Future direction and current capabilities of FTS software

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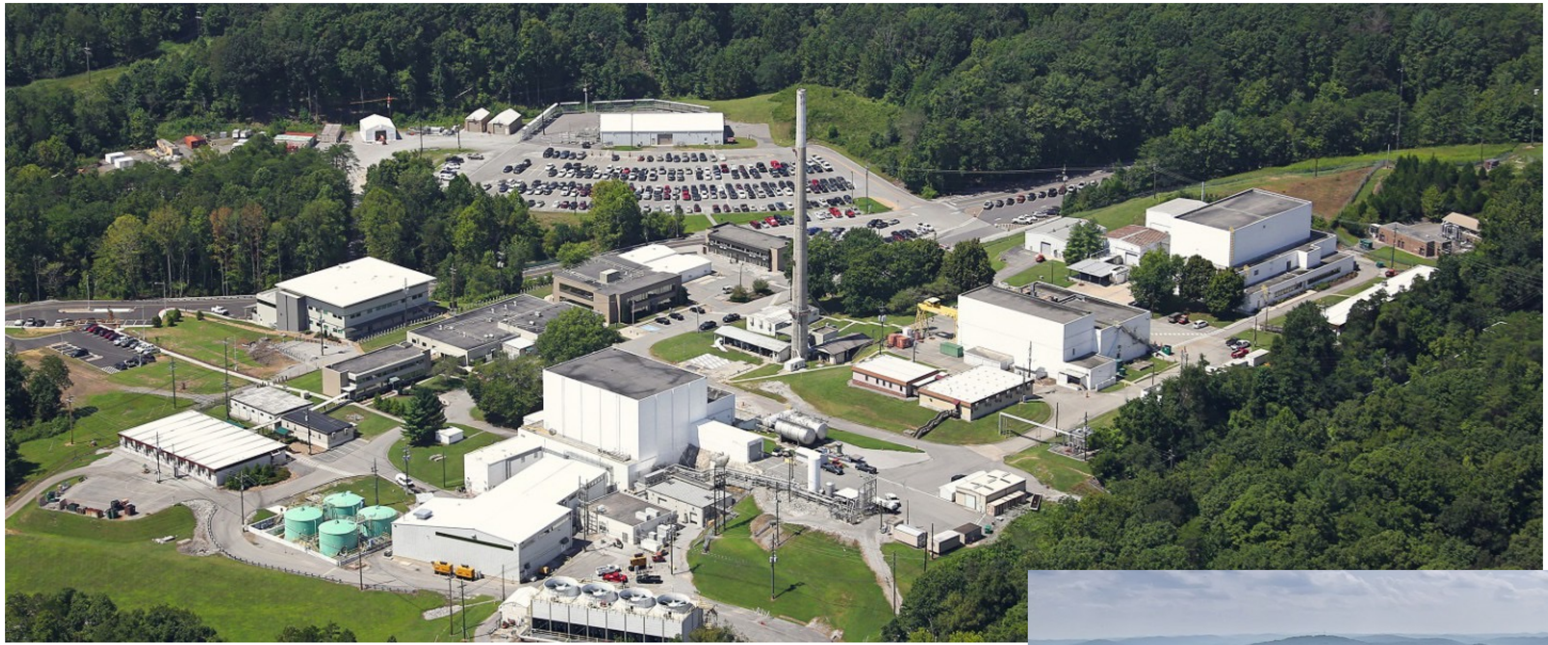
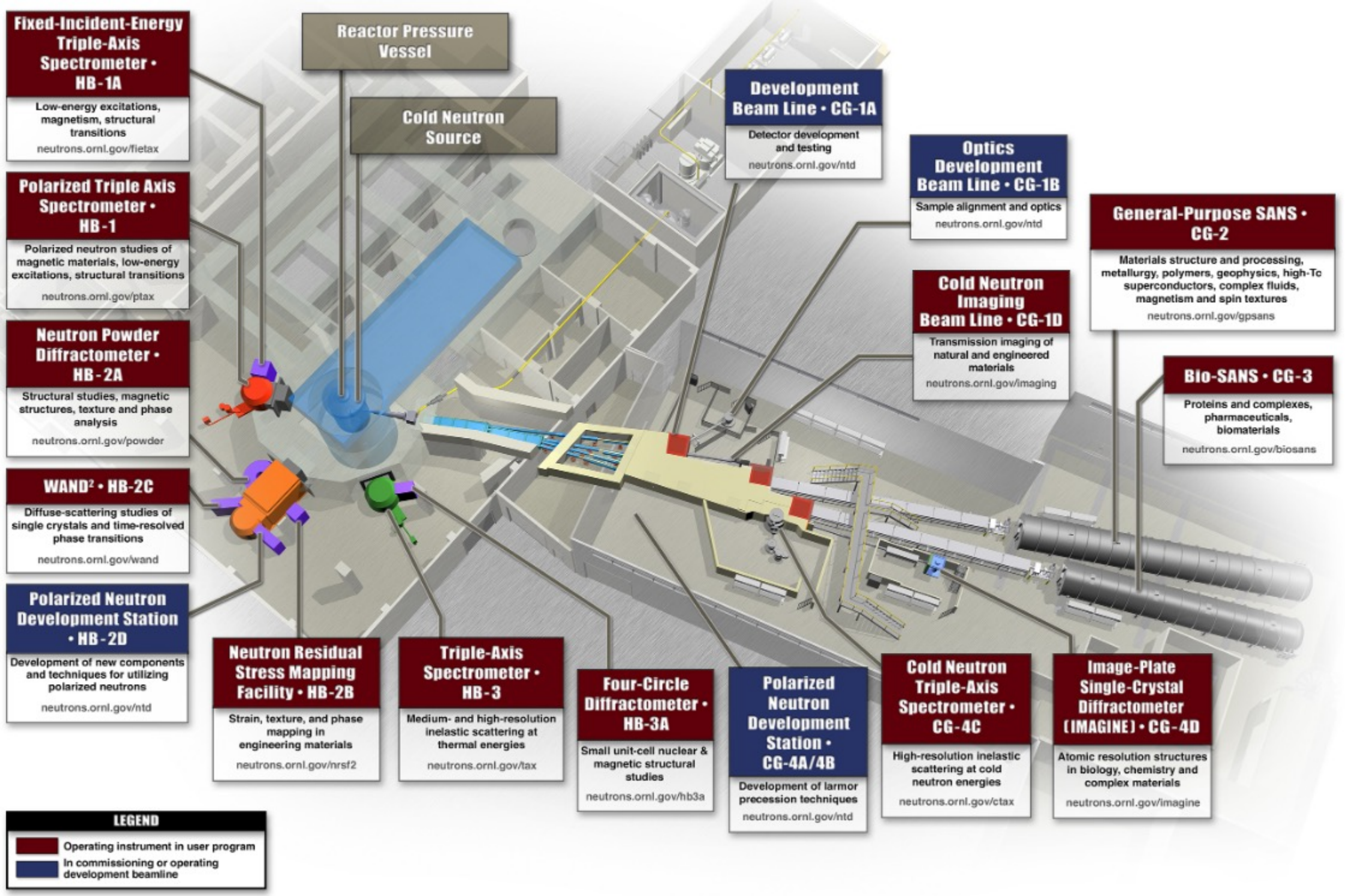
Neutron Sciences Directorate User Facilities



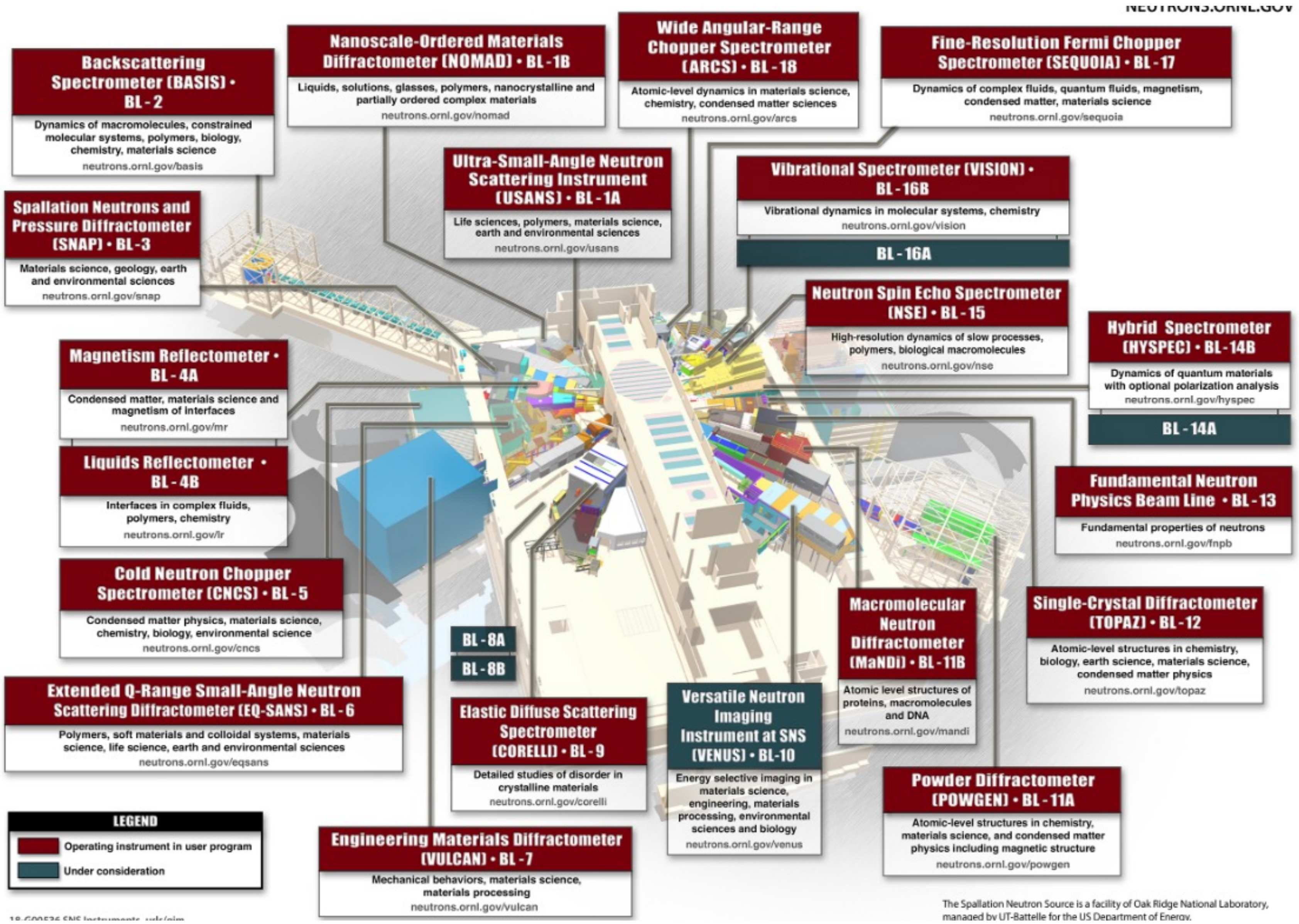
High Flux Isotope Reactor
(HFIR)

Spallation Neutron Source
(SNS)

Beamlines at HFIR



Beamlines at SNS



NScD facility user workflow – happy path

1. Come up with an idea
2. Write a beamtime proposal
3. Create "detailed" experiment plan
4. Measure data
5. Reduce data (remove instrument specifics from measurement)
6. Analyze data (gain insight)
7. Publish paper

Advancing all elements of the neutron data life cycle at SNS and HFIR

Acquisition

Data acquisition and instrument controls software upgrade

ADARA enabling streaming and live data

Reduction

Data reduction in *Mantid*

Automatic data reduction and web monitoring

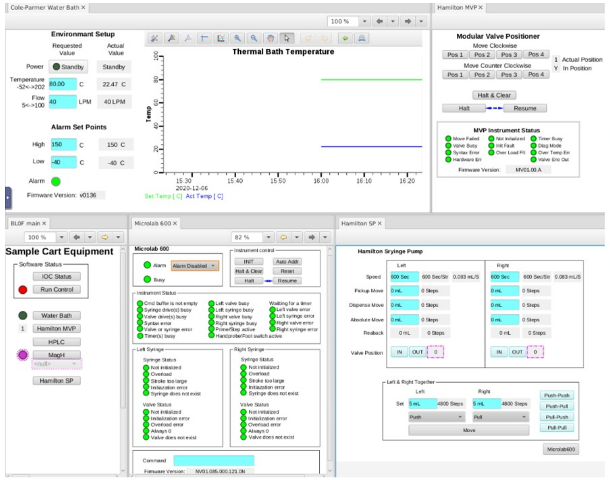
Visualization

Analysis, Modeling & Simulation

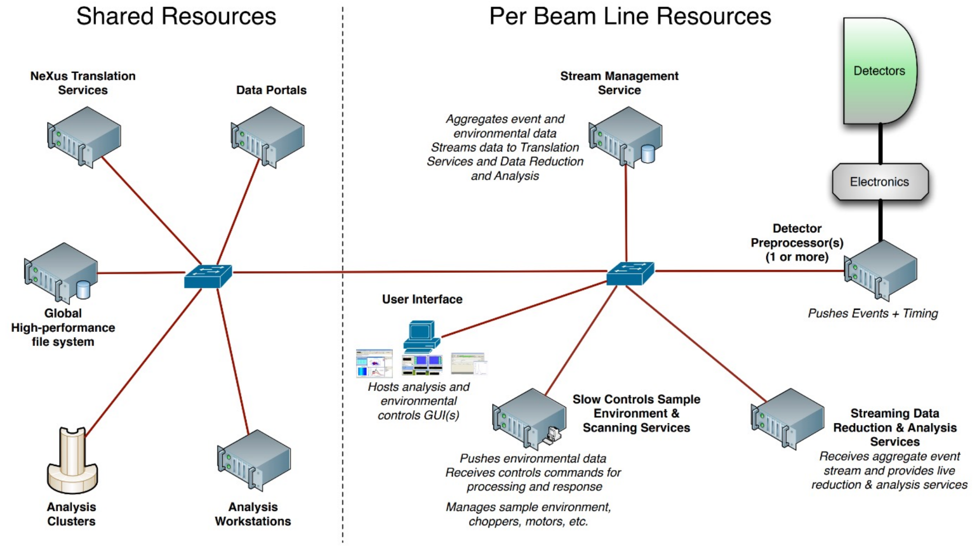
Partnering with community on development of analysis codes

Connecting to advanced materials modeling using HPC

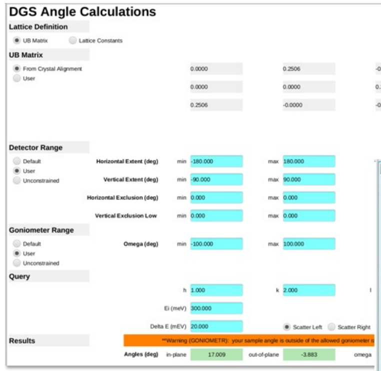
DAQ & Controls



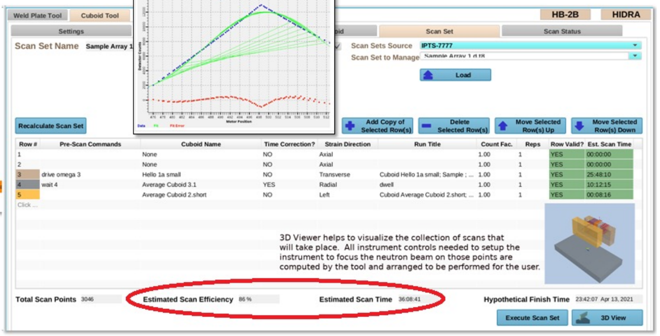
Mobile Sample Environment Controls interface



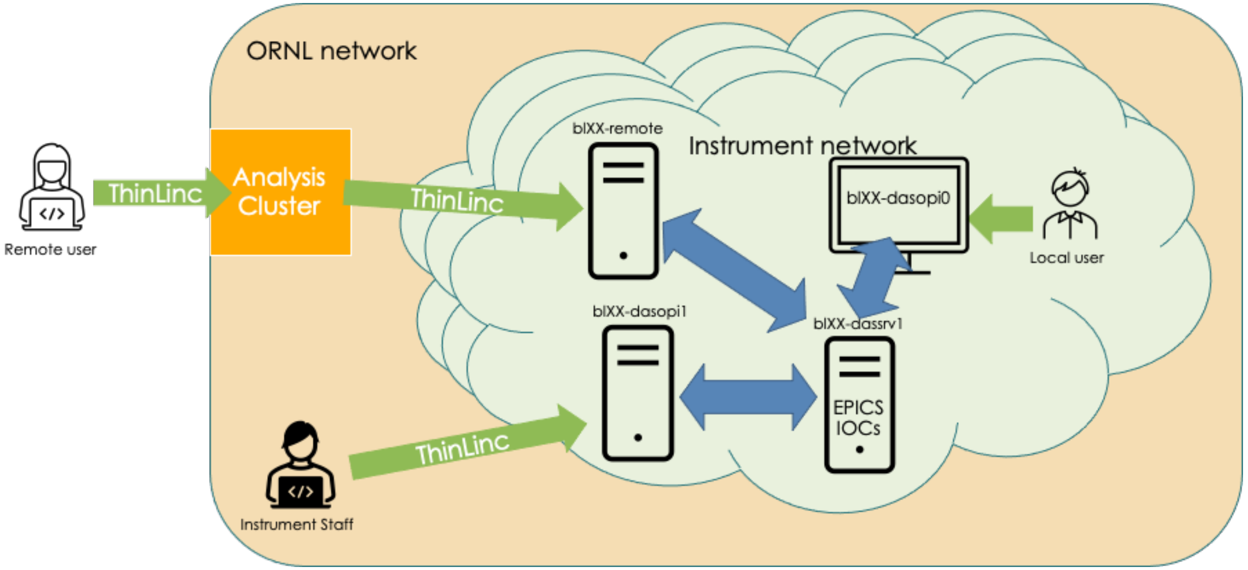
DAQ & Controls Architecture for SNS Instruments



Save users' time and increase efficiency of neutron beam time used.



Tools to scan the instrument in scientific coordinate systems.

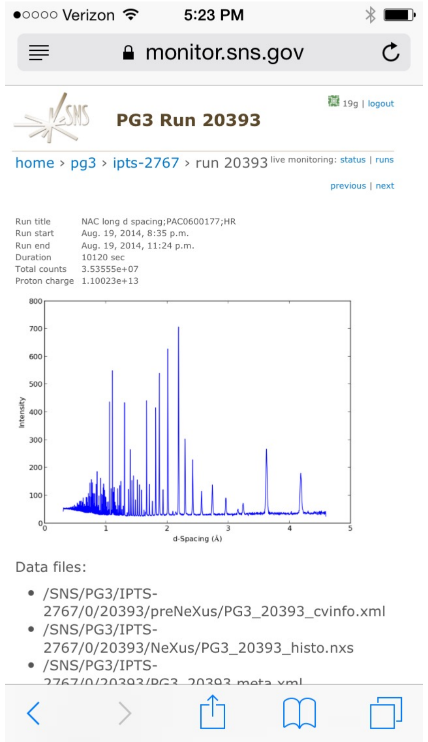


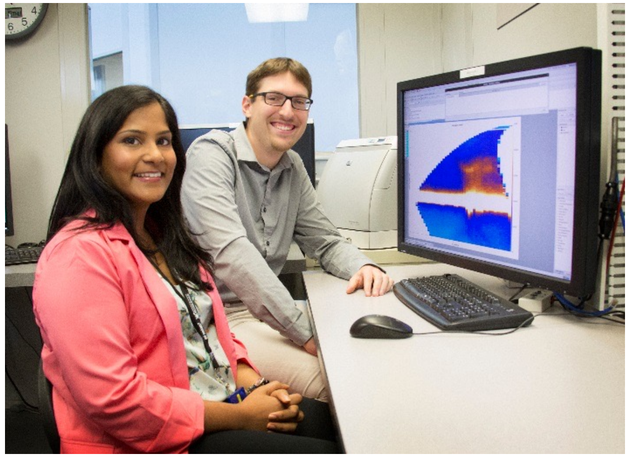
Experiment planning tools within the experiment control interface

Architecture for **Full remote control** of Beamlines

Live data and automatic reduction provide easy access to reduced data

- Automatic data reduction available on all SNS beam lines.
- Users have immediate access to data in meaningful instrument independent units after a run is finished.
- Interactive plotting under development.
- Remote access through website http://monitor.sns.gov





- Dalini Maharaj and Edwin Kermarrec from McMaster University look at live data of Ba_2YOsO_6 on SEQUOIA
- ADARA project enables viewing of data in user defined coordinates in real time

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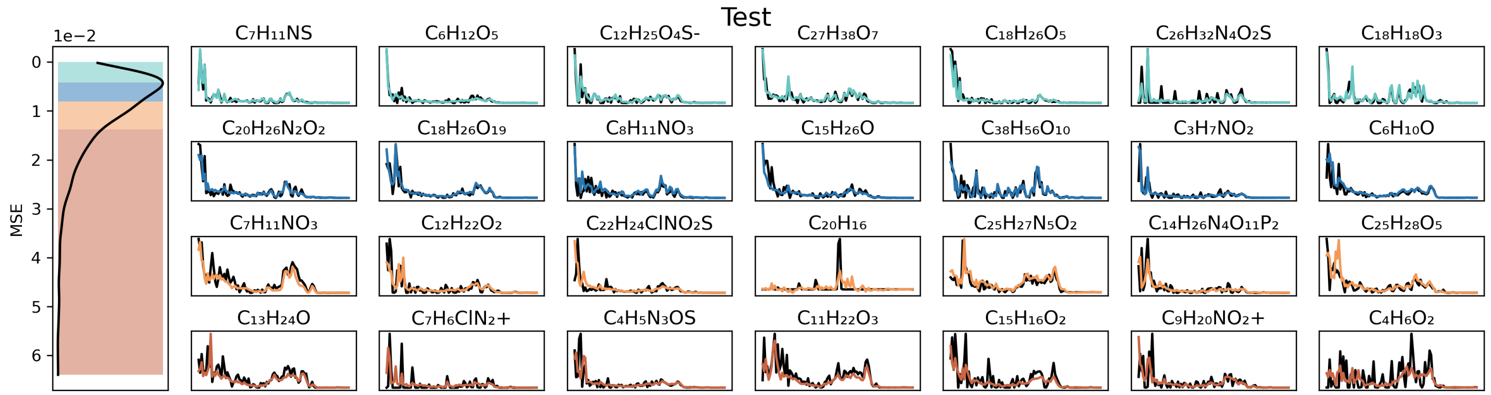
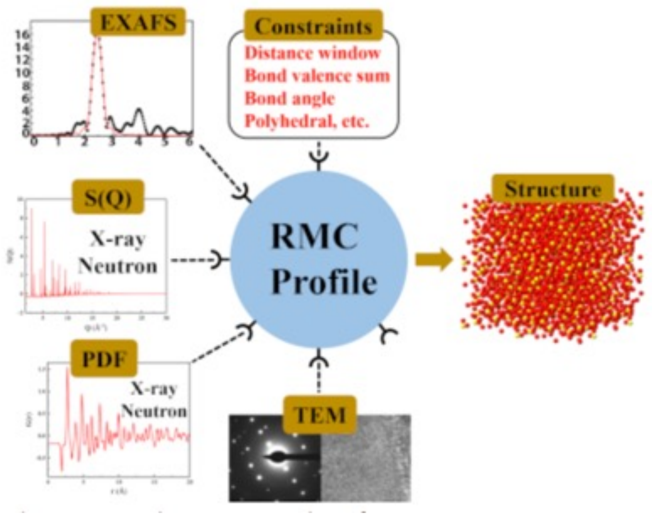
Data Analysis Plan

- Response to the Review of Data Reduction, Handling and Analysis.
- Development of **first** strategic plan for data analysis.
- Plan will identify priority areas and funding will be allocated using the established science productivity review process.
- Plan is a "***living document*** *that will evolve over time, it is important to initiate the process with a well-thought-out strategy, buy-in from the user community, and clear understanding of priorities ..*"
- Critical to our future and to maximize science knowledge from neutron scattering.

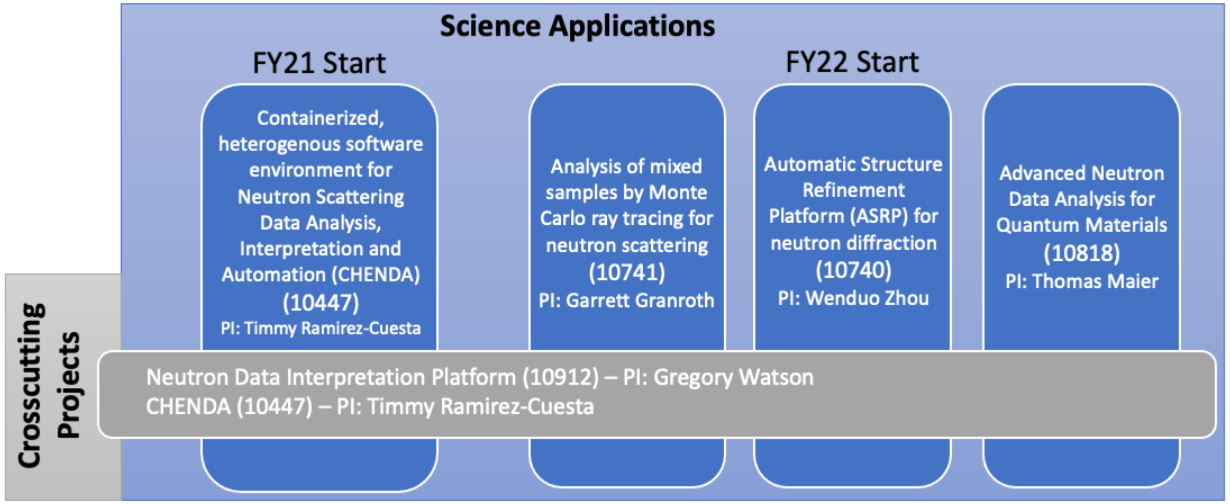
Data analysis examples



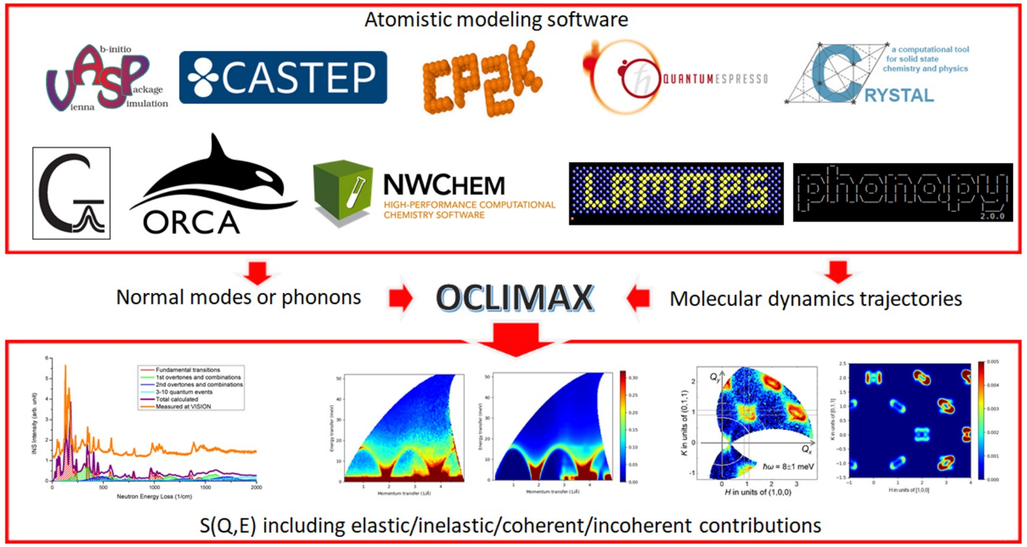
LDRD funded research to develop ML/AI systems for chemical spectroscopy - CNN developed to predict spectroscopic data from crystal structure



RMCProfile for total scattering data analysis



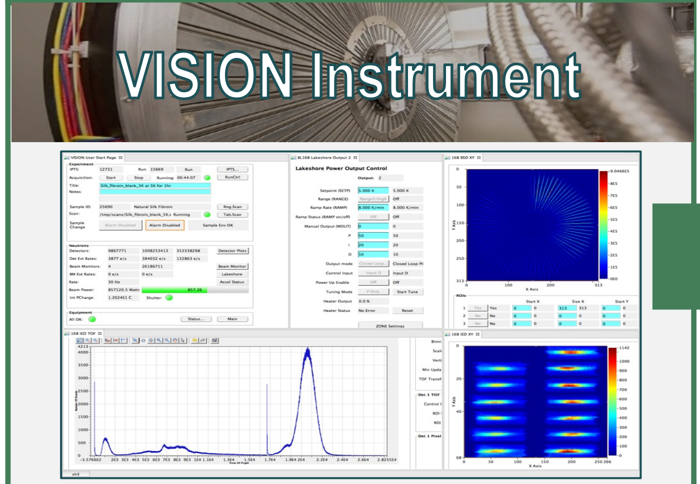
LDRD funded Neutron Data Interpretation Platform
- UI for workflow management & plugins for selected science impact areas.



OCLIMAX code integrates HPC into the analysis workflow for chemical spectroscopy

Workflow from data collection, reduction and analysis to modeling enabling automation and advanced analysis

Data acquisition Instrument control

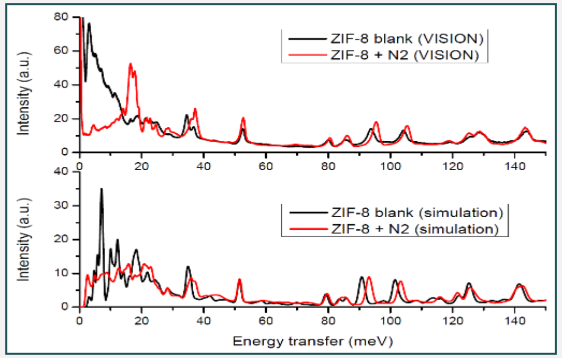


control system studio

ADARA

EPICS

Automatic Data Reduction



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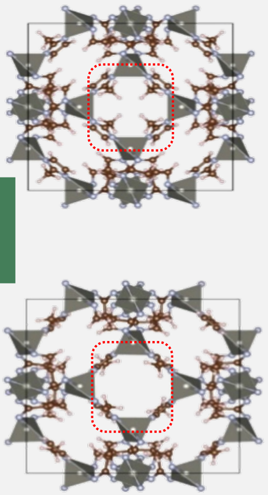
Data Analysis & Materials Modeling



VirtuES Cluster

ACUMEN

CADES
Compute & Data Environment for Science

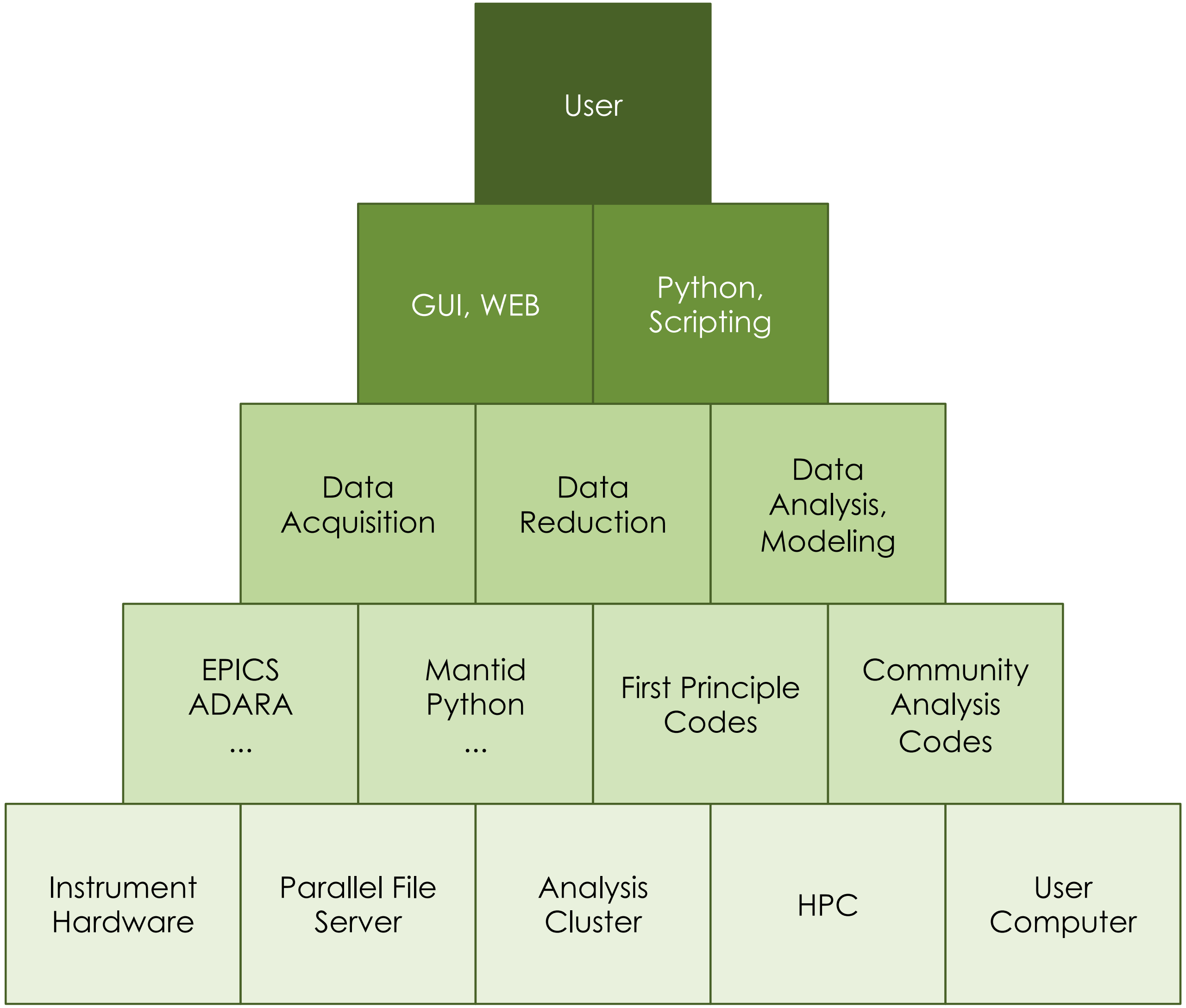
Experiment steering
Human or automatic

Refinement

Data published in M.E. Casco, Y.Q. Cheng, L.L. Daemen, D. Fairén-Jiménez, E.V. Ramos-Fernández, A.J. Ramirez-Cuesta, and J. Silvestre-Albero, Chem. Comm. (2016) 52, 3639

ICEMAN

Designing for the future



- **Algorithm development** and R&D in close collaboration with mathematicians, theorists and modelers.
- Create **code base** that can leverage current and future computing and HPC architectures as needed.
- **Workflow engines** and **web based user interfaces**.
- **Seamless integration** of instrument control, DAS, reduction and analysis & modeling for feedback & steering.

Future opportunities & (some) Lessons Learned

- Strategy to provide infrastructure and support to ensure users leave facility with reduced and analyzed data.
- Leverage current and future research for ML/Ai for the neutron science program.
- Move towards a data pipeline approach.
  - DAQ and data reduction can be combined allowing closer to real-time visualization.
  - Concept can be extended into analysis for certain "standard" cases – ML/AI could help here.
- Scientific computing is an investment.
  - Emphasis should be placed on affordability, production quality and UX.
  - Code bases that are large are expensive to maintain and that limits headroom.
  - Leverage community collaboration – understand this too comes at a cost.
- Support for operations limits flexibility for maintenance and refactoring code.
  - If underlying performance becomes an issue, it is slow to rectify.
  - Use construction phase schedule wisely.
- Carefully plan where event mode data collection is used.
  - A single raw data file of event list data can be cumbersome to process and manage.
  - Not all experiments benefit from event mode data for analysis.