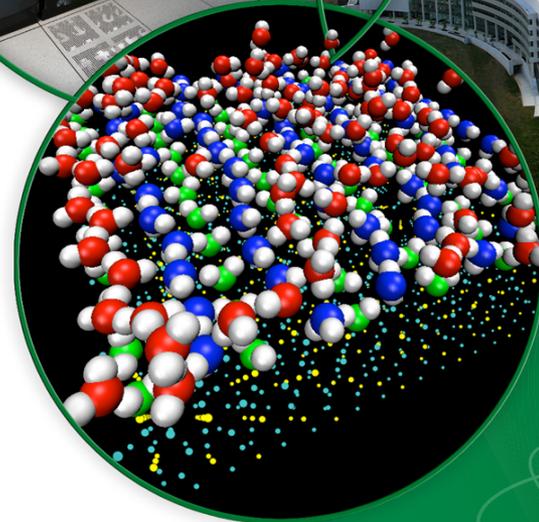


Accelerating Scientific Discovery at the Spallation Neutron Source

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

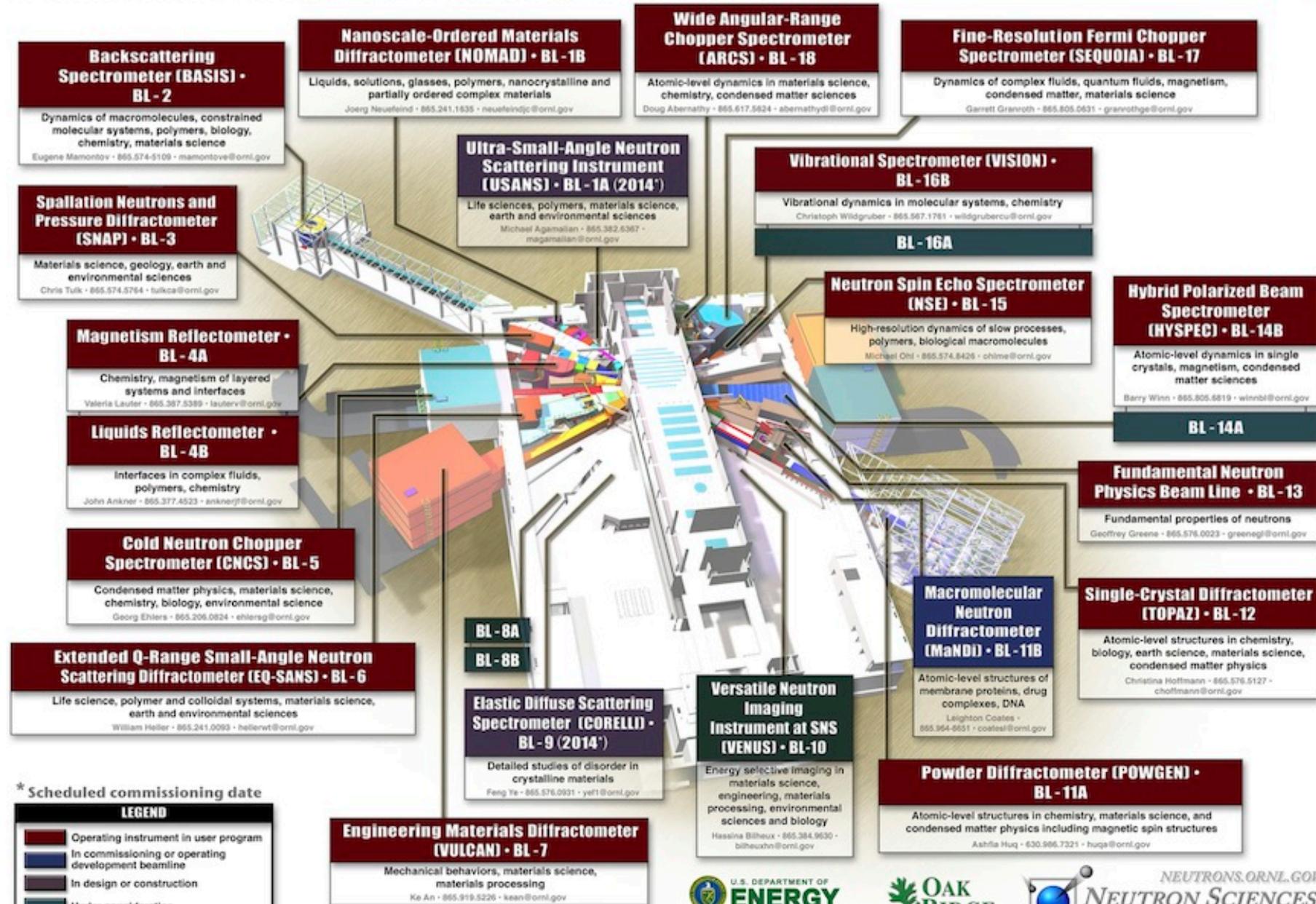
Spallation Neutron Source:
World's most powerful
accelerator-based neutron source

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



* Scheduled commissioning date

LEGEND

- Operating instrument in user program
- In commissioning or operating development beamline
- In design or construction
- Under consideration

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

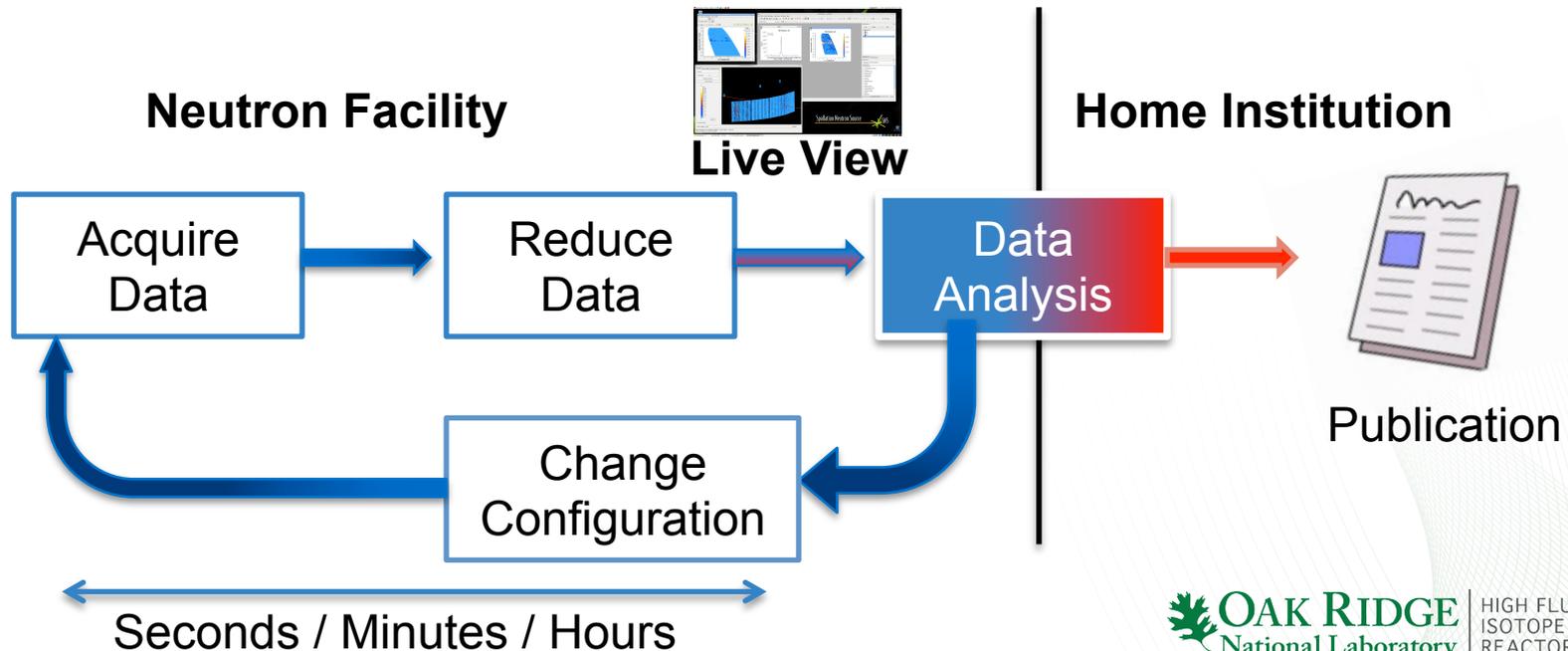
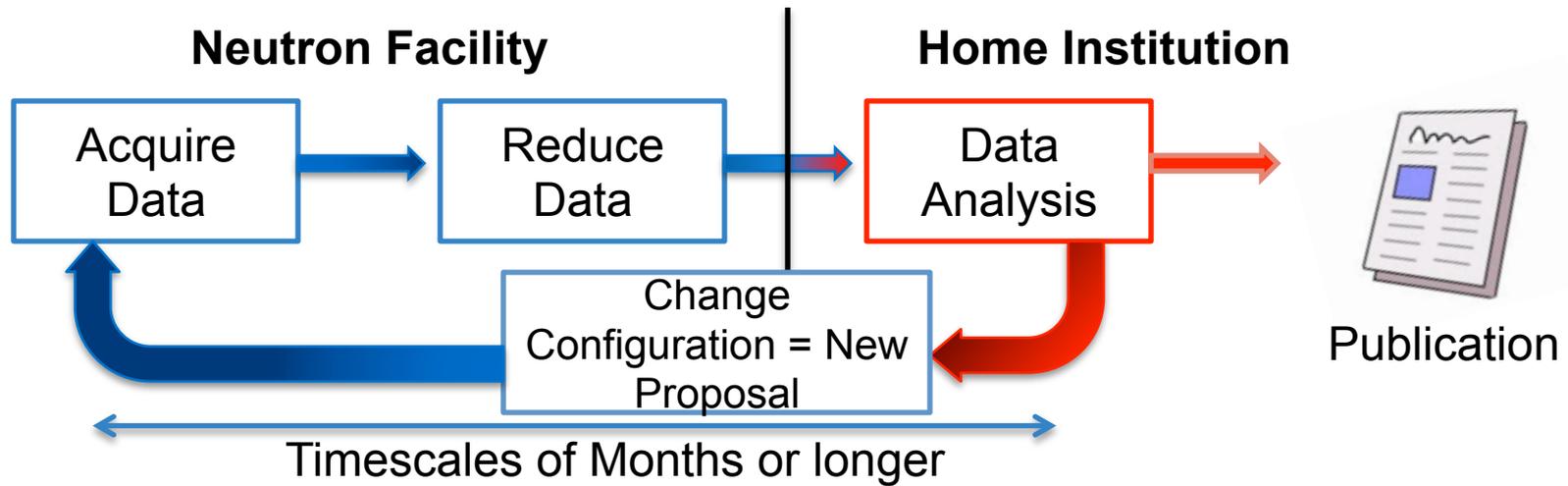


User Facility

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



Improving Productivity = Changing the Workflow



Our Mission... what do we aspire to do?

SNS is an experimental user facility

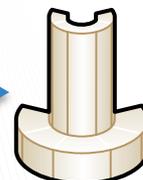
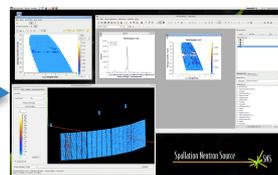
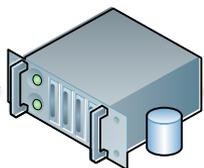
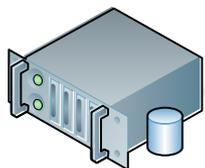
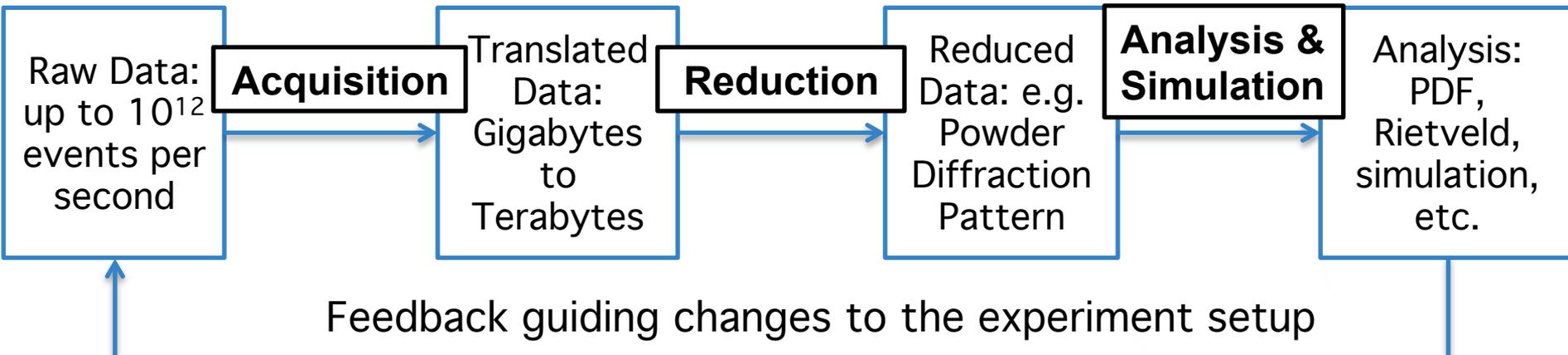
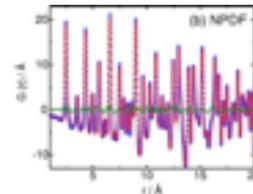
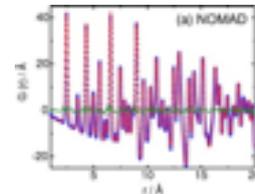
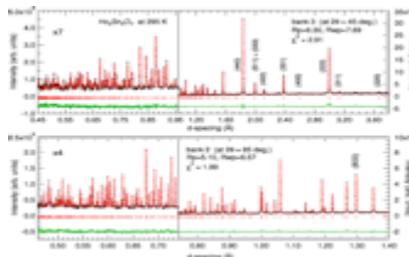
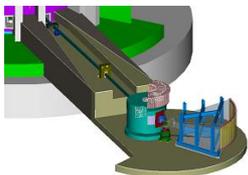
What should we aspire to... create a data infrastructure that gives users

- 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



Data captured and stored on multiple systems at the beamline

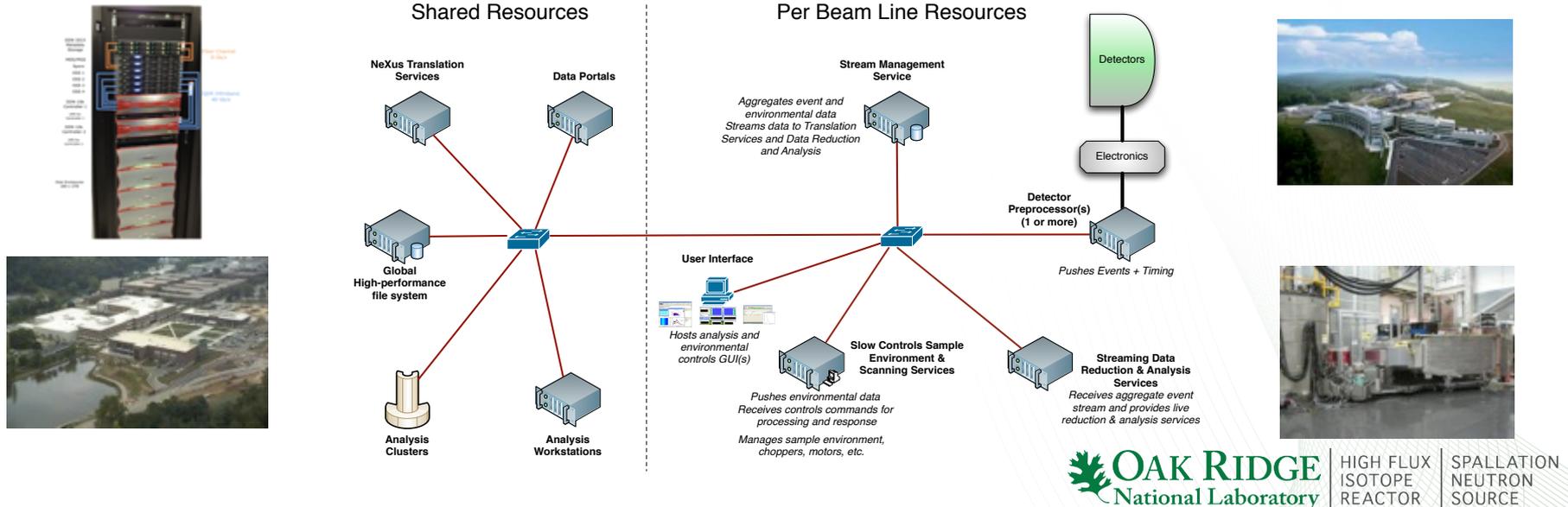
After completion of a "run" data is aggregated on a single system, translation begins

Once data is aggregated reduction begins using a workstation

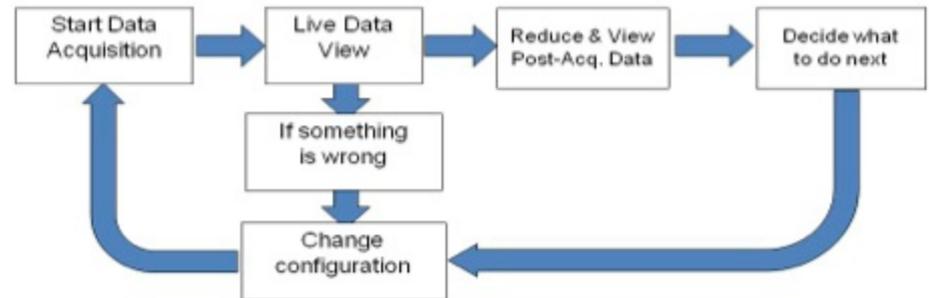
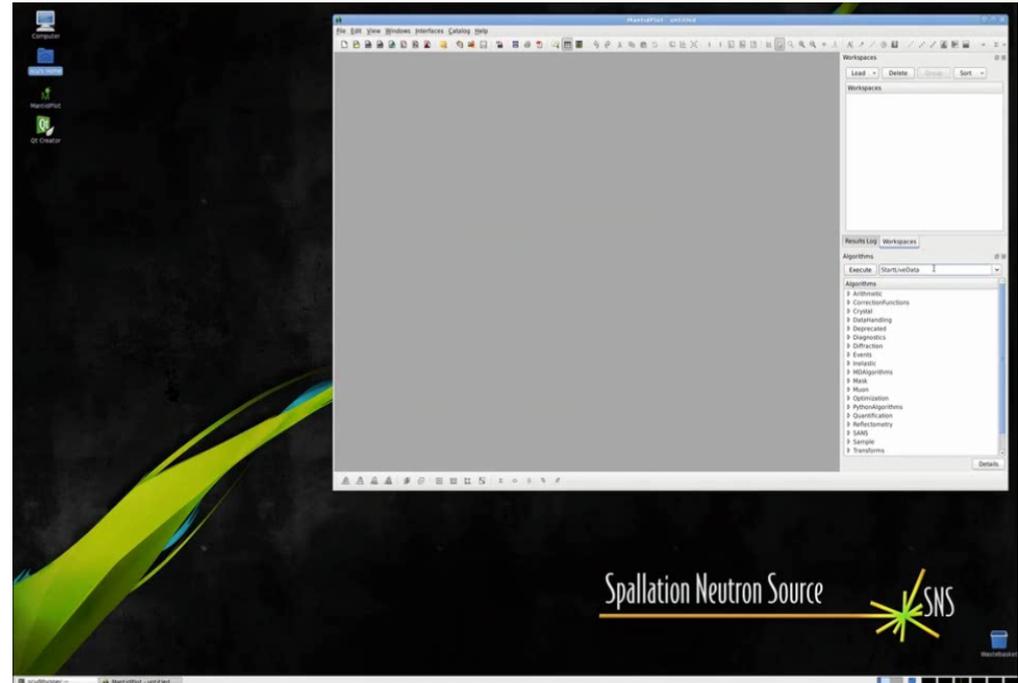
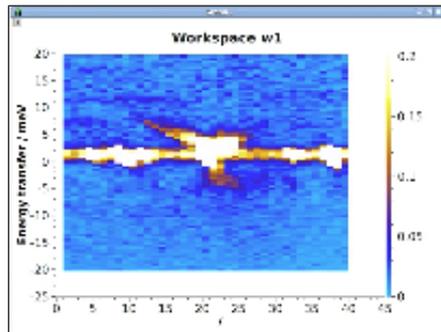
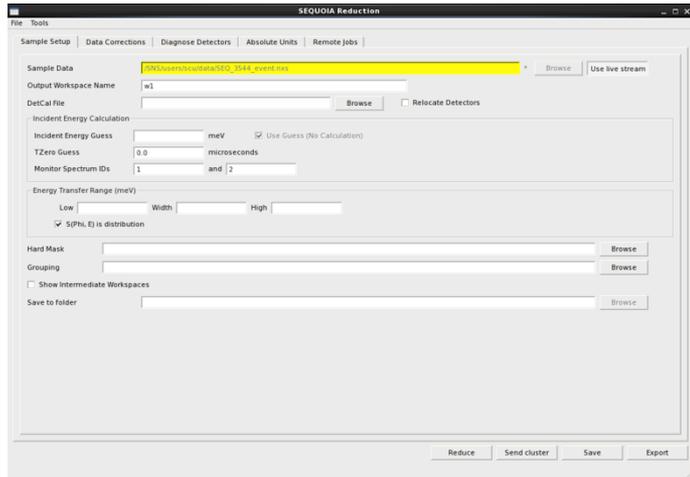
Analysis and Simulation using mid-scale compute

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



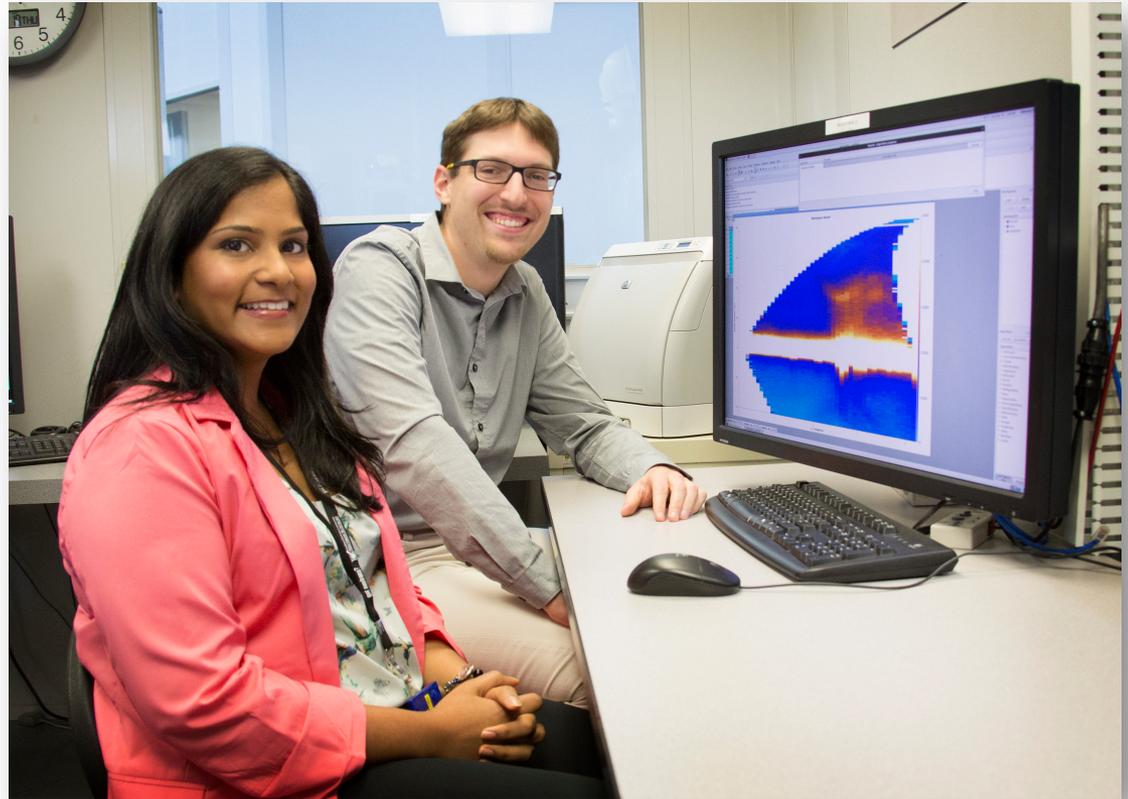
'Live' Reduction & Analysis



Optimal Experimental Design
Computational "Steering" (Decision Support System)

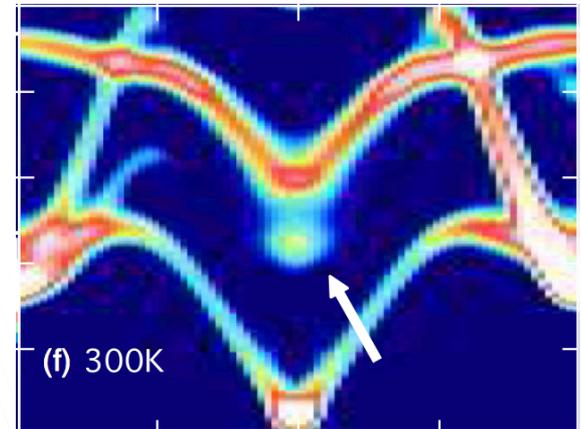
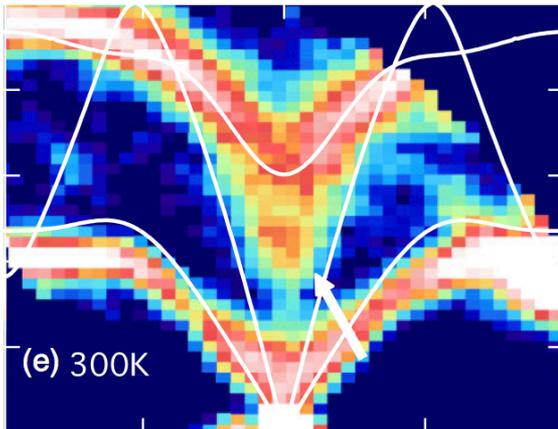
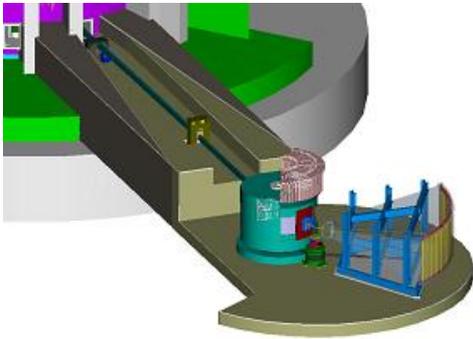
USERS watch their data live on SEQUOIA

- 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



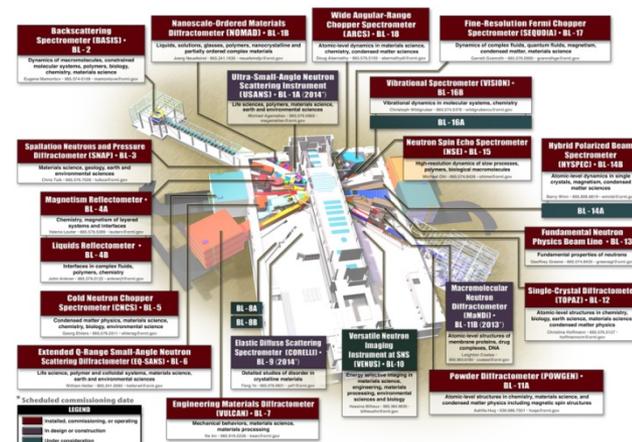
Center for Accelerating Materials Modeling

- 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



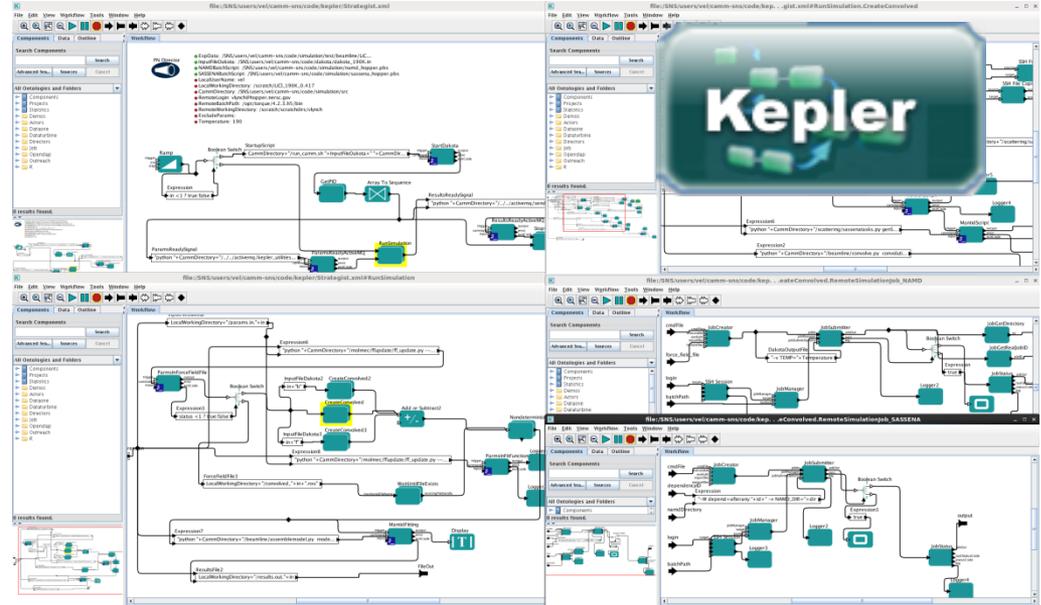
Validation, Refinement & SNS

- 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.

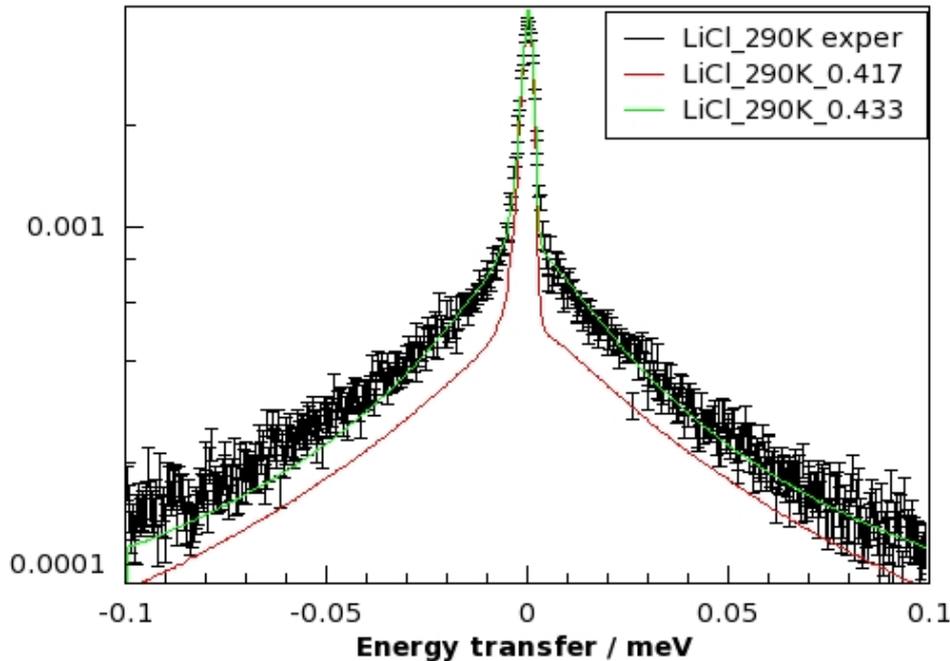


Modeling LiCl data with workflow

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



LiCl_{290K} Q=0.9

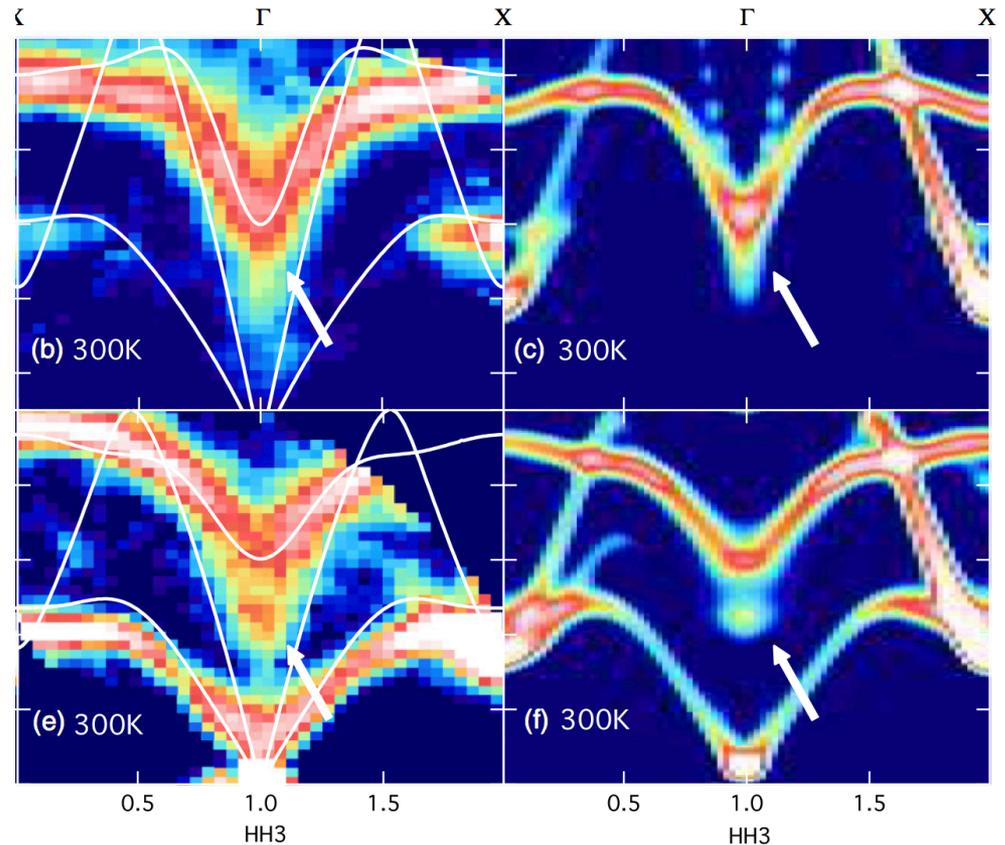


<<<<< Best data captured at function evaluation 2
 Confidence Interval for c0 is [7.7181005978e-01, 7.9133911535e-01]
 Confidence Interval for b0 is [3.5683719031e-05, 4.1095168905e-05]
 Confidence Interval for e0.0 is [4.7649690032e-03, 5.0604743707e-02]
 Confidence Interval for e0.1 is [3.8658107943e-02, 4.0925369124e-02]
 Confidence Interval for e0.2 is [3.2393364793e-02, 3.4198221349e-02]
 Confidence Interval for eshift is [2.2784599458e-04, 2.7276832227e-04]
 Confidence Interval for FF1 is [4.3254547020e-01, 4.3403369489e-01]



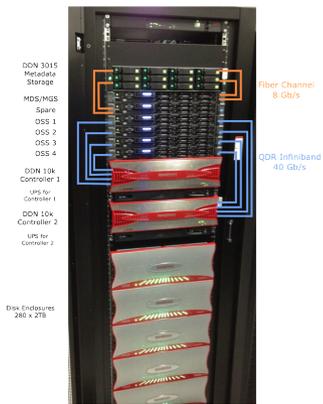
A VERY Recent Example

- 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.

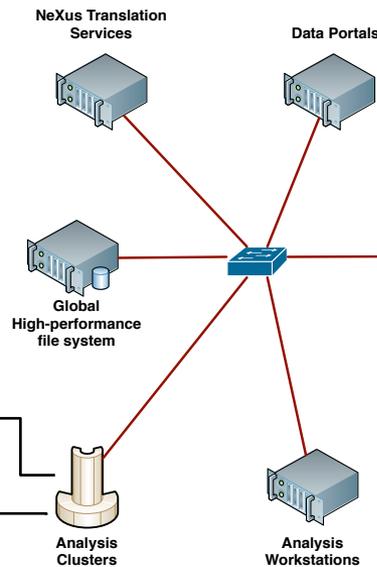


A Neutron Sciences & Computing Partnership

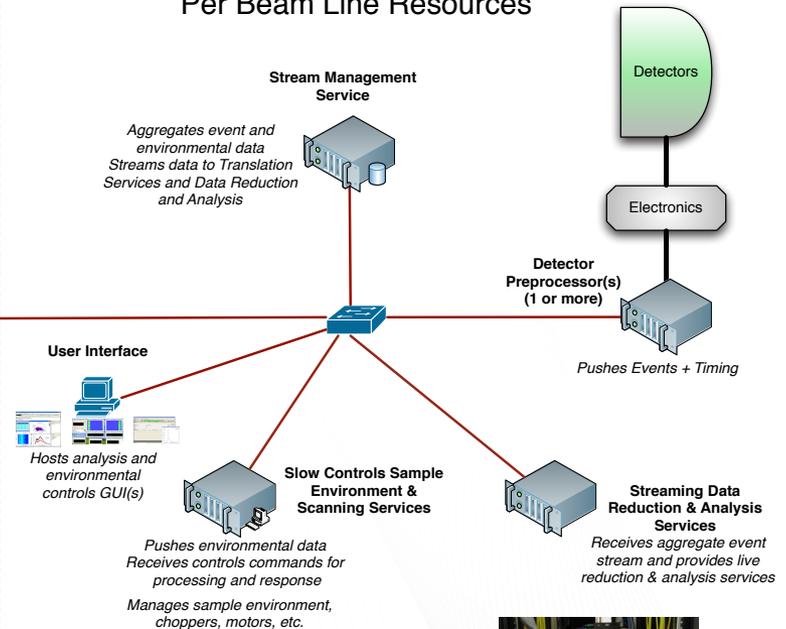
- CADES provides core compute and data capabilities for SNS users
 - Center wide parallel file system, HPC compute & utility compute
 - Expertise in HPC, data analysis, visualization, and computer science



Shared Resources



Per Beam Line Resources



Chadwick (196 cores)
 Fermi (512 cores)
 OIC (256 cores)
 Titan (300K cores + 18K GPUS)



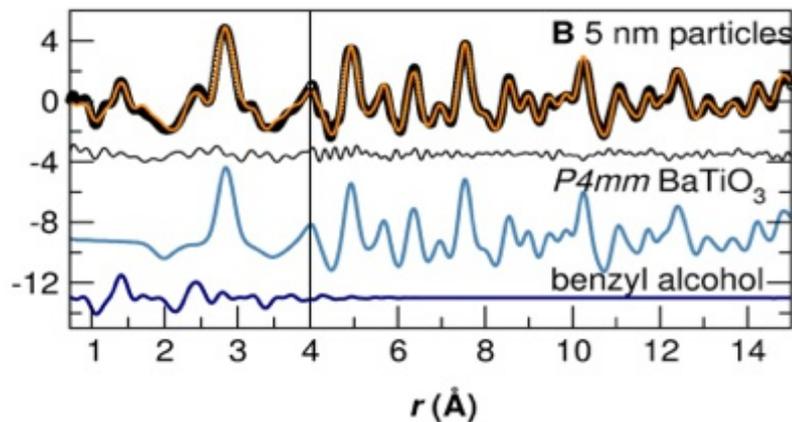
Login node workstations
 32 cores, 256Gb



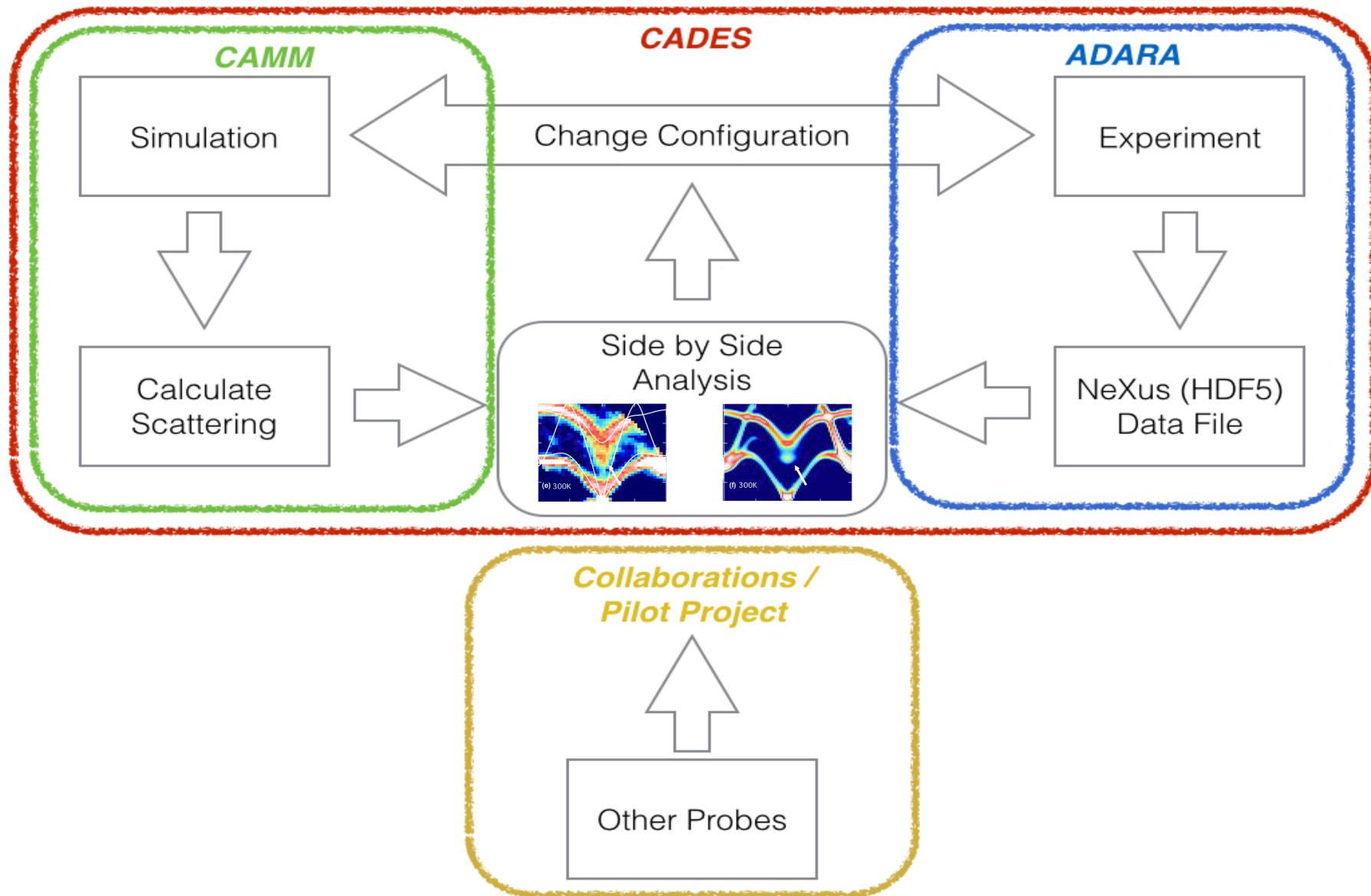
Beam line workstations
 32 cores, 256Gb

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



Acknowledgements

ADARA – Funded by Laboratory Directed Research & Development at ORNL
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