

# DANSE and Neutron Scattering at ORNL

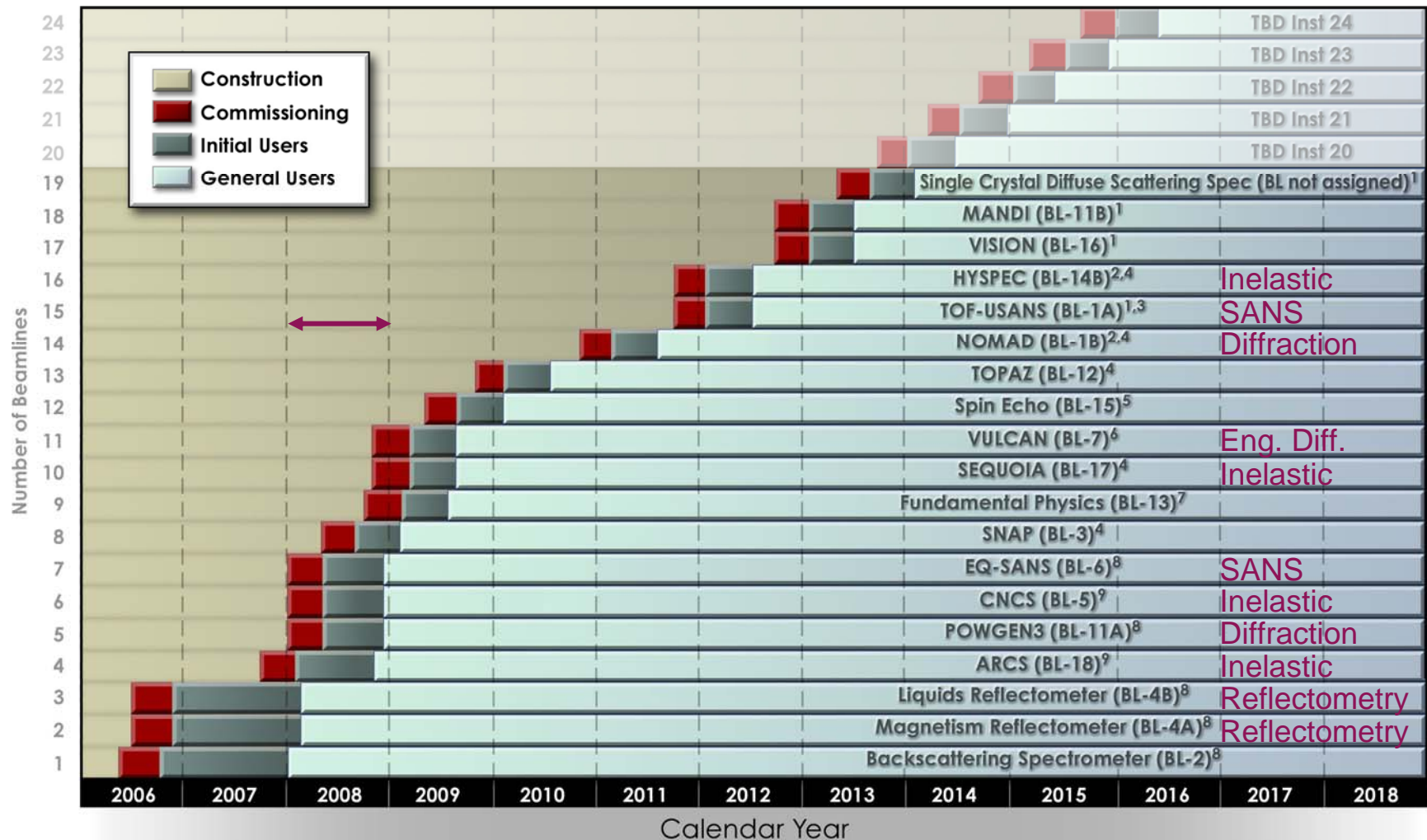


**Ken Herwig**  
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**Neutron Scattering Science Division**  
**Oak Ridge National Laboratory**

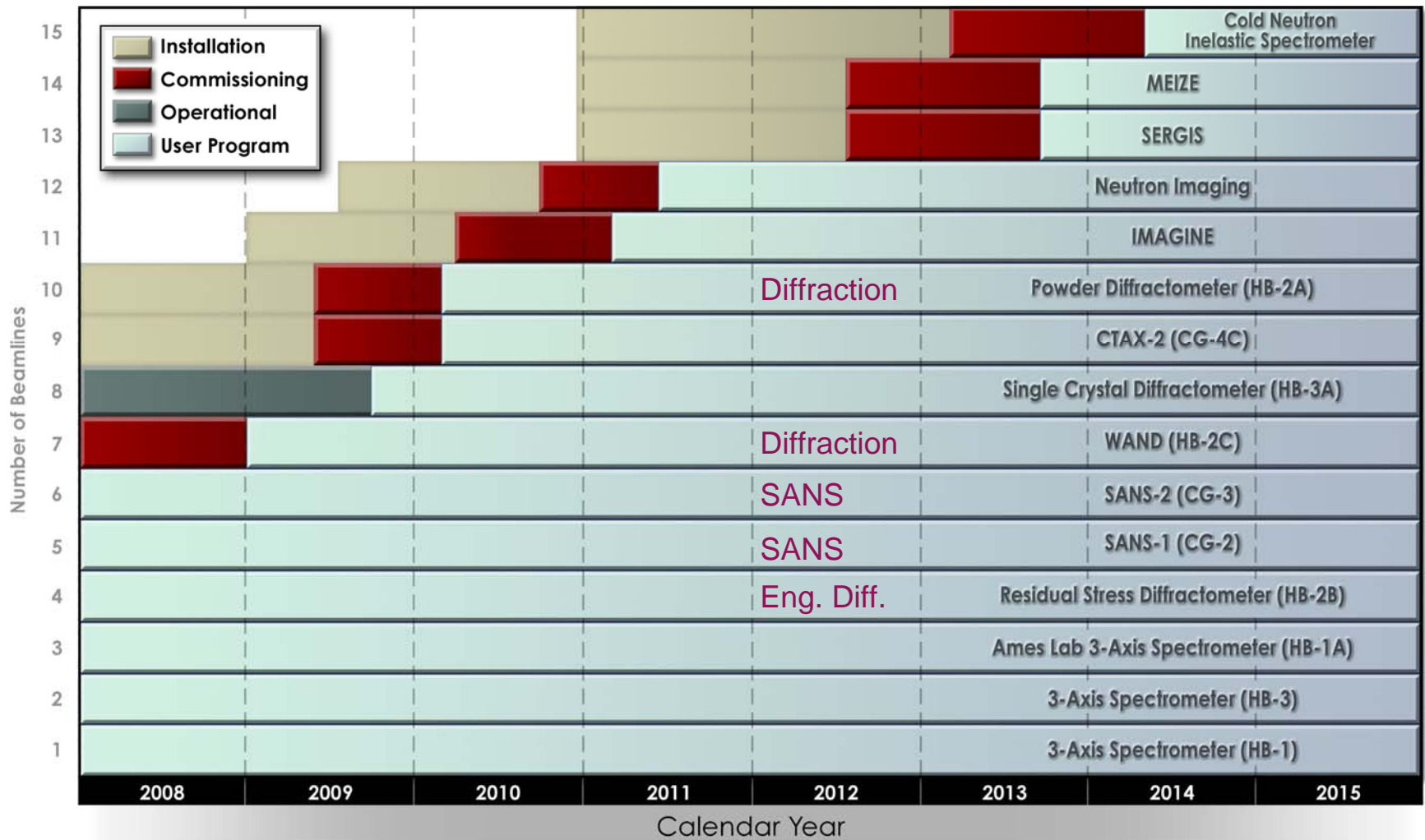
# SNS and DANSE Partnership

- **SNS relies on DANSE for advanced science applications for analysis of neutron scattering data**
- **DANSE represents a key partnership with the Neutron Scattering User Community**
- **Interactions**
  - **SNS will host individual DANSE science teams this summer – dialog and demonstration**
  - **SNS representative participates in Friday DANSE management teleconference**
  - **7 DANSE team members have UCAMS (ORNL domain access) and others have XCAMS (general user access)**

# Commissioning SNS Instruments – 2008 is a banner year

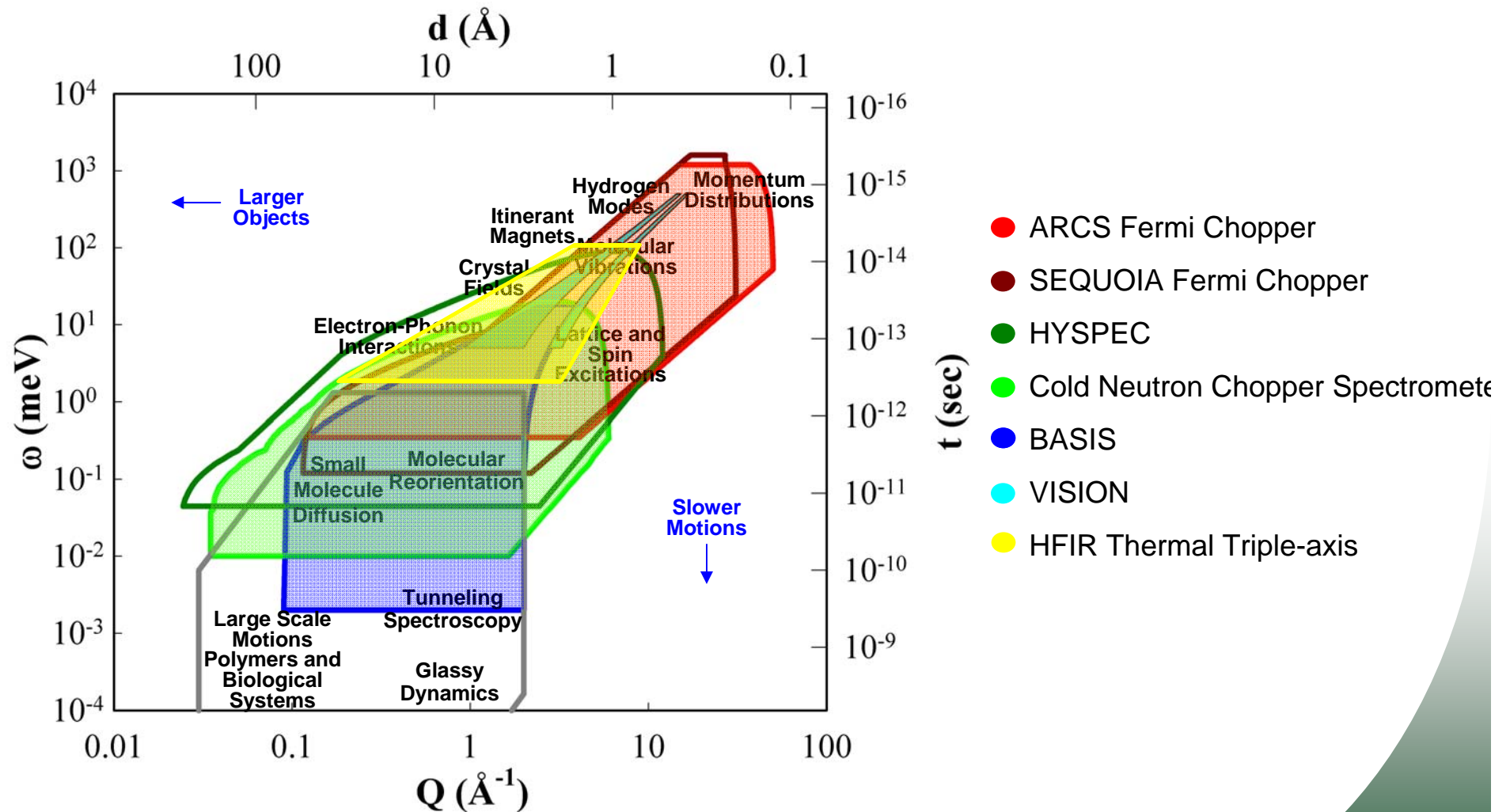


# New Instruments in the User Program at HFIR

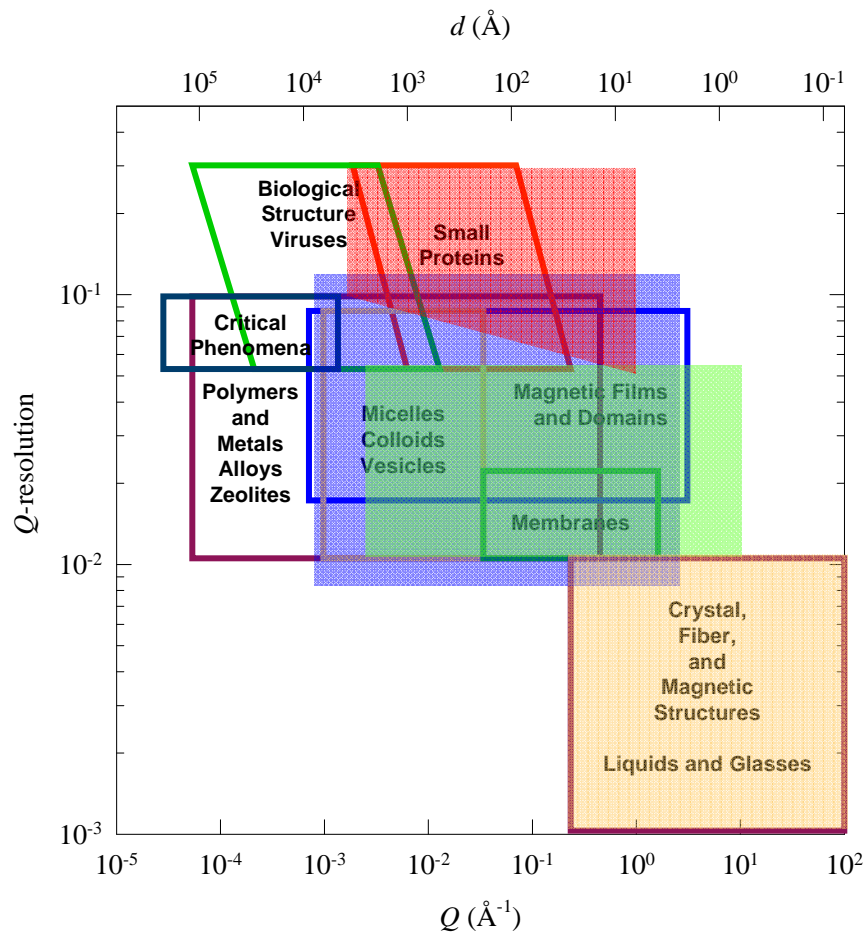


07-G01412A/arm

# The ORNL Inelastic Instrument Suite Will Cover the Dynamics Landscape Within 2008



# Building Science Capabilities in the ORNL Elastic Instrument Suite



- **Liquids Reflectometer**
- **Magnetism Reflectometer**
- **HFIR SANS**
- **SNS EQ-SANS**
- **Diffractometers:**  
**WAND, SNAP, HFIR NRSF2,**  
**POWGEN**  
**HFIR Powder, Vulcan**

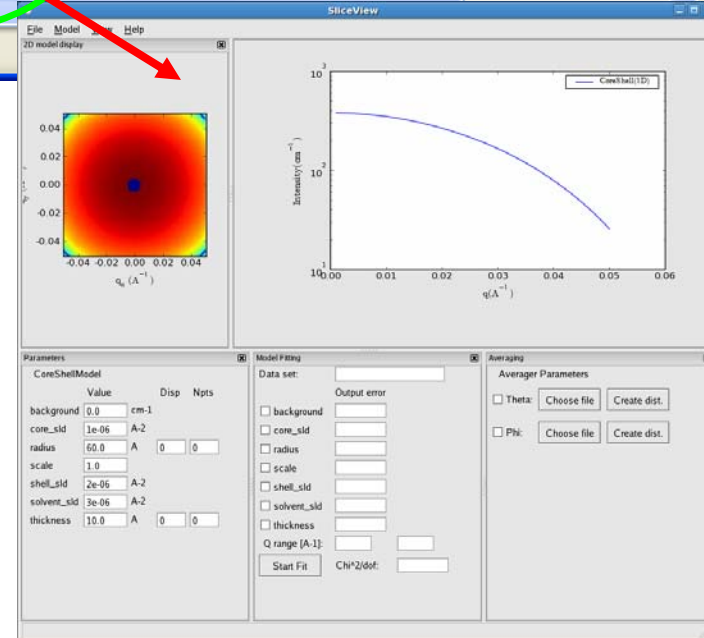
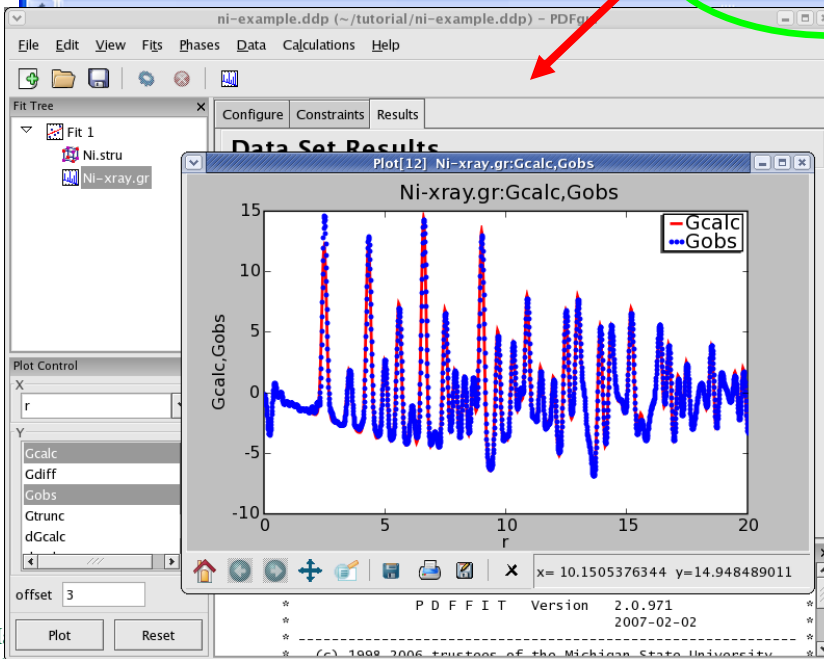
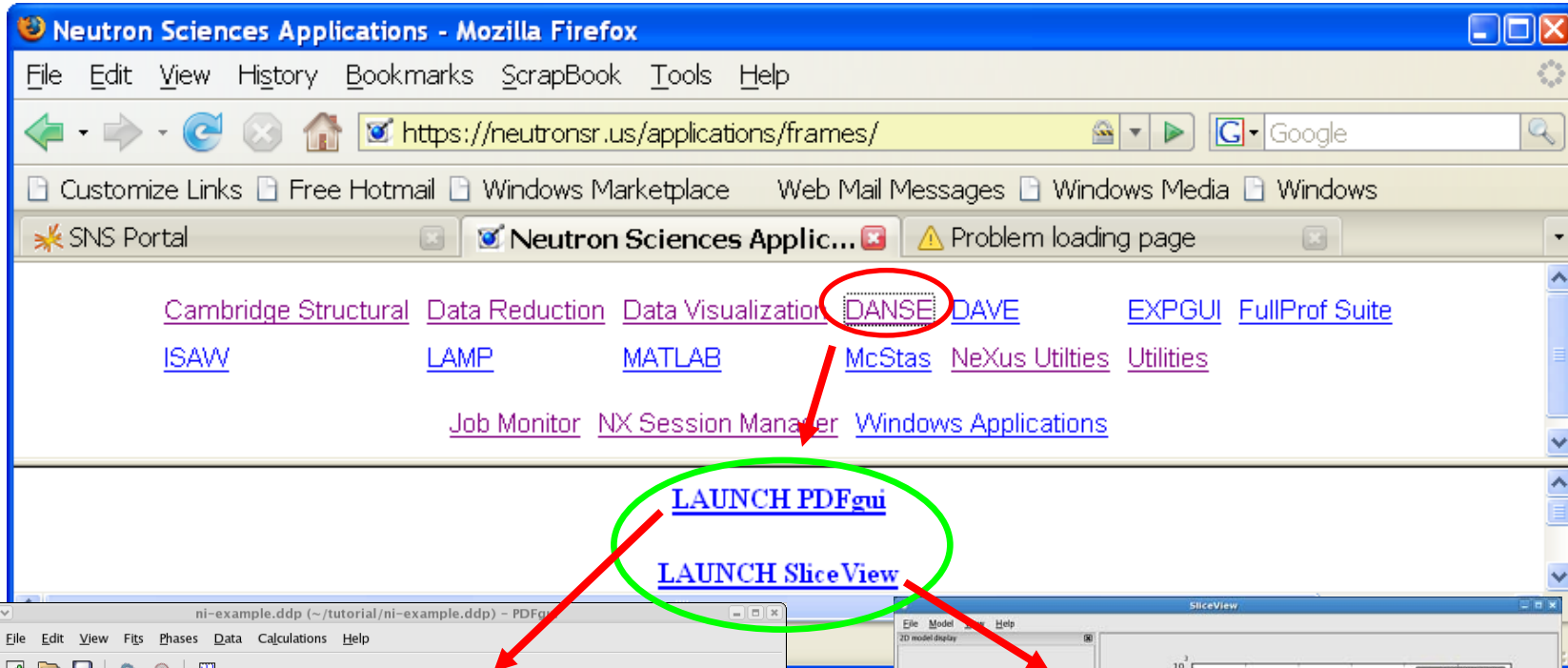
# SNS Delivering Computing Infrastructure to Meet Current Instrument Needs

- **Data Management**
  - Access
  - Archive/catalog
  - Provide common work space for collaborations
- **Data Reduction**
  - Backscattering (BASIS) – crystal analyzer
  - Reflectometers
  - ToF-SANS
  - Diffraction – via ISAW tool
  - Observations
    - Iterative Process – strong engagement with Instrument Team
    - Large data sets and execution speed are issues
- **Analysis Portal**
  - Hosting applications
  - Instrument simulations

# Opportunities that need to be addressed

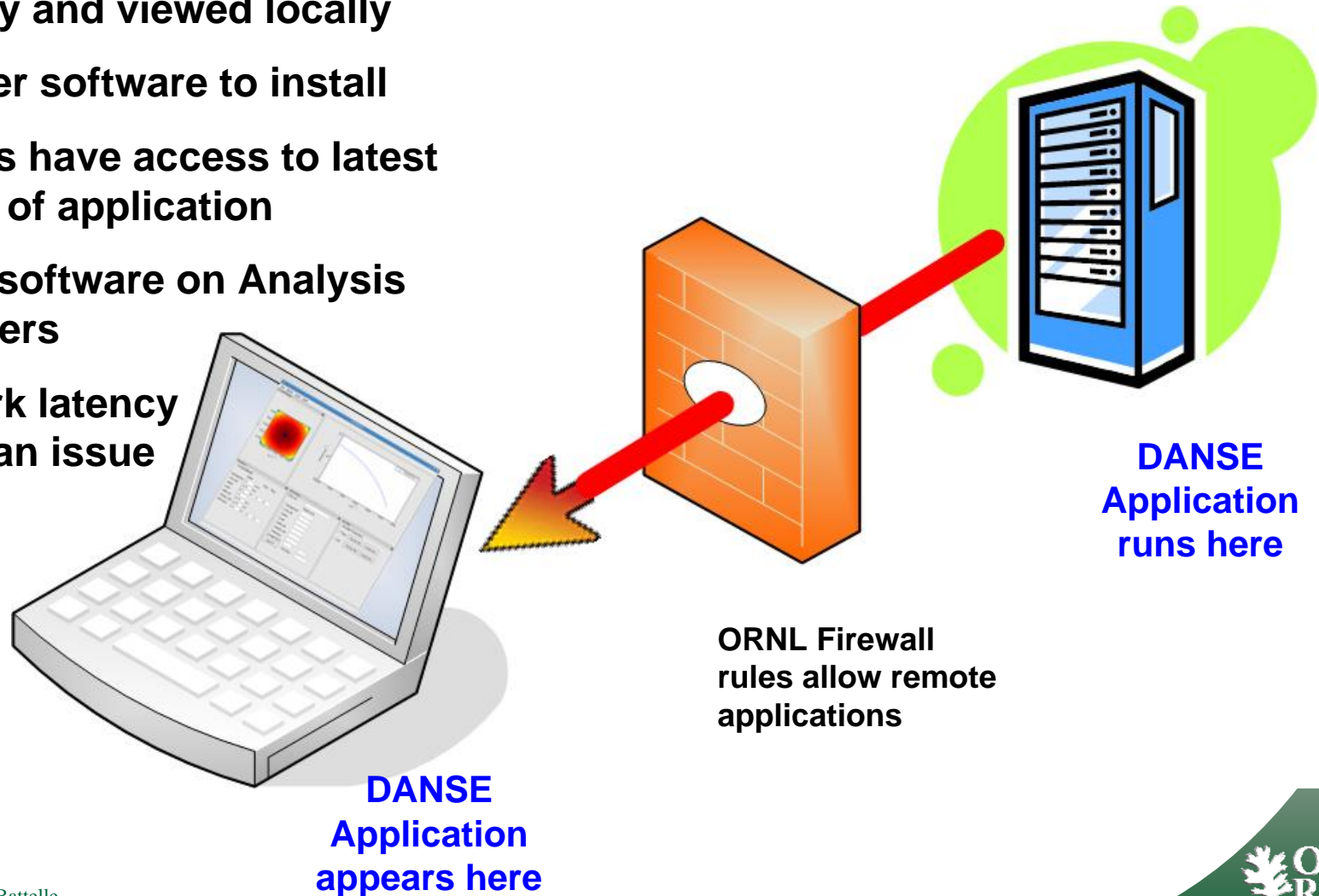
- **Single Crystal**
  - Elastic – diffraction
  - Inelastic – collective excitations
  - Diffuse – Corelli (2013)
- **Chemical Sciences Applications**
  - Chemical Spectroscopy – Vision (2011-2012)
  - Quasielastic Neutron Scattering (BASIS and CNCS)
- **Liquids/Amorphous Materials Diffraction**
  - Enormous data sets
  - Sophisticated data corrections
- **Future**
  - Neutron spin-encoded techniques – Neutron Spin Echo, SERGIS
  - Neutron Imaging/Tomography – (commercial visualization software?)

# DANSE Applications in Portal



# Remote Applications – Thin Client

- In use today!
- Applications hosted remotely and viewed locally
- No user software to install
- Always have access to latest version of application
- Same software on Analysis computers
- Network latency can be an issue



# Work In Progress – Web Services

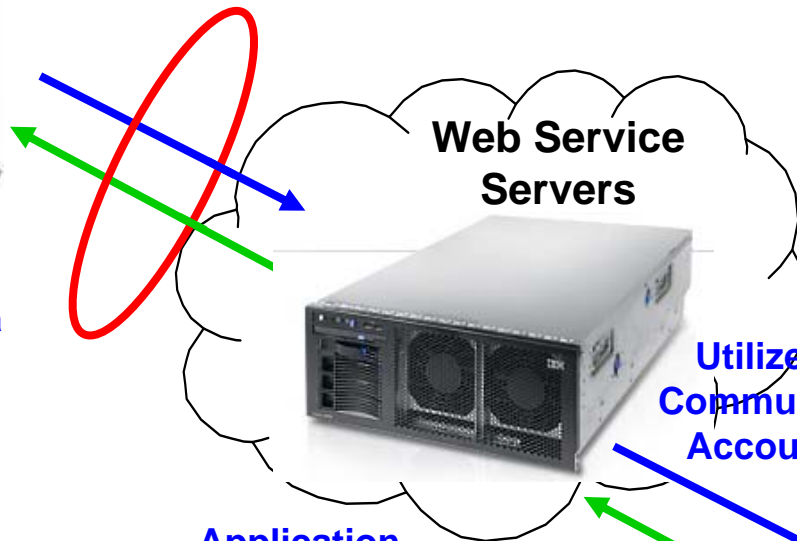
## Web Service enabled application



### Thick Client:

- User needs to install a “thick client” or a DANSE WS enabled application
- Work locally
- Utilize remote applications as desired
- Can access data remotely
- Virtual Organizations facilitate collaboration

ORNL Firewall



Web Service Servers

Utilizes Community Account

### Application Manager:

- Aware of which jobs it can manage
- Decides where to run jobs
- Manages data movement
- Provides monitoring info

Utilization of National Cyber-Infrastructure resources to serve neutron scattering scientific research

Backend compute resource

DANSE processing software installed



# Hardware Infrastructure

- **Oak Ridge Institutional Cluster**
  - 28 nodes, 8 cores/node
  - 16 GB/node
  - Linux
- **Compute Servers**
  - 8 and 16 processors with up to 56 GB
- **TeraGrid**
  - Local 32 node cluster
  - Small allocation on grid at large
- **FY09 – Provide a development platform to facilitate migration of DANSE software to ORNL for users**
  - Adapt to ORNL architecture
  - Promote collaboration
  - Migrate applications to more computer power as appropriate - OIC



# Summary

- **SNS relies on DANSE to provide advanced analysis software**
- **Increased engagement with DANSE science teams and SNS/HFIR Instrument scientists is in progress**
- **DANSE migration to ORNL**
  - **SNS is committed to hosting DANSE software**
  - **SNS will provide the hardware infrastructure suited to deploying DANSE software**
  - **SNS will support continued development and maintenance of DANSE software**
- **DANSE is one of our key partnerships with the Neutron Scattering User Community**

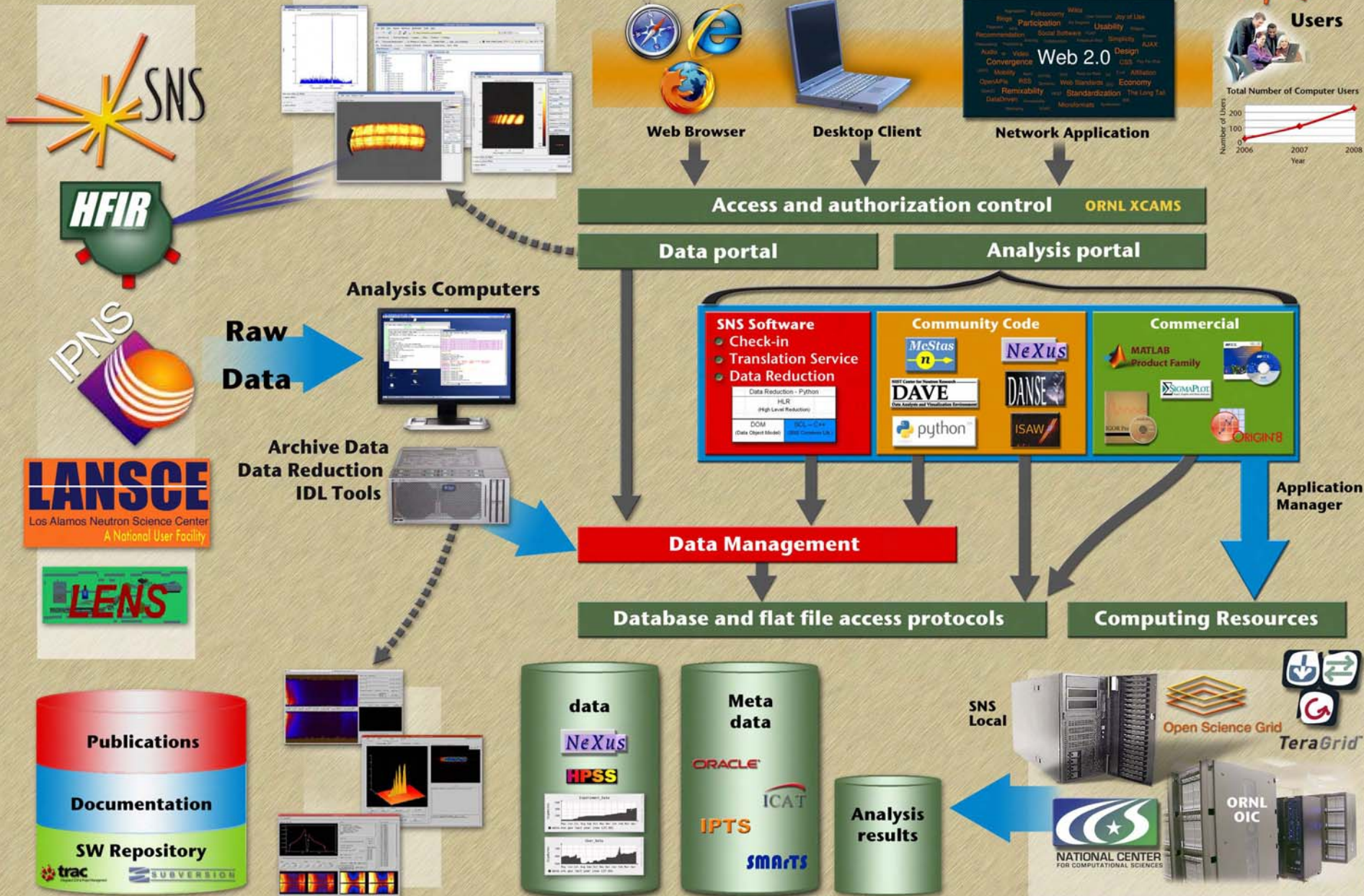
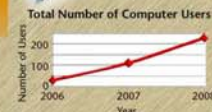


[neutrons.ornl.gov](http://neutrons.ornl.gov)

# Backup Material



Users





# Data Search

**Search Criteria**

SNS REF\_L Search Reset

file\_name proposal... Search C... Search C... Search C... Search C... Search C...

.nxs 225

**Search Results**

URI	file_name	TITLE	SAMPLE...	CREATE...	INSTRUME...	FILE_NA...	PROPOSAL...	FORMU...	PI
/SNS/REF_L/IPTS-225/4/4119/NeXus/REF_L_4119.nxs	proposal_id	As Cast...	PVDMA Fil...	2007-08-...	REF_L	REF_L_...	IPTS-225		
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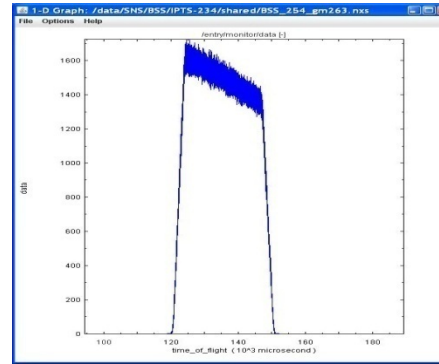
StatusBar

[Security Notice](#)

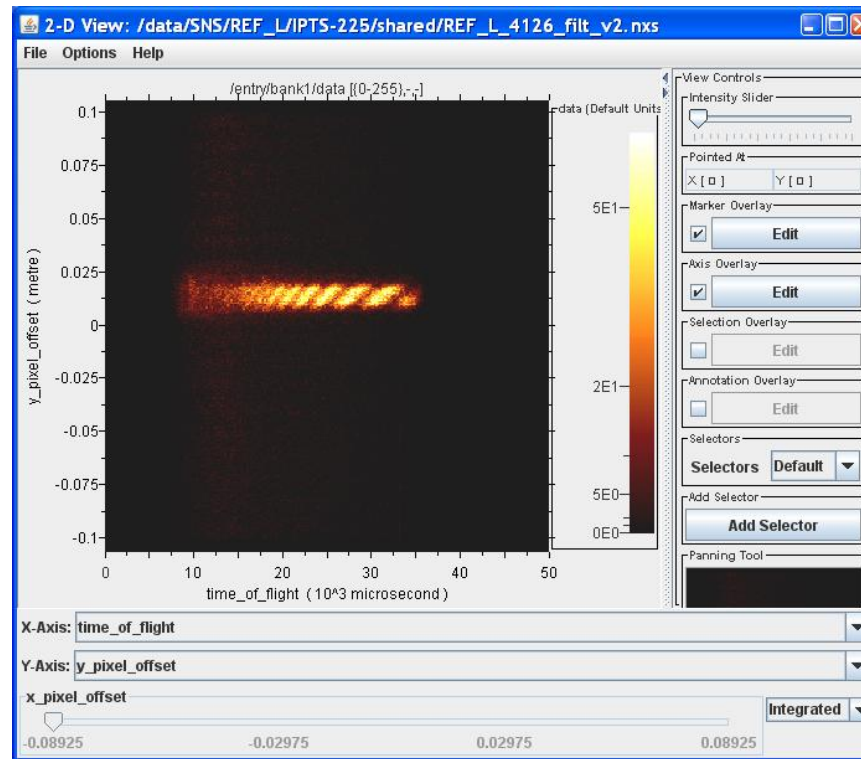
Applet gov.ornl.sns.portal.PortalApplet started neutrons.ornl.gov

# Data Visualization

- Visualization
- Table
- 1-D Graph
- 2-D View
- 3-D Volume



Monitor data for Backscattering Spectrometer

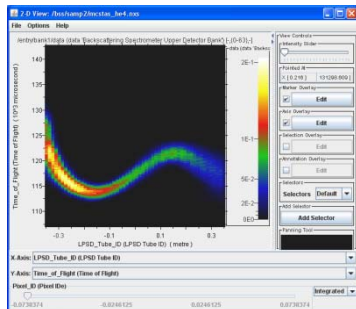


Reflectometer Y vs TOF data – integrated over X

- Re-host ISAW visualization tools within the portal
- Provide 1D, 2D, and table views
- “Portal backend” handles sending data to the visualization tool – sending all data can be too large!

# Simulation Portal Development

- **McStas simulation tool** available via portal, for simulating backscattering experiments
- **Utilizes community account on TeraGrid**
- **Produces NeXus files**
- **Simulation Tab**
  - Pull-down menu for selecting TeraGrid resources...
  - Set min/max/step input parameters

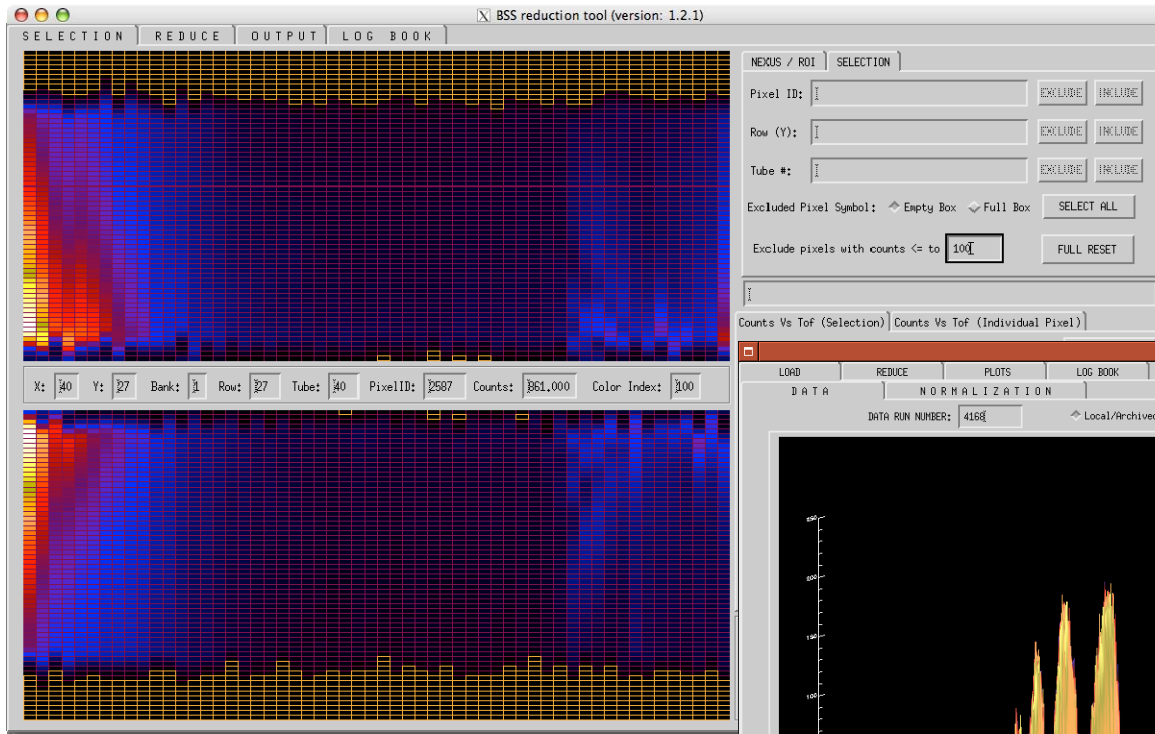


Simulation Tab

The screenshot shows the SNS Portal web interface in a Windows Internet Explorer browser. The URL is <https://snsportal.ornl.gov/snsportal/>. The 'Simulation' tab is selected and highlighted with a red circle and a red arrow. The interface includes a 'Resource Declaration' section with a '# CPUS' field set to 10 and a 'TeraGrid computer' dropdown menu set to 'tg-login.ncsa.teragrid.org'. Below this is a 'Moderator Source File' field containing 'source\_sct091\_tu\_02\_1.dat'. The 'Number of Neutrons' field is set to 1 e 7. The 'Energy Range' section has 'Min' set to 2 and 'Max' set to 2.16. The 'TOF Offset' field is set to 0. The 'Reusing Neutrons' section has 'Max Number to Reuse' set to 1 e 10 and 'Rep Count' set to 100. A 'Run' button is visible at the bottom of the configuration area. The status bar at the bottom indicates 'Applet gov.ornl.sns.portal.PortalApplet started' and 'Local intranet'.

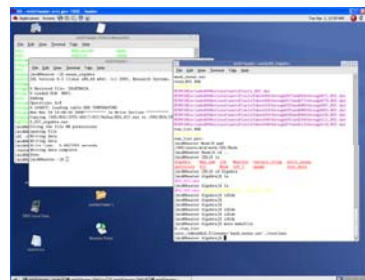
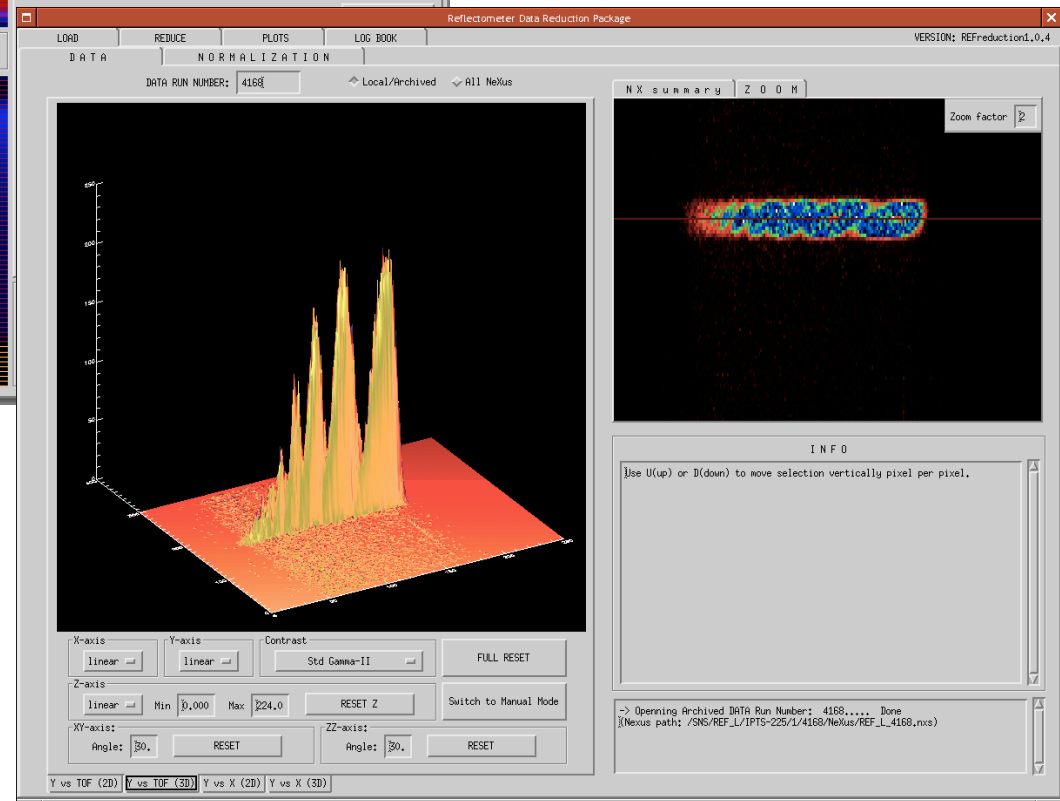
# Data Reduction – Local and Remote

## Backscattering Data Reduction



SNS has been developing data reduction software as needed.

## Reflectometry Data Reduction



NoMachine client and desktop applications