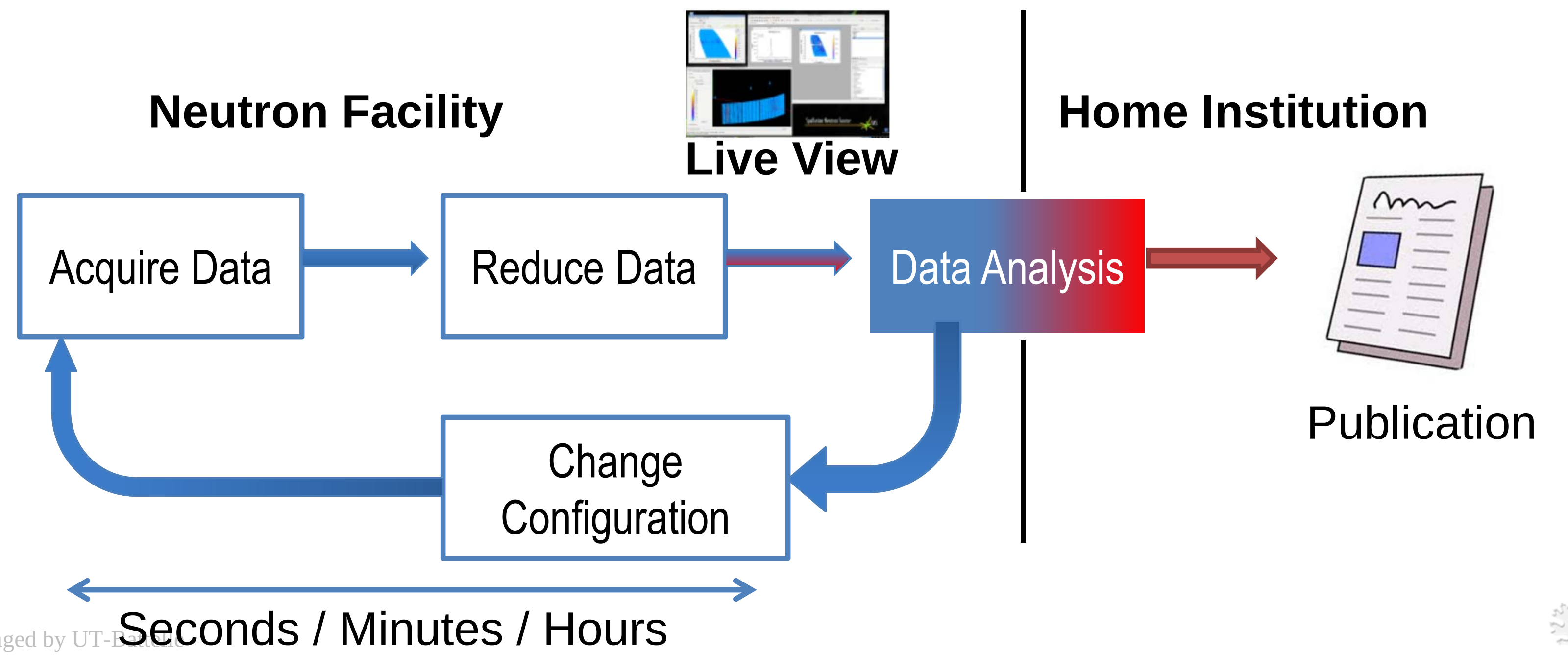
After completion of a "run" data is aggregated on a single system, translation begins

Once data is aggregated reduction begins using a workstation

Analysis and Simulation using mid-scale compute

Improving Productivity = Changing the Workflow

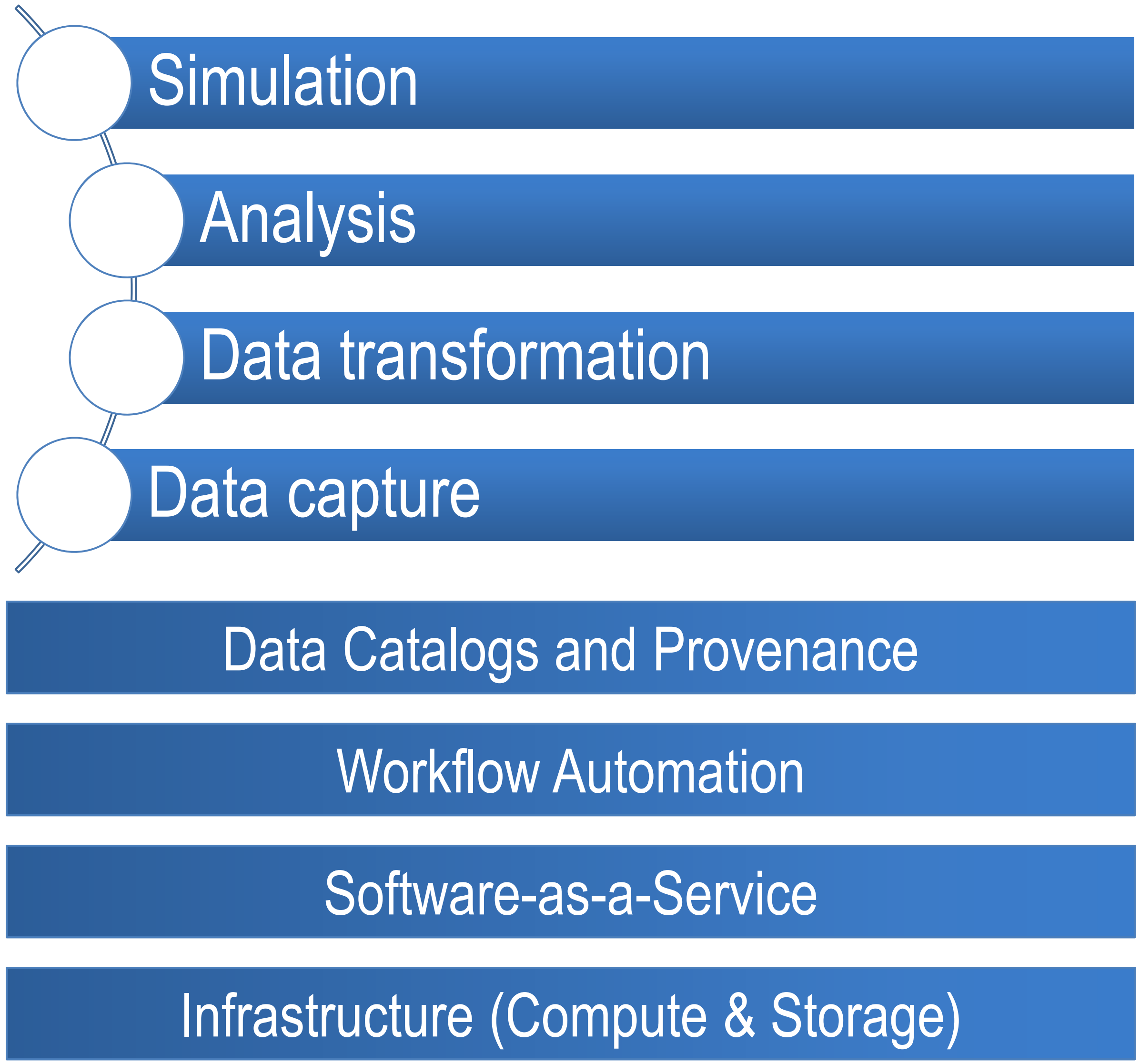




Challenges

- Advanced data infrastructure and the staff for operations
- Data capture and aggregation from a diverse sensors
- Data transformation/reduction in near real-time for live view
- Coupling of advanced analysis/simulation
- Cataloging of experiment results to include provenance
- Remote access to data and compute resources
- Long-term stewardship and public access

A Knowledge Discovery Architecture for Neutron Science



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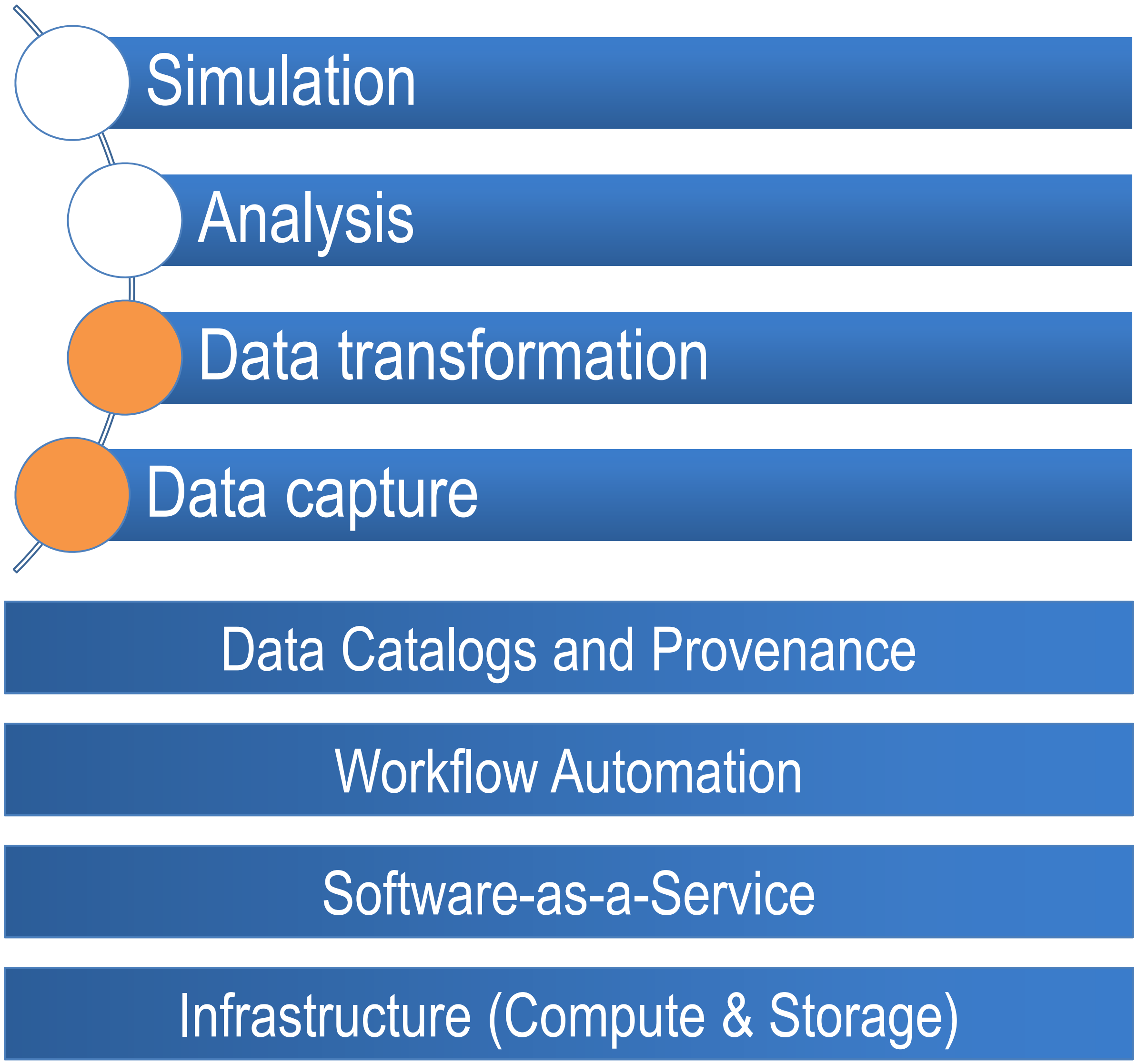
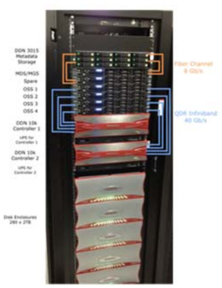
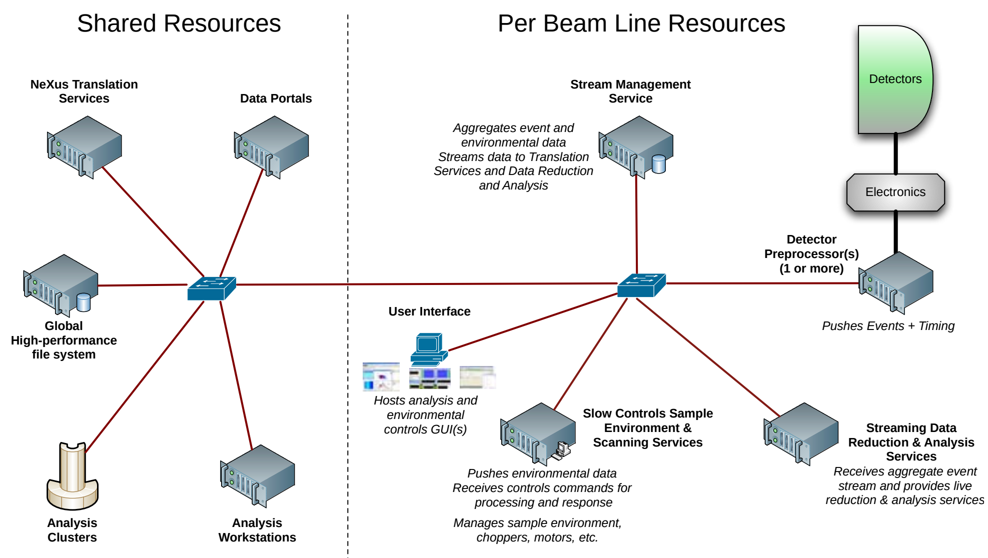


Data Capture and Transformation

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 modify MANTID (data reduction) to read from the data stream live from SMS
  - *Streaming Reduction Service (SRS)*
- 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)*
- Files are created on an HPC infrastructure for subsequent parallel analysis and data reduction





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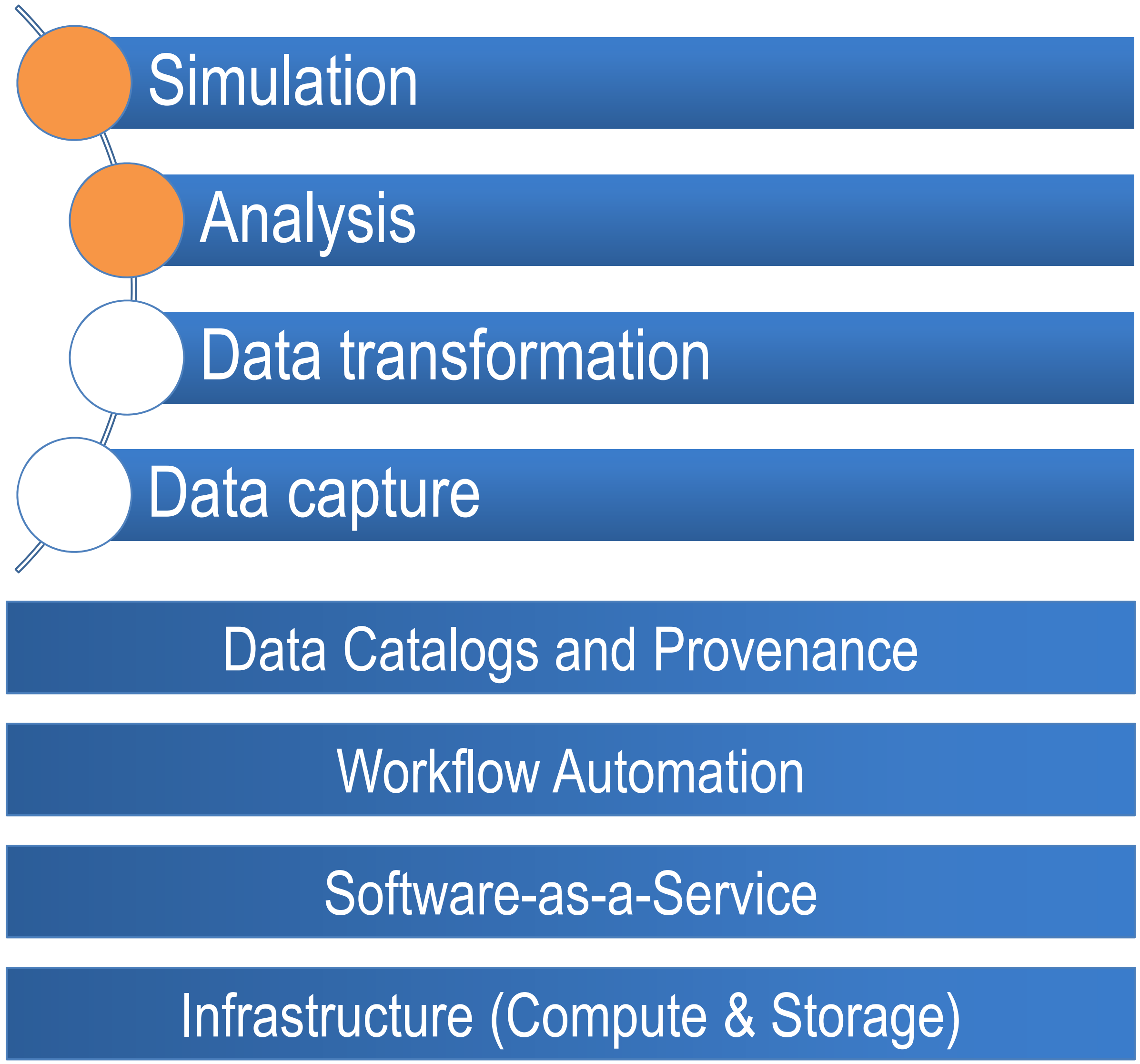
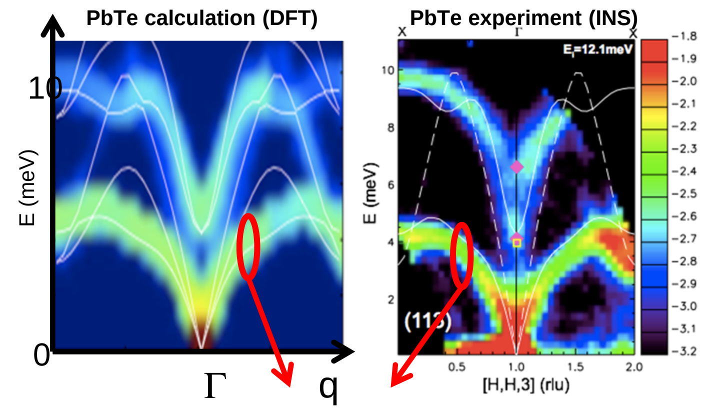


Data Analysis and Simulation
- Center for Accelerating Materials Modeling

- The CAMM will integrate materials modeling/simulation (MD/DFT) directly into the chain for neutron scattering data analysis, **offline** and **online** (in near real time)
- Developing workflows for refinement, integration of MD codes, **neutron scattering corrections** ..
- The CAMM is working with ORNL's Materials Science and Technology Division to study coarse grained MD simulations of polymers PEO-AA (CNMS), *ab-initio* MD simulations for ferroelectrics/thermoelectrics



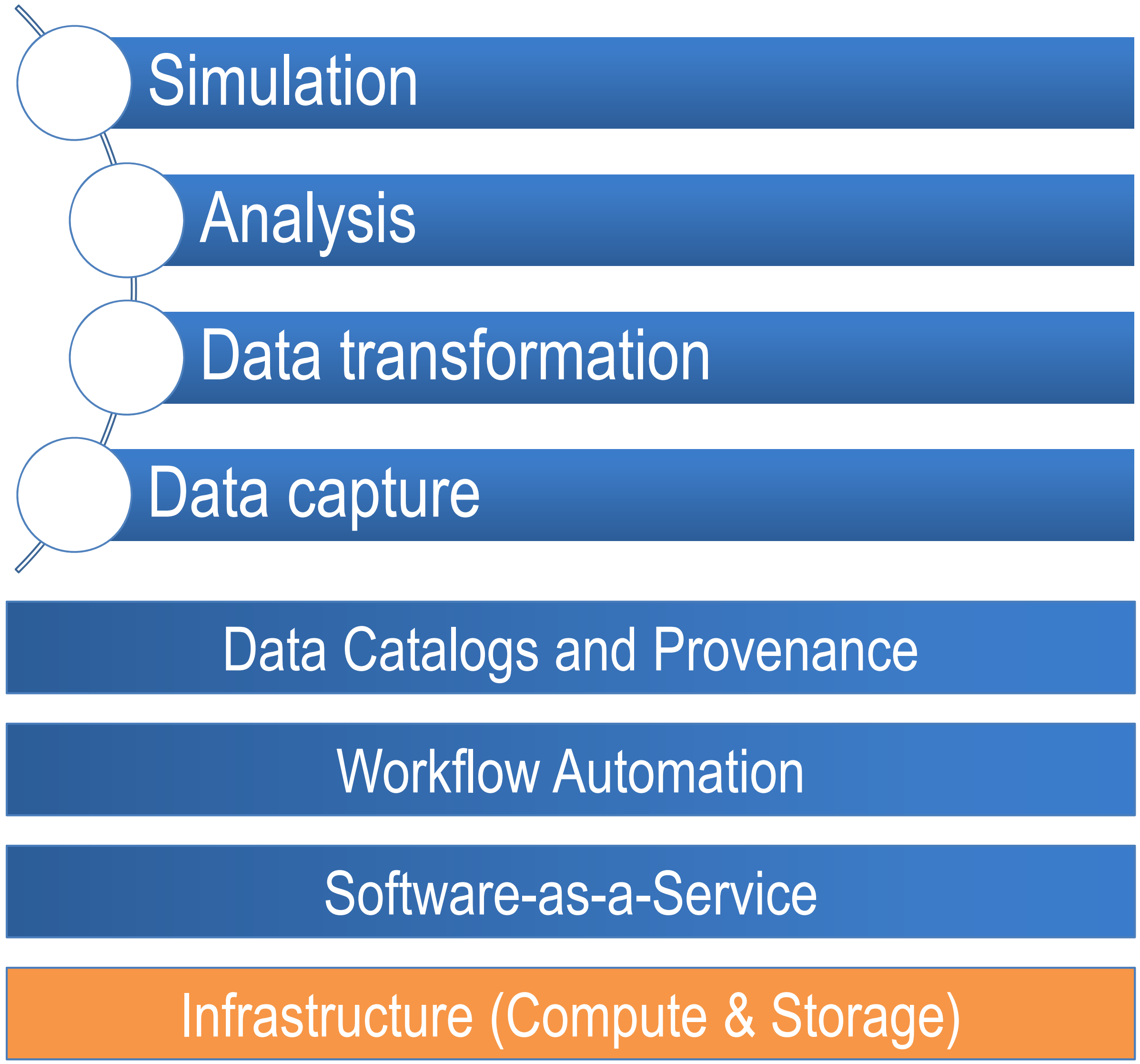
Focus on *width* of dispersions:
- measured line widths need corrections for instrument resolution effects.
- will support development of reliable line width predictions.

Delaire et al., *Nature Materials* (2011).

The Center for Accelerating Materials Modeling (CAMM)

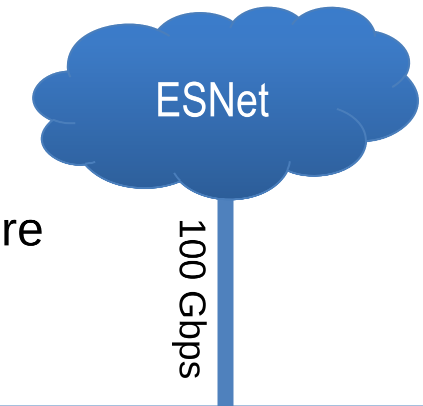
- *Partnership between ORNL's Neutron Sciences, Physical Sciences and Computing and Computational Sciences Directorates*
- *Studying force field refinement from quasi-elastic and inelastic neutron scattering data*
- *CAMM formed in response to BES proposal call for* Predictive Theory and Modeling

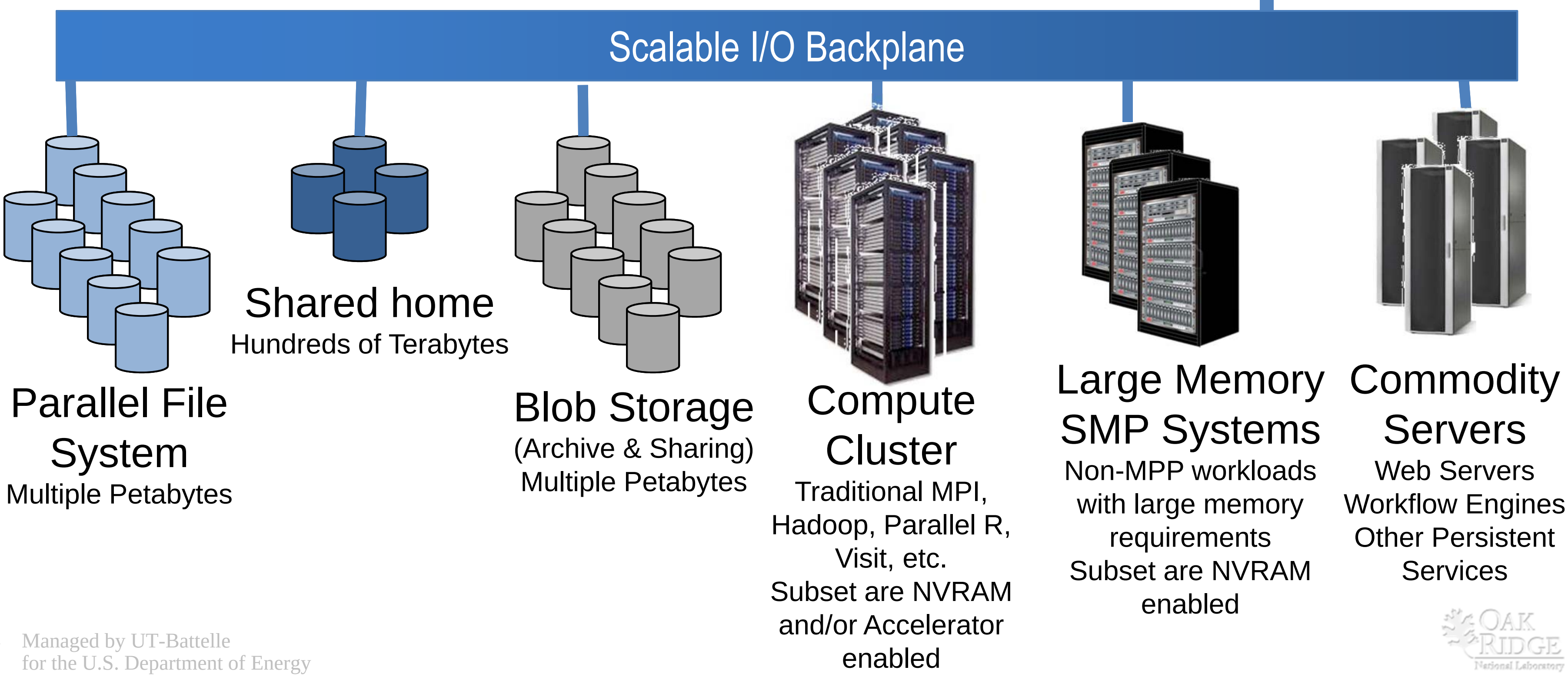
A Knowledge Discovery Architecture for Neutron Science



Compute and Data Infrastructure

- Flexible: tailored software stacks coupled with workload appropriate compute
- Elastic: meet point-in-time storage and compute requirements
- Ability to provision persistent services for data capture services, portals, databases, etc.





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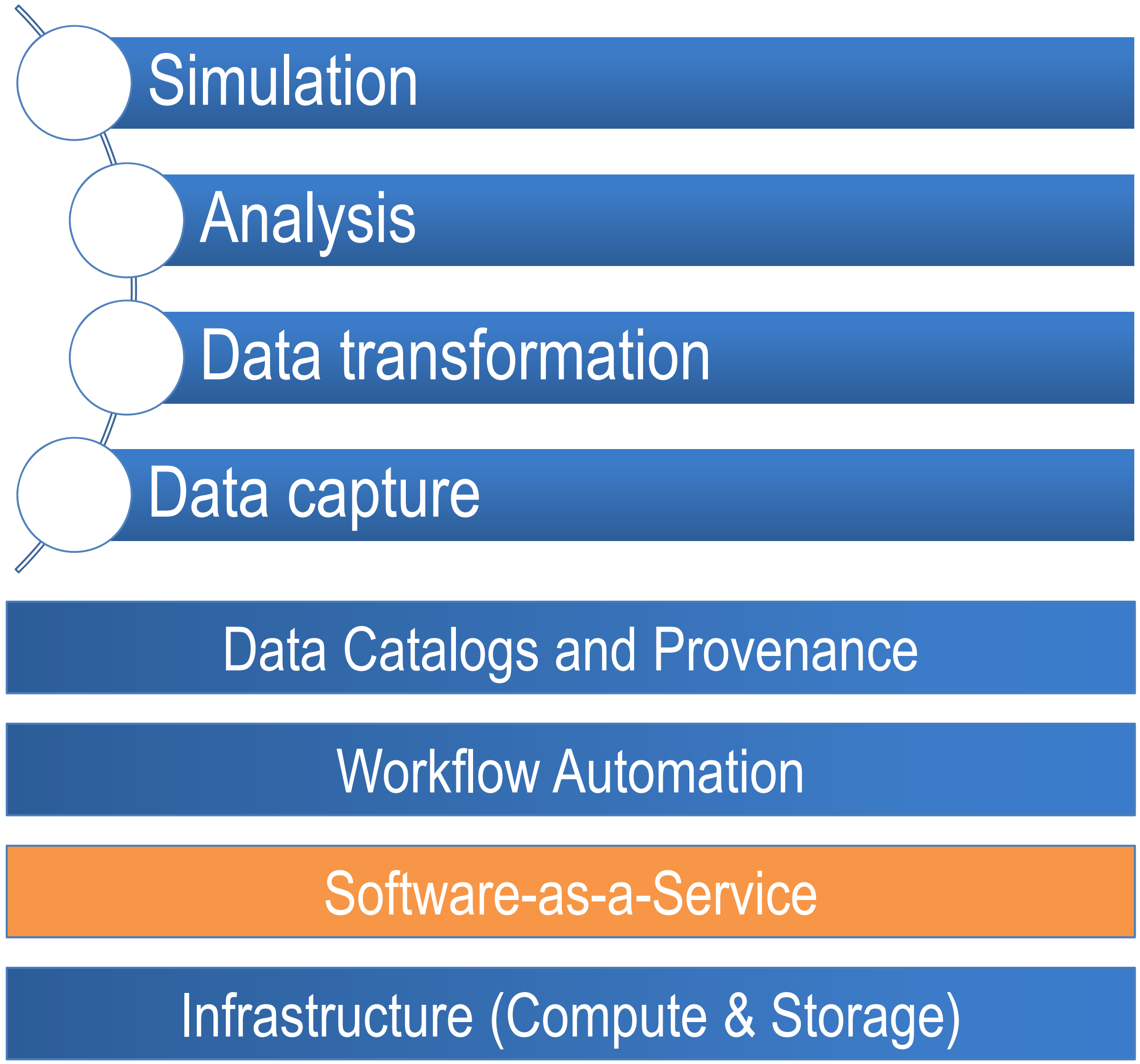
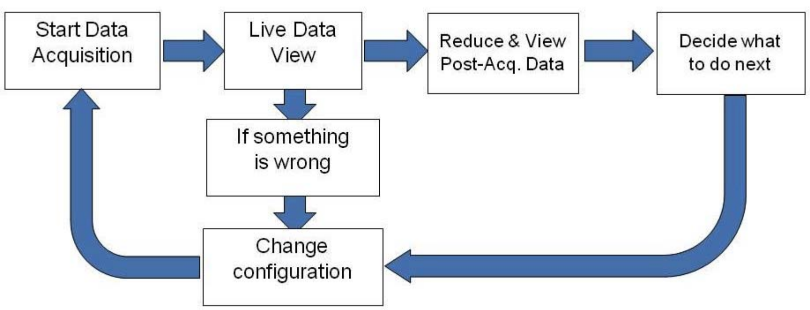
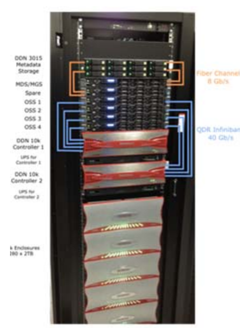


Software-as-a-Service Platform

- A hybrid HPC cluster and software-as-a-service “cloud”
- Full HPC software stack and parallel file system environment
- Unlike traditional HPC, users are insulated from this environment
- Parallel reduction algorithms are configured and ready to run
  - Leverages Mantid in a “Framework” mode and runs this data parallel
- These reductions are available for execution from anywhere via MOAB web-services
- Users continue to interact with Mantid for reduction as they always have on their workstation or via thin-client
  - Mantid executes reduction remotely through MOAB web-services
- Other software services will be required - modeling and simulation





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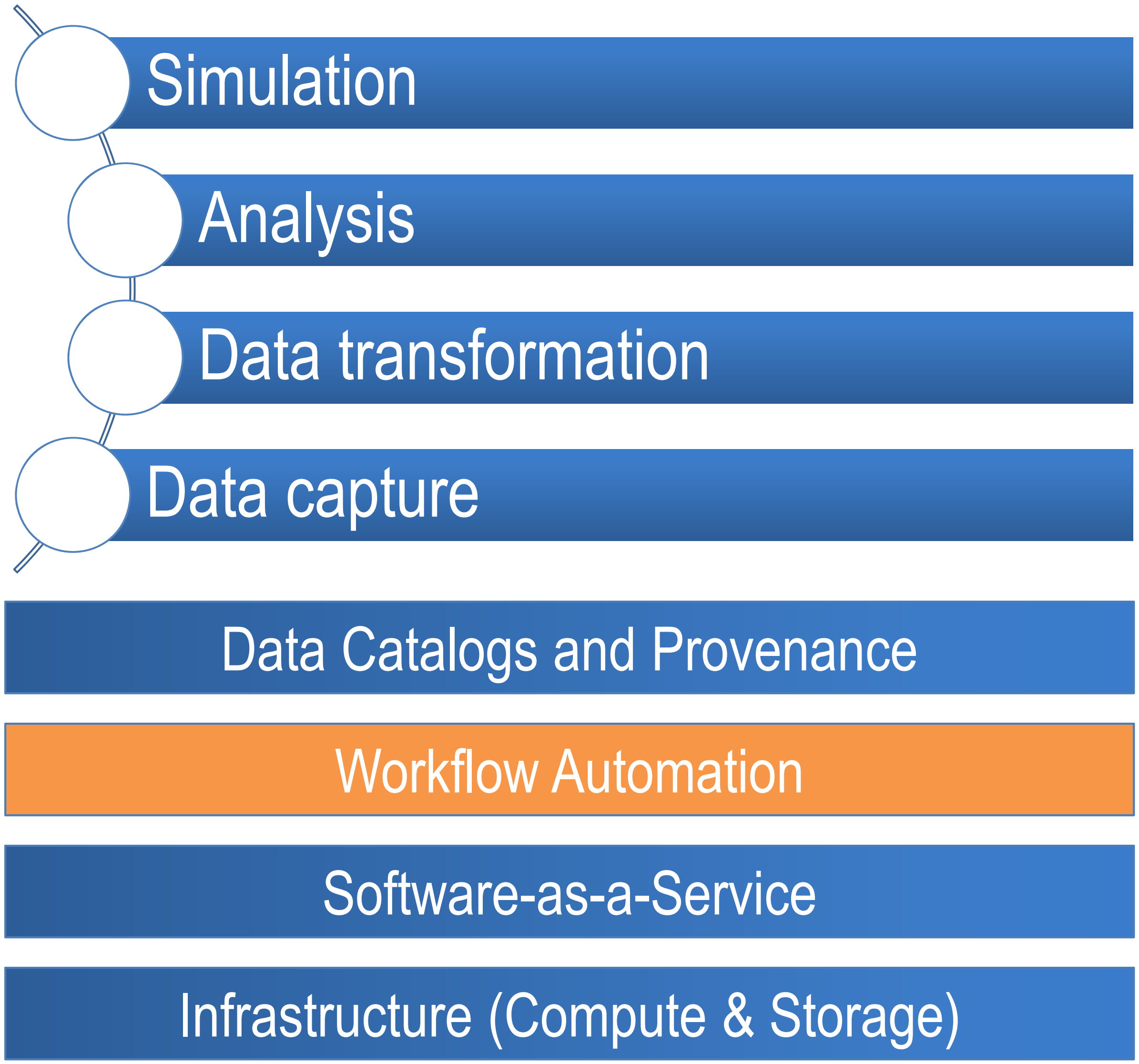
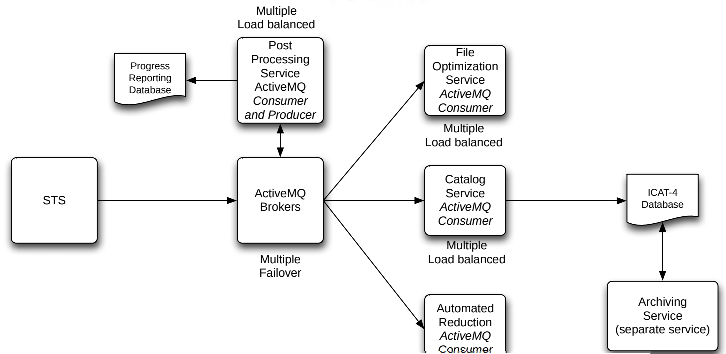
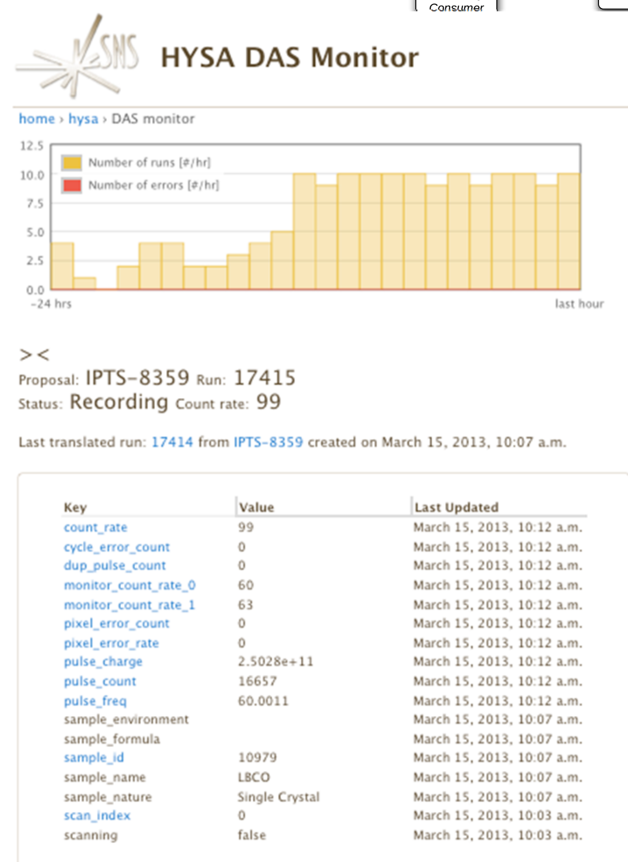


Workflow Automation

- The Workflow Manager handles data cataloging, automated reduction, and archiving of datasets post acquisition
- Built on Apache ActiveMQ allowing loosely coupled architecture
  - Resilience through durable messages and clustered message brokers
  - Load balancing of tasks across resources through message queues
- Tasks within the workflow are handled by independent processes running on one or more systems
- Each task type maps to an ActiveMQ queue, to activate a task you simply send a message to that queue
- A director process manages the workflow sending messages to these queues
- Workflows are defined and stored within the director's redundant MySQL system





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cycle_error_count	0	March 15, 2013, 10:12 a.m.
dup_pulse_count	0	March 15, 2013, 10:12 a.m.
monitor_count_rate_0	60	March 15, 2013, 10:12 a.m.
monitor_count_rate_1	63	March 15, 2013, 10:12 a.m.
pixel_error_count	0	March 15, 2013, 10:12 a.m.
pixel_error_rate	0	March 15, 2013, 10:12 a.m.
pulse_charge	2.5028e+11	March 15, 2013, 10:12 a.m.
pulse_count	16657	March 15, 2013, 10:12 a.m.
pulse_freq	60.0011	March 15, 2013, 10:12 a.m.
sample_environment		March 15, 2013, 10:07 a.m.
sample_formula		March 15, 2013, 10:07 a.m.
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sample_name	LBCO	March 15, 2013, 10:07 a.m.
sample_nature	Single Crystal	March 15, 2013, 10:07 a.m.
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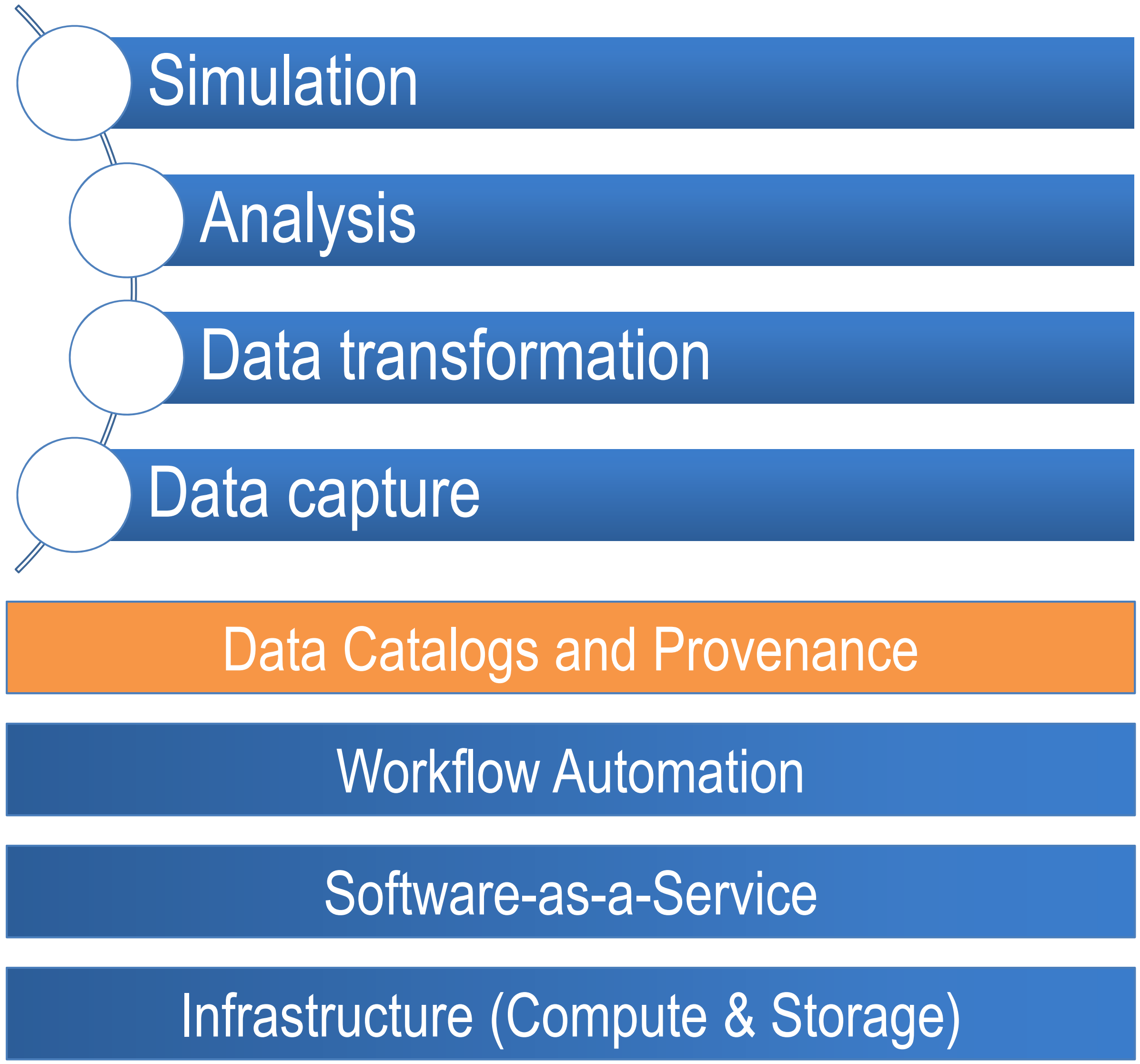
A Knowledge Discovery Architecture for Neutron Science



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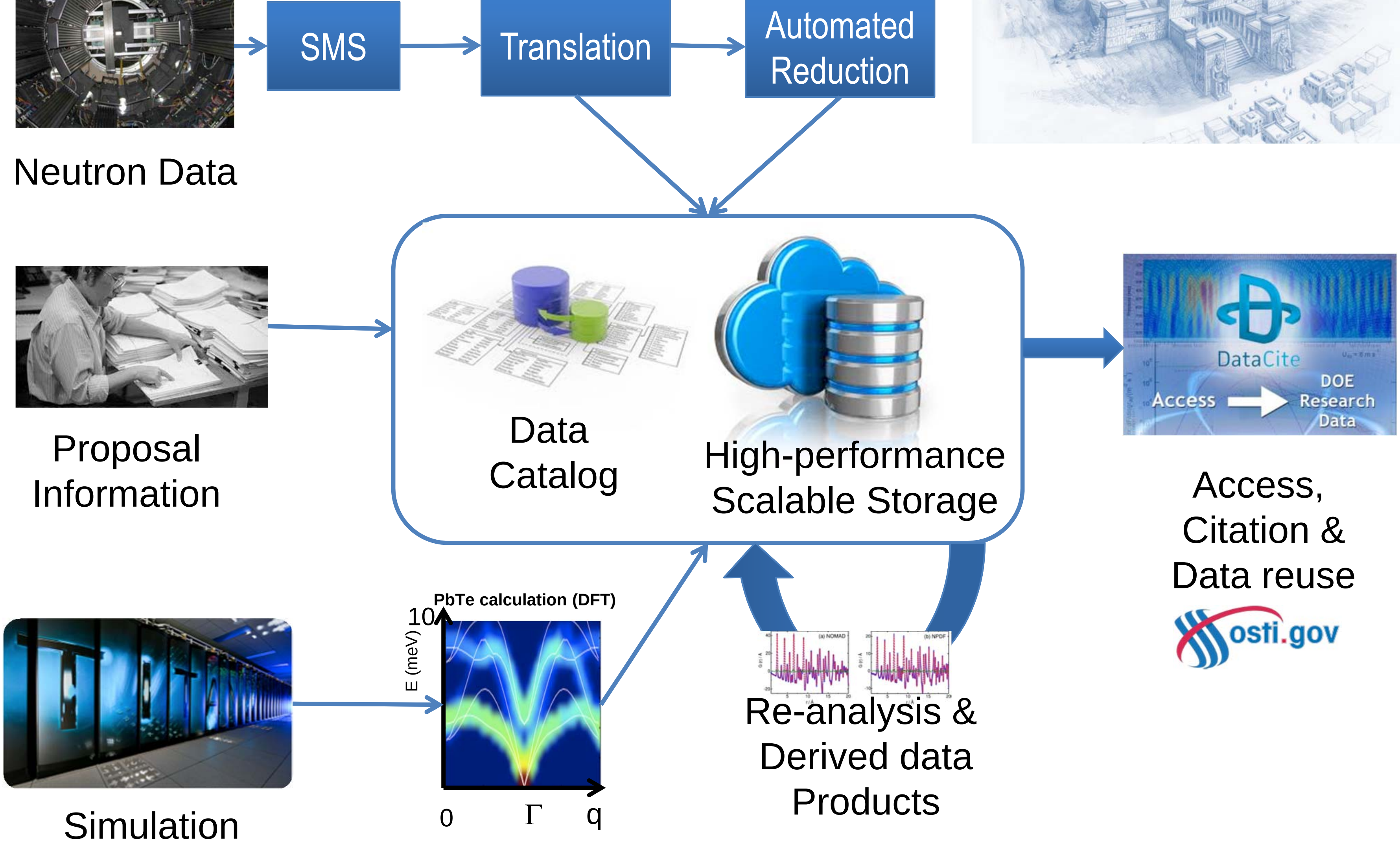
Data Catalogs and Provenance



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