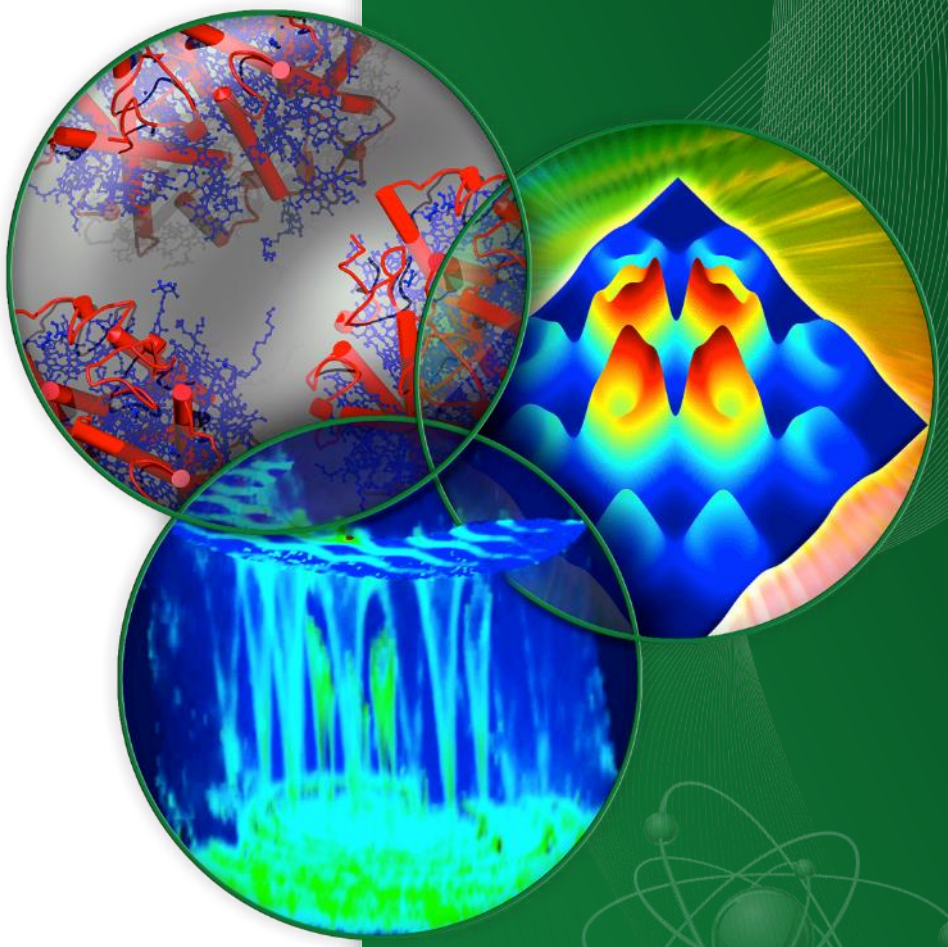
Neutron Data Analysis and Visualization Division

Overview



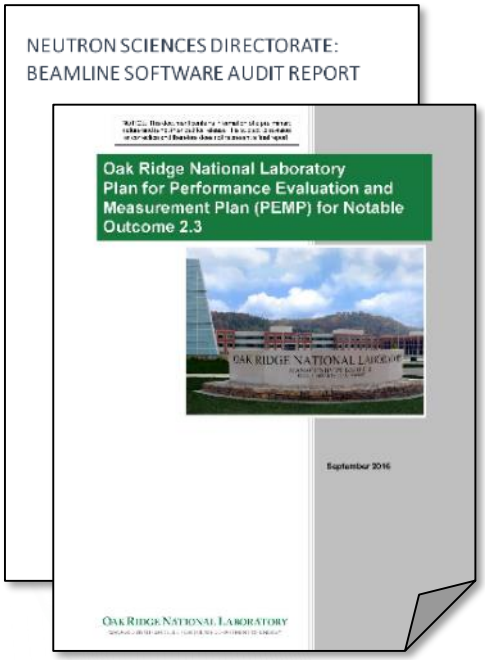
Thomas Proffen,
NDAV Division Director

ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Addressing user community needs for data collection, reduction, and analysis

Notable outcome	Actions
Deliver and start implementing a comprehensive plan to address the day-to-day needs of the HFIR and SNS user communities for data collection, reduction, and analysis 	September 19: Plan briefed to DOE-HQ • Requirements and standards established for data collection, reduction, and analysis software and tools • Assessment of every HFIR and SNS beam line to determine data and software needs • Scientific programmers embedded with each instrument team • Comprehensive plan developed to address software needs for next 3 years • Plan integrated into Scientific Productivity Process Ongoing: Plan implementation • Data acquisition and instrument control, data reduction and data management software upgrades are in progress at HFIR and SNS



Key elements of approach

- Form a cross cutting steering group
- Manage to standards and requirements
- Implement auditing, review, and progress tracking
- Integration of teams from DAS, data, and analysis/visualization
- Embedding of software scientists with beamlines
- Clear roles and responsibilities
- Integrated software and data plan for NScD
- Effective use of feedback and quality control
- Systematic approach to training

Steering group is defining and coordinating actions

Originally convened in October 2015 by directorate

Core group meets every second week and full group meets monthly

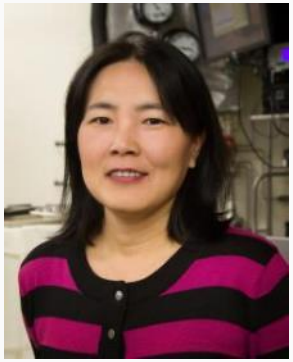
Thomas Proffen,
NDAV Division Director

Garrett Granroth,
Scientific Data Analysis
Group Lead

Shelly Ren,
Science Information
Systems Team Lead

Steve Hartman,
Data Acquisition
Group Lead

Steve Kulan,
HFIR Data Acquisition
Team Lead



Wei Tian,
HB1A HFIR scientist

Changwoo Do,
EQ SANS scientist

Ashfia Huq,
Chemical Crystallography
Group Lead

Mark Lumsden,
TOF Spectroscopy
Group Lead

Guiding principles and standards

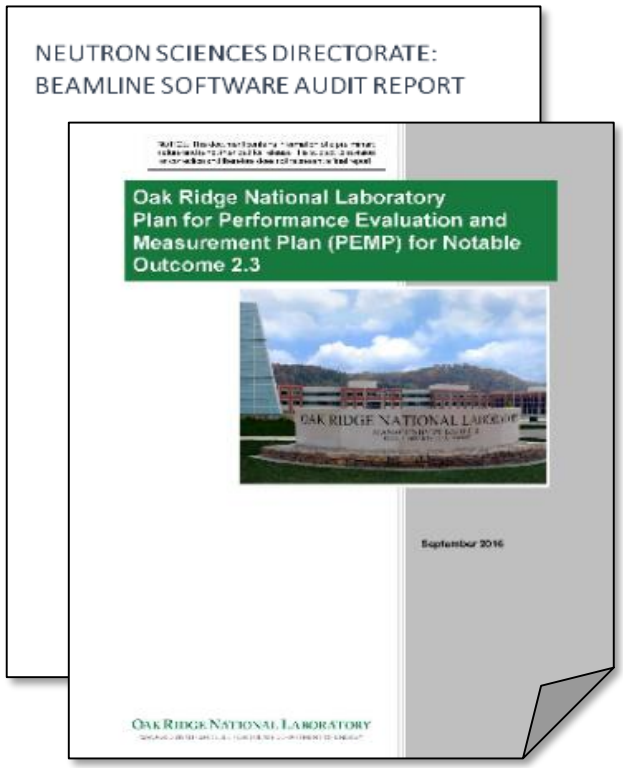
- PhD level students need to be able to run standard experiments independently after initial training on the beamline.
- Understanding the ‘contract’ between us and the users.
- Standards, ongoing quality control and assurance.
- Responsive to community feedback.
- Unified user experience across all aspects.
- Automation

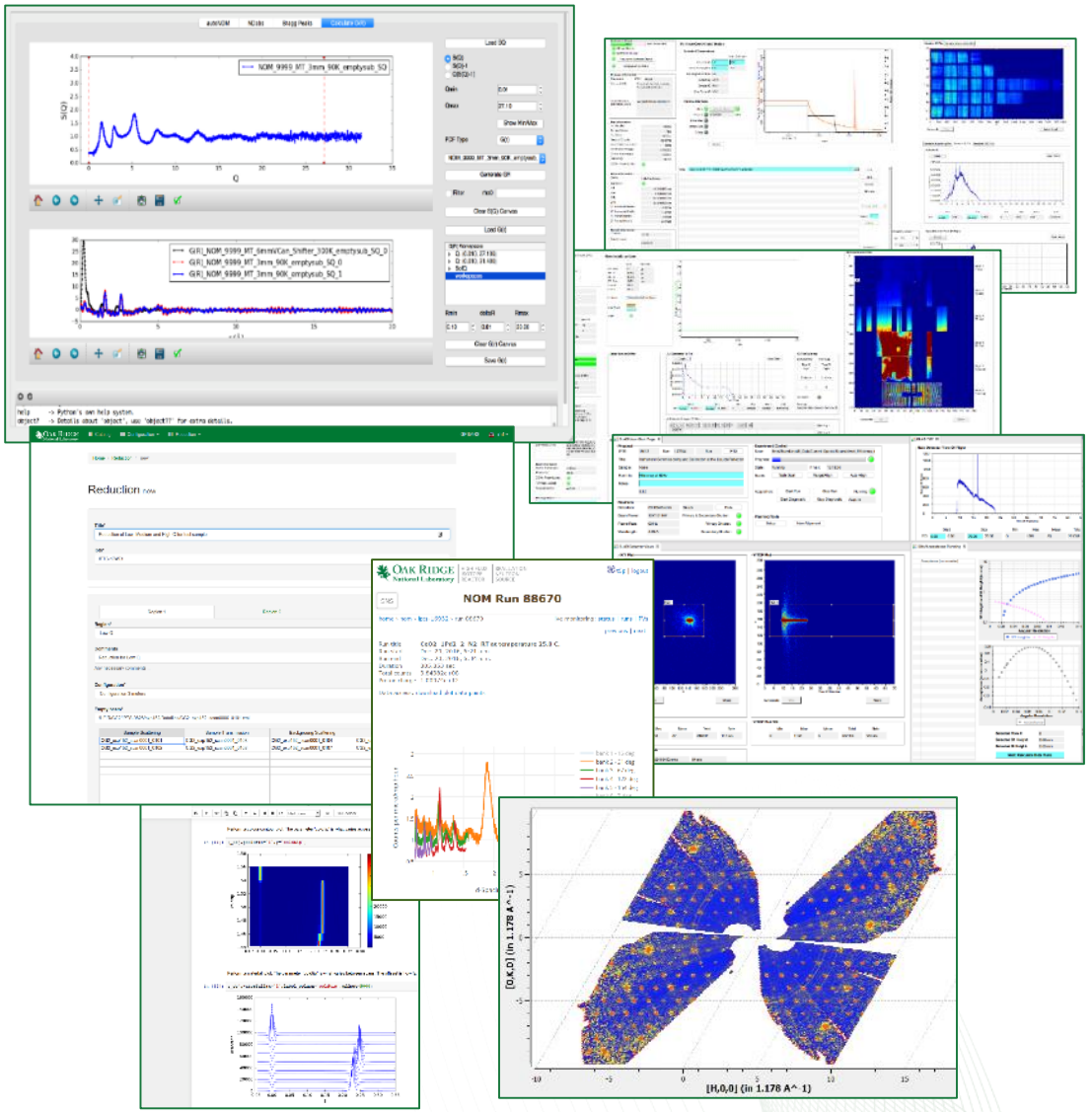
Audits of all SNS and HFIR instruments

- **Internal audits in early 2016**
- **Instrument findings**
  - **NOMAD**: DAS upgrade, auto data reduction, beam/sample alignment…
  - **MANDI**: lack of planning tools, non-optimal method of peak integration…
  - **HIFR SANS**: develop unified & fully benchmarked auto data reduction process using Mantid…
  - **IMAGING**: Interface with computational resources at SNS for data archive/processing, auto reduction
- **Facility wide**
  - Documentation
  - Instrument calibration
  - Adopt common data archiving and computational resources for data processing of instruments at HIFR and SNS
  - Develop suite-based DAS and data reduction software

75 pages…

Software and Data Management Plan





- Download the plan at http://ns-staff.ornl.gov/ (under *Helpful Info*)

Embedding of NDAV staff with instrument teams

Goal: *Create effective teams around scientific instrument software to ensure the most effective, user friendly and cutting edge tools being developed and deployed.*

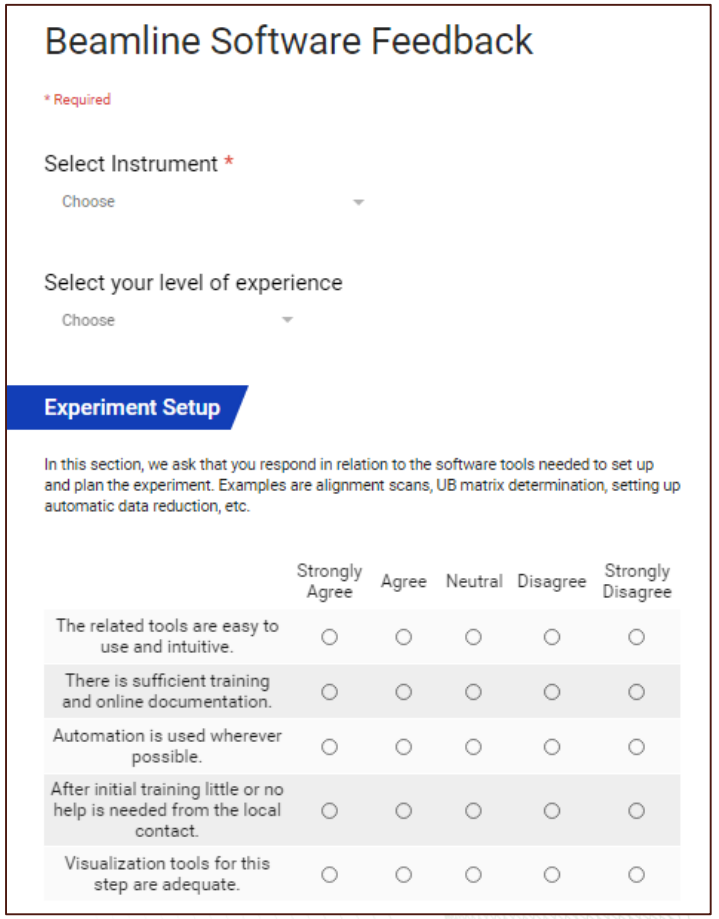
- Adding a scientist with expertise in software and analysis to the team.
- Know the computational needs of the beamline
  - Developed in collaboration with users and instrument staff
  - Help develop an actionable plan to meet those needs.
  - Be integral in executing the plan.
- Participate in experiments
- Introduce the instrument staff to new codes/ features in codes

Embedded NDAV Staff

NDAV Staff	Instrument(s)			
Jean Bilheux	Imaging			
Jose Borreguero	Basis			
Mathieu Doucet	EQSANS	USANS	REFL	REFM
Garrett Granroth	HB-1A	HB-1	HB-3	CTAX
Steve Hahn	Vision			
Ricardo Leal	BIOSANS	GPSANS		
Jiao Lin	ARCS	SEQUOIA		
Vickie Lynch	TOPAZ	MANDI	Imagine	
Peter Peterson	NOMAD	Powgen	SNAP	
Andrei Savici	HYSPEC	CNCS		
Ross Whitfield	Corelli	WAND		
Wenduo Zhou	Vulcan	HB-2B	HB-2A	HB-3A

Instrument Software Feedback Form rolled out at SNS and HFIR

- User Software Feedback Form rolled out for all SNS and HFIR beamlines
- Covering feedback for
  - Experiment setup
  - Data Reduction
  - Data Analysis and Modeling



Beamline Software Feedback

* Required

Select Instrument *

Choose

Select your level of experience

Choose

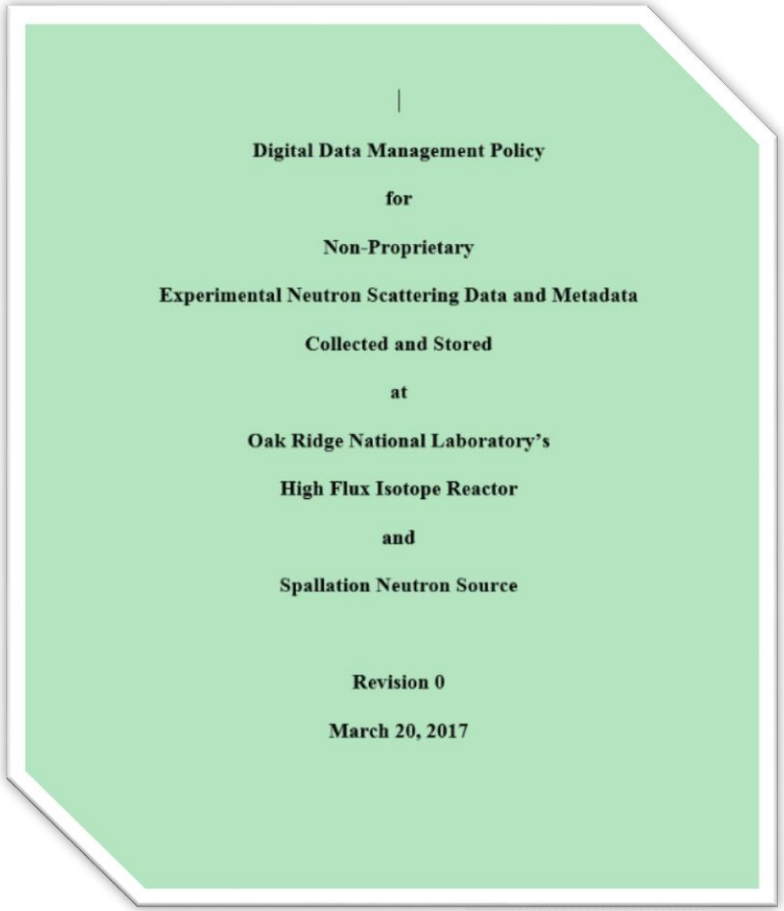
Experiment Setup

In this section, we ask that you respond in relation to the software tools needed to set up and plan the experiment. Examples are alignment scans, UB matrix determination, setting up automatic data reduction, etc.

	Strongly Agree	Agree	Neutral	Disagree	Strongly Disagree
The related tools are easy to use and intuitive.	○	○	○	○	○
There is sufficient training and online documentation.	○	○	○	○	○
Automation is used wherever possible.	○	○	○	○	○
After initial training little or no help is needed from the local contact.	○	○	○	○	○
Visualization tools for this step are adequate.	○	○	○	○	○

Data Management Policy

- Elements of SNS/HFIR data management policy:
  - **Raw data and meta data**: Kept on disk for 3 years and on long term archive another 5 years.
  - **Reduced data**: Kept on disk for 3 years.
  - **Files on scratch space** (current share): Kept for 6 months after last use.



Digital Data Management Policy

for

Non-Proprietary

Experimental Neutron Scattering Data and Metadata

Collected and Stored

at

Oak Ridge National Laboratory's

High Flux Isotope Reactor

and

Spallation Neutron Source

Revision 0

March 20, 2017

Computing resources available to users

- **Analysis cluster**
  - ‘Automatic’ access
  - 4 year renewal cycle
- **CADES resources** (by request)
  - VIRTUES cluster for VISION users
    - 50 nodes / 1600 cores / DFT codes
  - ORNL resources
- **HPC resources** (by request)
  - TITAN
  - NERSC

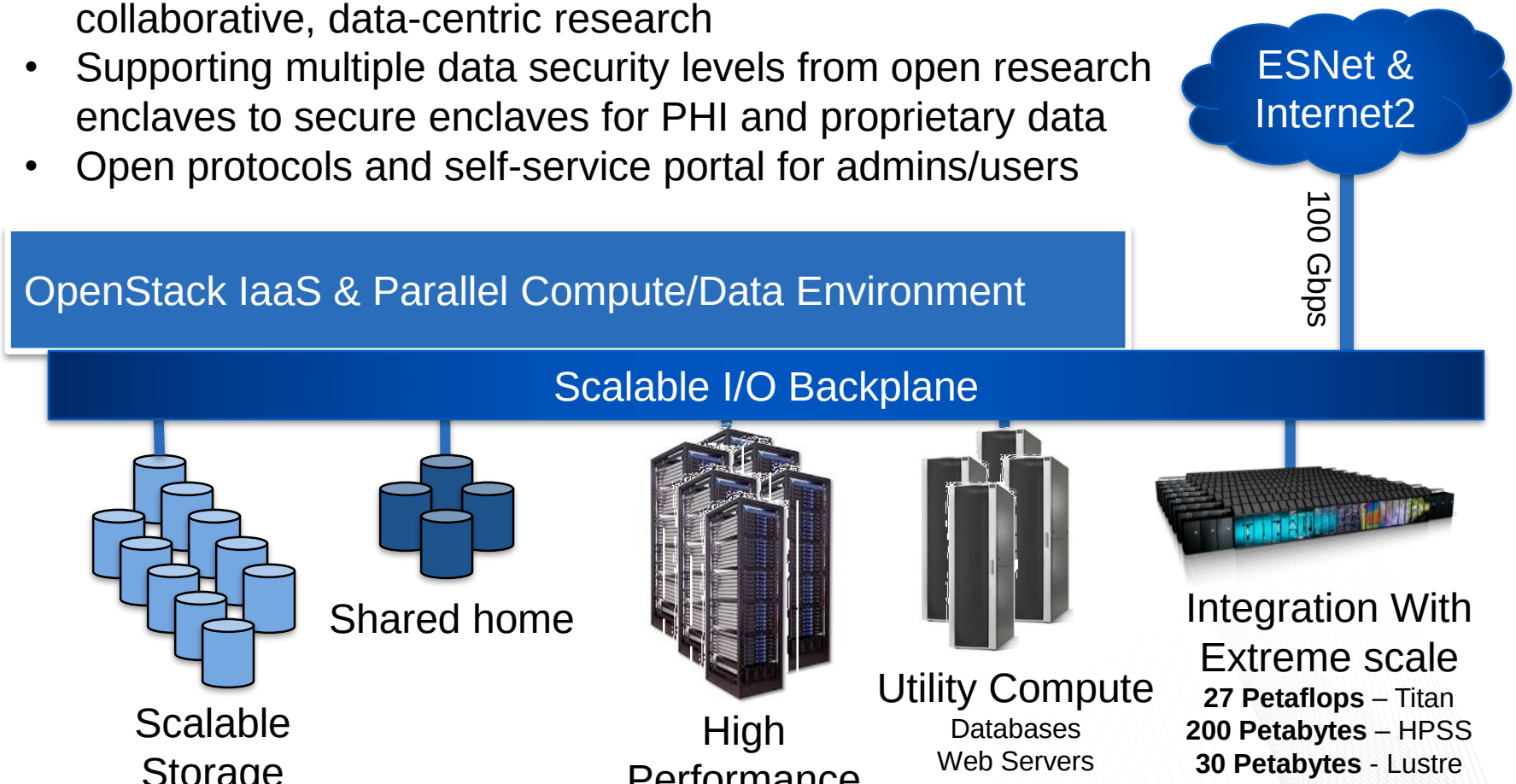
CADES
Compute & Data Environment for Science

NERSC

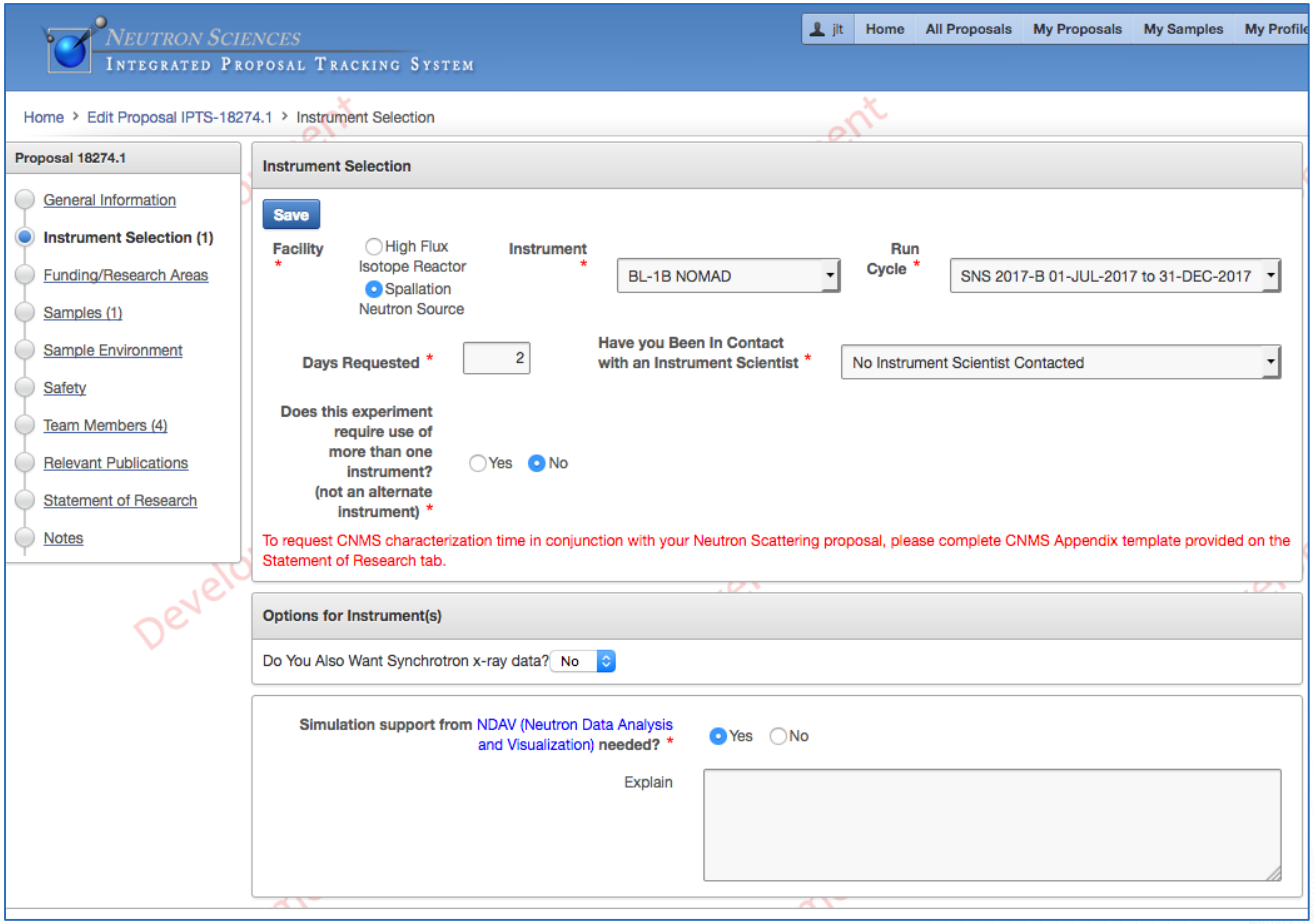
- Plan to allow users to specify computing and modeling needs as part of the beamtime proposal

CADES Cloud Initial Infrastructure

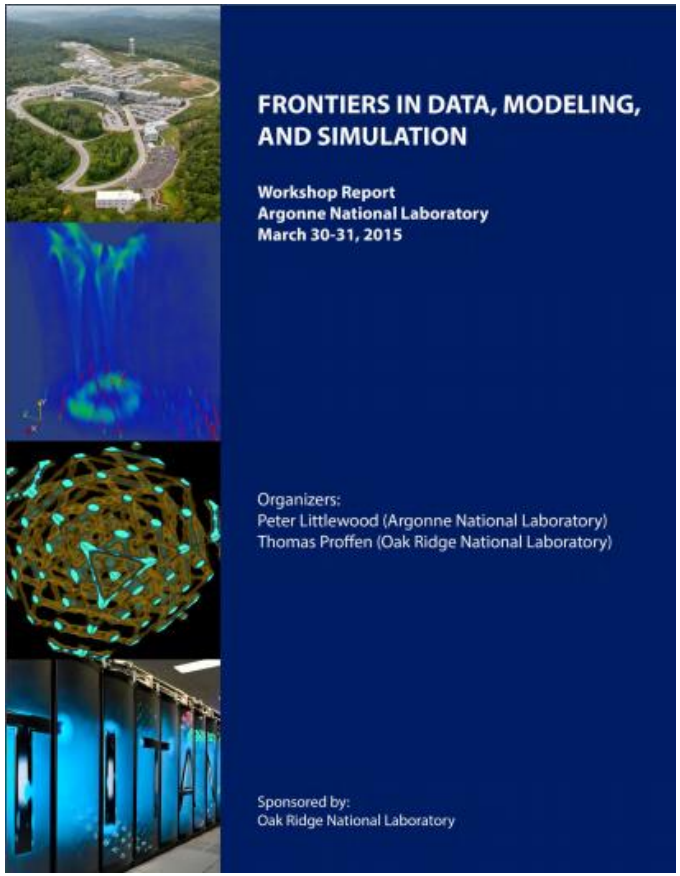
- A Data Intensive computing environment serving multiple projects and use cases
- A rich software stack enabling highly integrated, collaborative, data-centric research
- Supporting multiple data security levels from open research enclaves to secure enclaves for PHI and proprietary data
- Open protocols and self-service portal for admins/users



Users can indicate need for simulation support in IPTS



Workshop report “Frontiers in Data, Modeling and Simulation” published



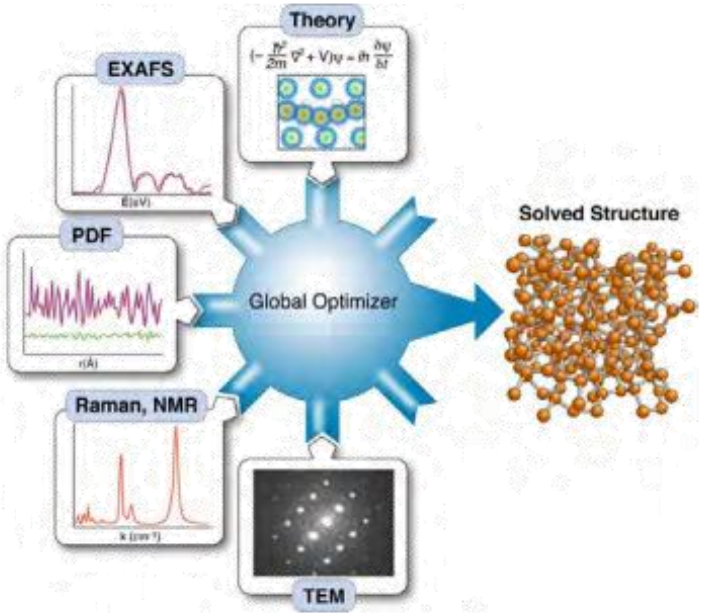
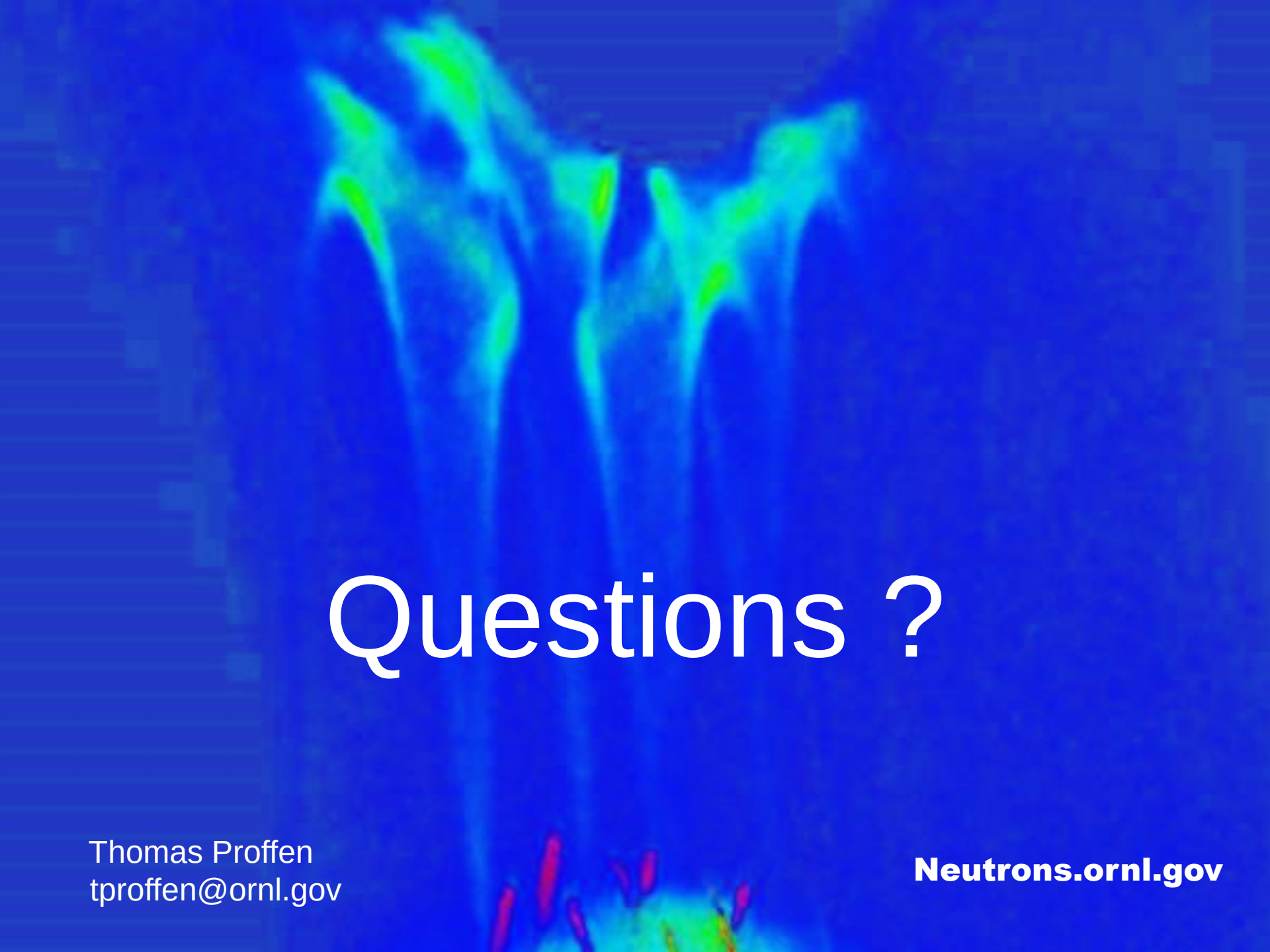


Figure 7. Schematic of the Complex Modeling Optimization paradigm of combining heterogeneous data sources to constrain a unique solution to marginally posed inverse problems, in this case the nanostructure inverse problem.

http://neutrons.ornl.gov/grand-challenge-workshops



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