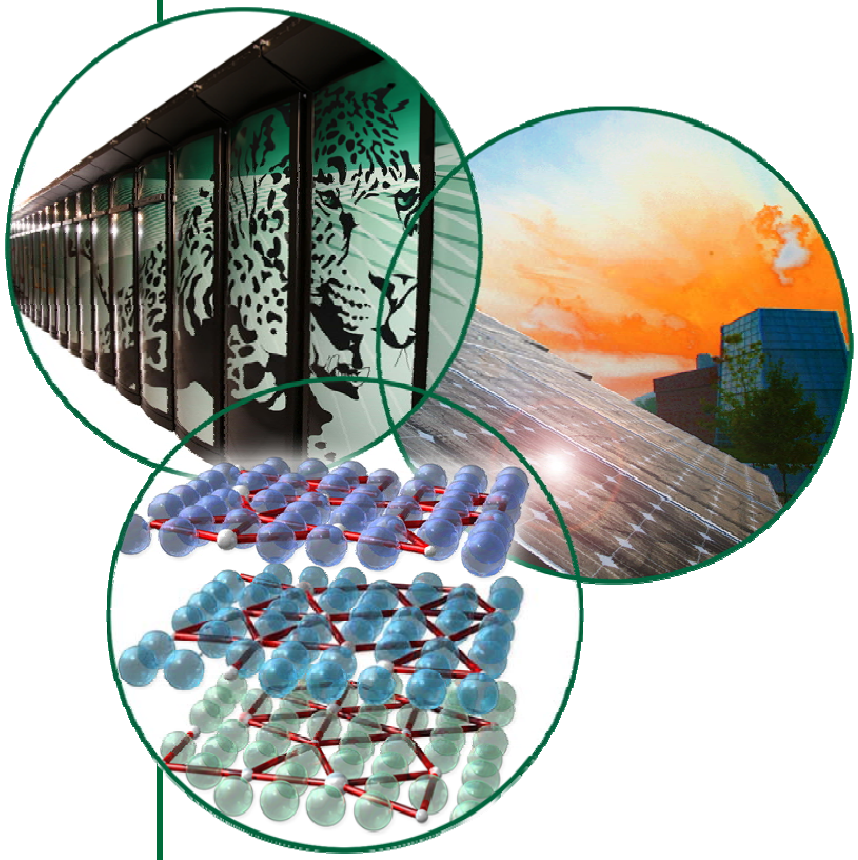
Scientific Computing at the SNS

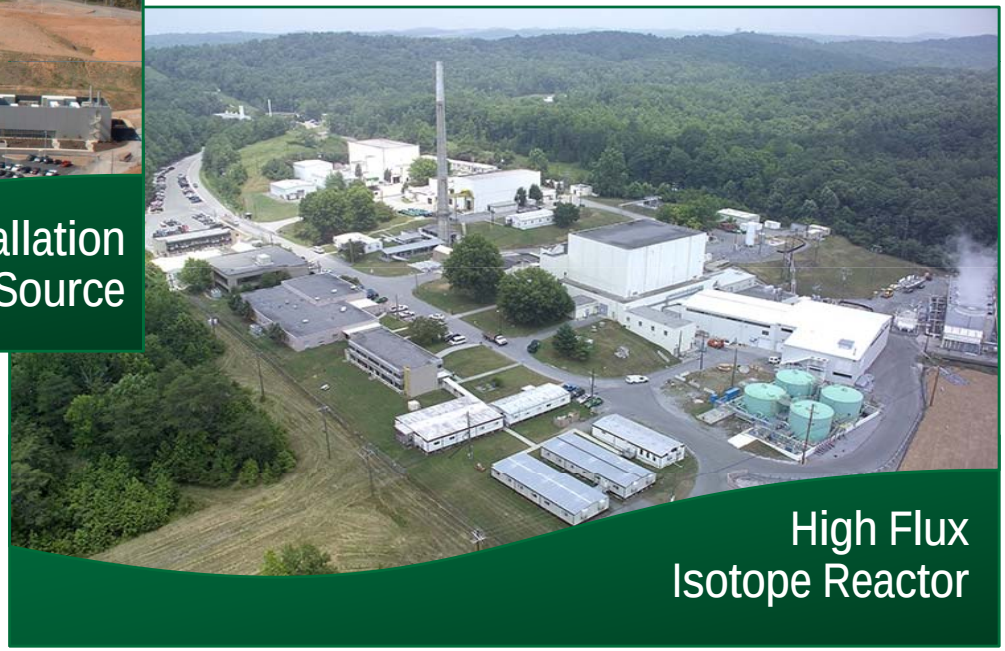
Stuart Campbell
Scientific Computing Group
Neutron Scattering Science Division



U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

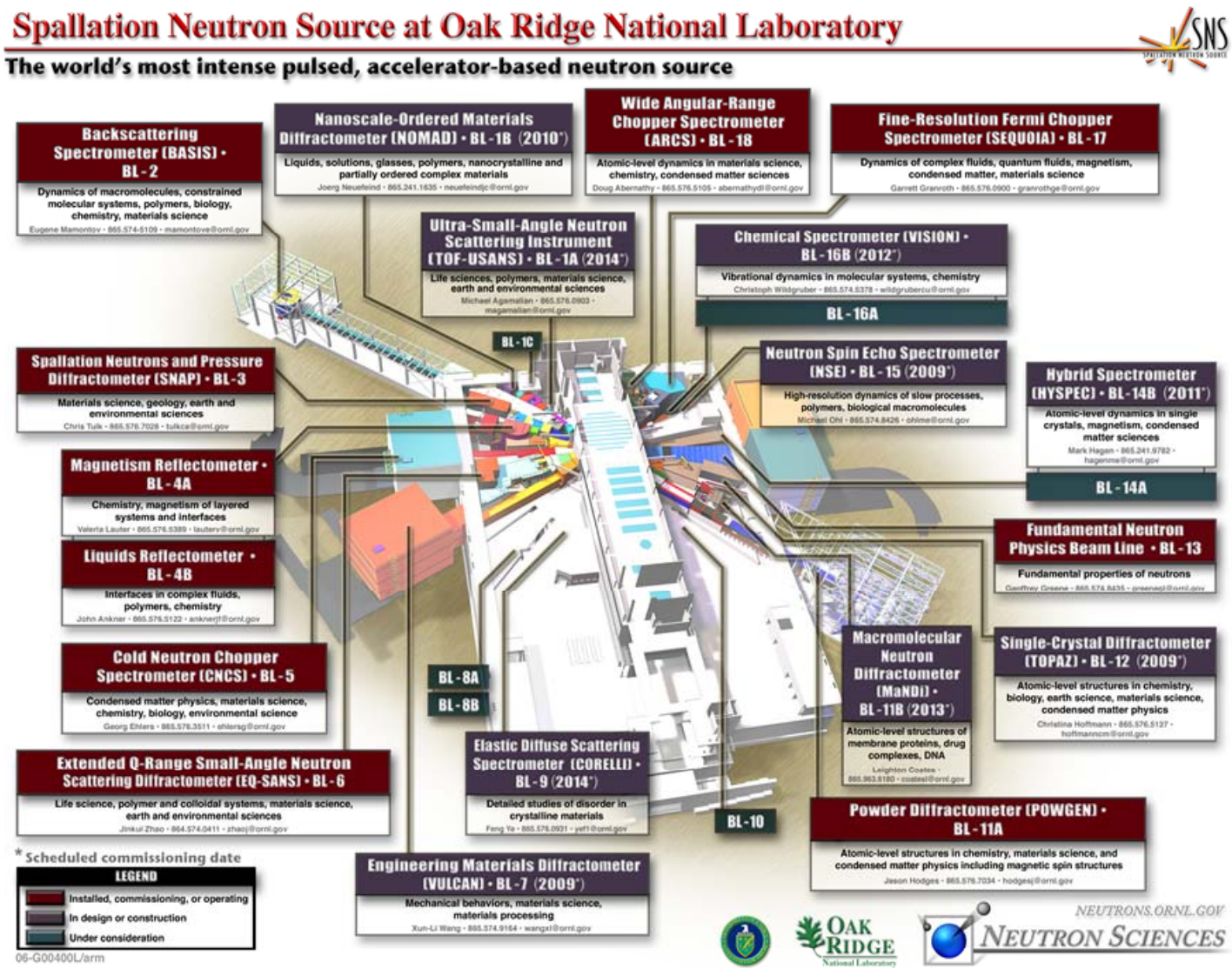
ORNL's two world-leading facilities for neutron science



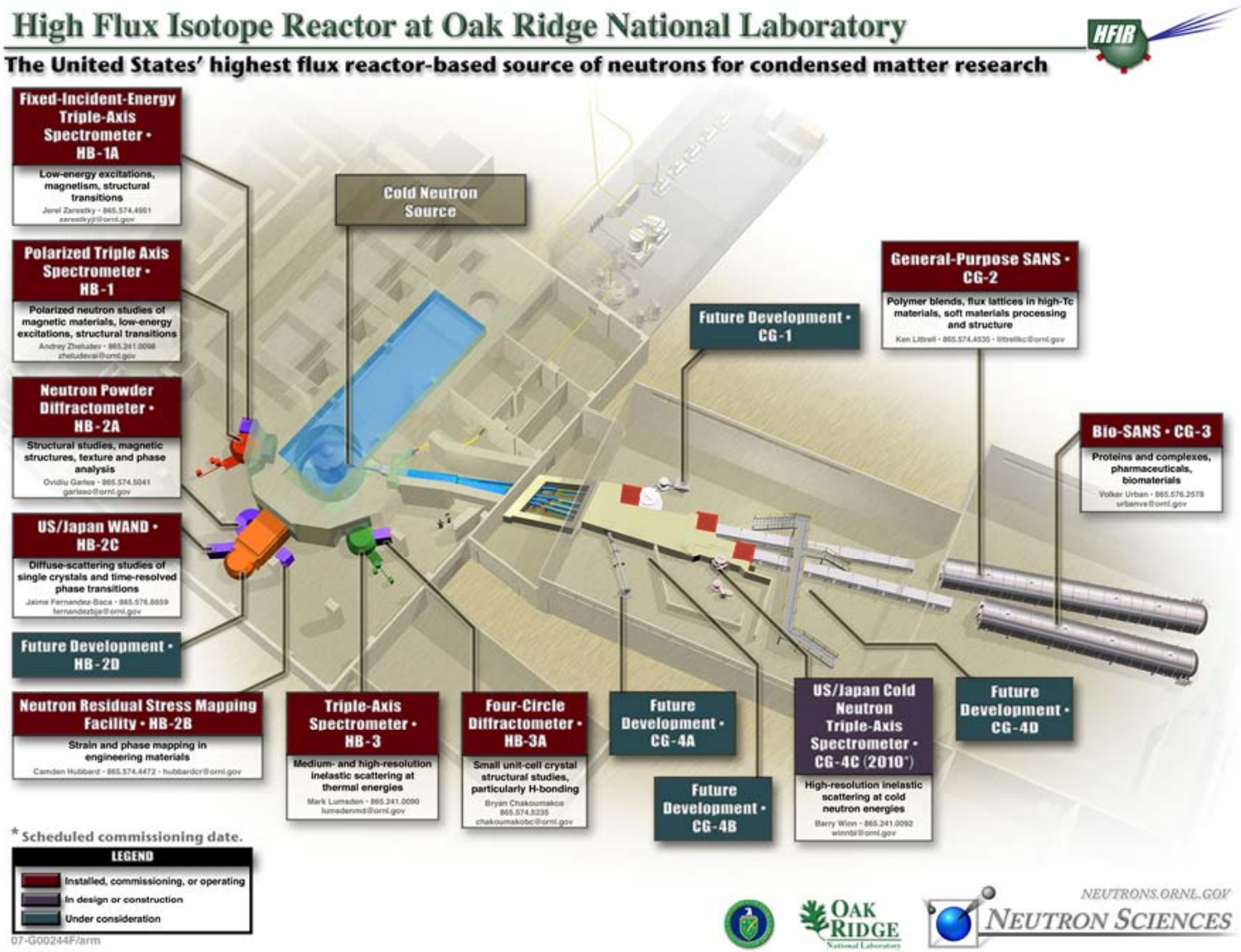
The Spallation Neutron Source

- Construction completed May 2006
- User operations began in 2007
- Design Power 1.4 MW: ~8× ISIS, the world's leading pulsed spallation source
- Room for 25 instruments spanning physics, chemistry, biology, and materials science
- Upgradable to higher power and a second target station

13 Operating Instruments



9 Operating Instruments



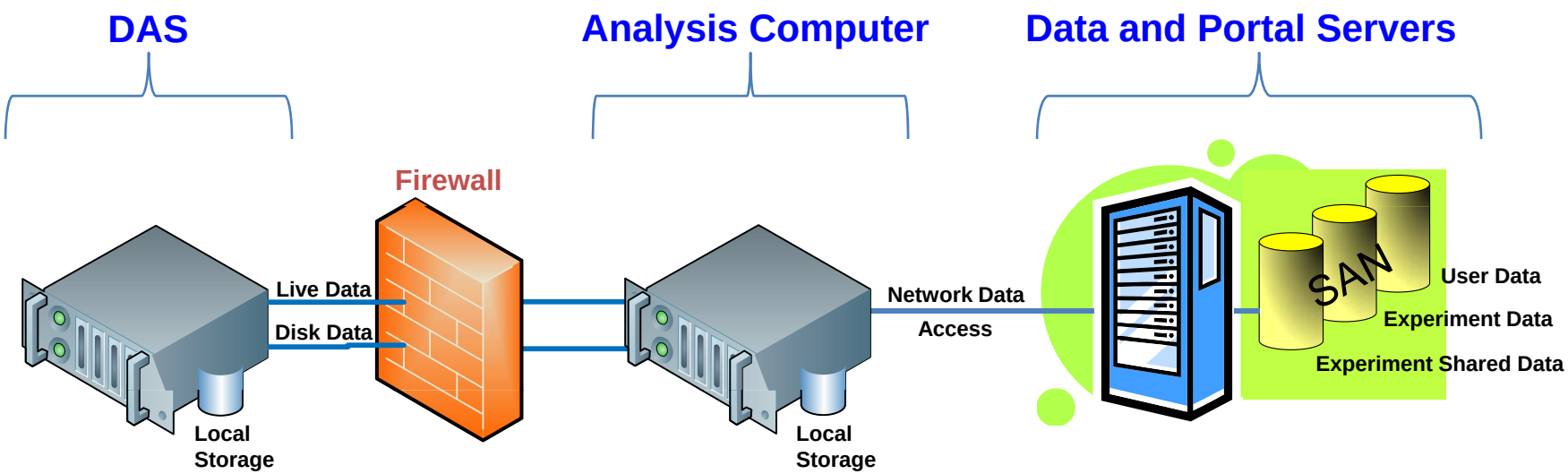
Scientific Computing Group Responsibilities

- Creation and cataloging of NeXus files following an experiment run – Translation and Live Cataloging
- Data Reduction
- Live Data Processing
- Visualization tools
- Data Access – via the portal
- Lines of Code developed:
  - Data Reduction including GUIs (40/60): ~450k lines
  - Data Translation and Live Cataloging: ~50k
  - Portal: ~100k
  - Utilities: 35k

Strategies:

- Generation I – up to now.
  - Establish stable software platforms for operating instruments
  - Leverage and, as necessary, adapt existing software
- Generation II – next 2 years
  - Transition to produce and provide a coherent suite of software across the instrument beam lines
  - More science focused
- Generation III – after 2 years
  - Advanced Simulations
  - Incorporation of “blue skies” software projects
  - …

Experimental Data Flow

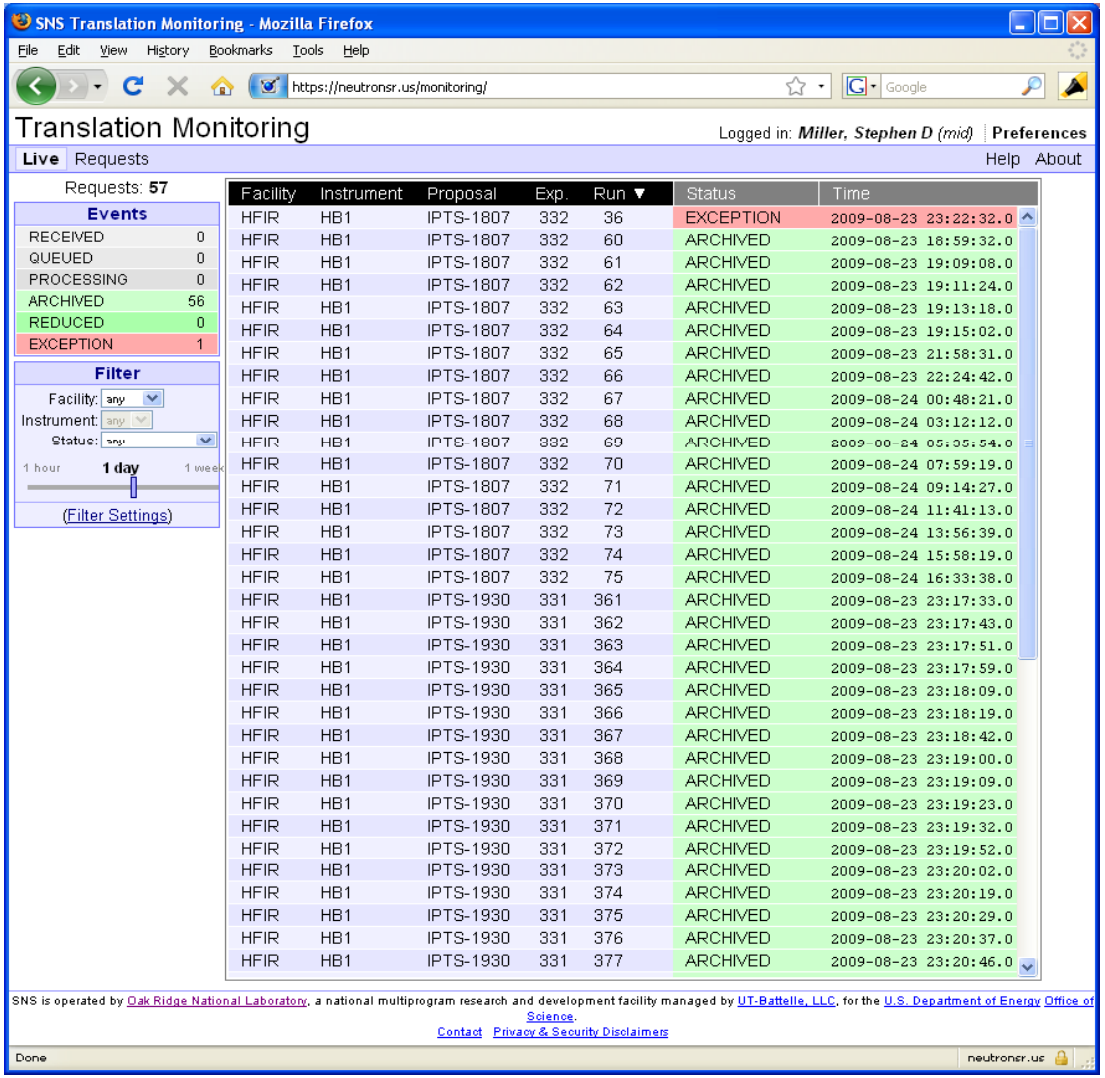


- Private Network
- Neutrons are collected in event mode
- Creates ~6 'pre-NeXus' files (different formats)
- Read only mount
- DAS computer sends out a message once a run is complete

- Translation service responds to end of collection message
- NeXus file created from preNeXus + geometry
- Data is then catalogued (ICAT)

- NeXus and preNeXus files are copied to central disk archive
- Data are available to users via computers and portal
- Data are network mounted for other computers to access
- Data is stored long term and backed-up

Translation Monitoring



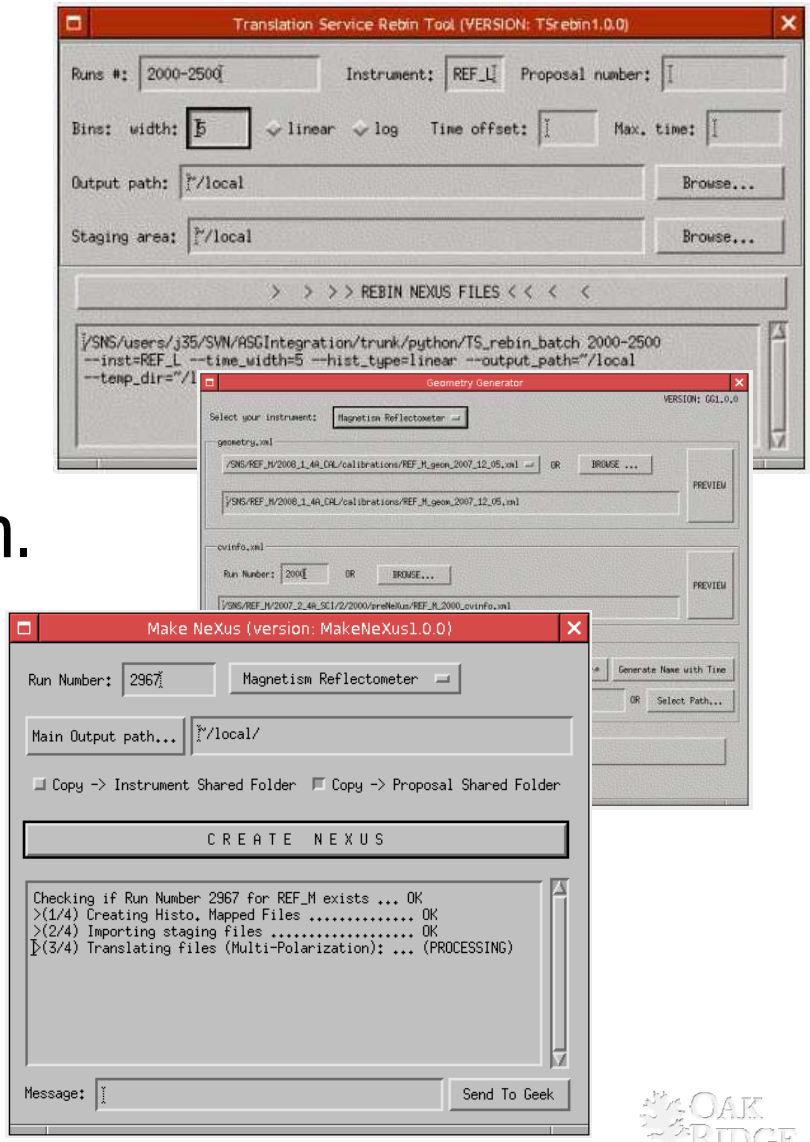
Facility	Instrument	Proposal	Exp.	Run ▼	Status	Time
HFIR	HB1	IPTS-1807	332	36	EXCEPTION	2009-08-23 23:22:32.0
HFIR	HB1	IPTS-1807	332	60	ARCHIVED	2009-08-23 18:59:32.0
HFIR	HB1	IPTS-1807	332	61	ARCHIVED	2009-08-23 19:09:08.0
HFIR	HB1	IPTS-1807	332	62	ARCHIVED	2009-08-23 19:11:24.0
HFIR	HB1	IPTS-1807	332	63	ARCHIVED	2009-08-23 19:13:18.0
HFIR	HB1	IPTS-1807	332	64	ARCHIVED	2009-08-23 19:15:02.0
HFIR	HB1	IPTS-1807	332	65	ARCHIVED	2009-08-23 21:58:31.0
HFIR	HB1	IPTS-1807	332	66	ARCHIVED	2009-08-23 22:24:42.0
HFIR	HB1	IPTS-1807	332	67	ARCHIVED	2009-08-24 00:48:21.0
HFIR	HB1	IPTS-1807	332	68	ARCHIVED	2009-08-24 03:12:12.0
HFIR	HB1	IPTS-1807	332	69	ARCHIVED	2009-08-24 05:35:54.0
HFIR	HB1	IPTS-1807	332	70	ARCHIVED	2009-08-24 07:59:19.0
HFIR	HB1	IPTS-1807	332	71	ARCHIVED	2009-08-24 09:14:27.0
HFIR	HB1	IPTS-1807	332	72	ARCHIVED	2009-08-24 11:41:13.0
HFIR	HB1	IPTS-1807	332	73	ARCHIVED	2009-08-24 13:56:39.0
HFIR	HB1	IPTS-1807	332	74	ARCHIVED	2009-08-24 15:58:19.0
HFIR	HB1	IPTS-1807	332	75	ARCHIVED	2009-08-24 16:33:38.0
HFIR	HB1	IPTS-1930	331	361	ARCHIVED	2009-08-23 23:17:33.0
HFIR	HB1	IPTS-1930	331	362	ARCHIVED	2009-08-23 23:17:43.0
HFIR	HB1	IPTS-1930	331	363	ARCHIVED	2009-08-23 23:17:51.0
HFIR	HB1	IPTS-1930	331	364	ARCHIVED	2009-08-23 23:17:59.0
HFIR	HB1	IPTS-1930	331	365	ARCHIVED	2009-08-23 23:18:09.0
HFIR	HB1	IPTS-1930	331	366	ARCHIVED	2009-08-23 23:18:19.0
HFIR	HB1	IPTS-1930	331	367	ARCHIVED	2009-08-23 23:18:42.0
HFIR	HB1	IPTS-1930	331	368	ARCHIVED	2009-08-23 23:19:00.0
HFIR	HB1	IPTS-1930	331	369	ARCHIVED	2009-08-23 23:19:09.0
HFIR	HB1	IPTS-1930	331	370	ARCHIVED	2009-08-23 23:19:23.0
HFIR	HB1	IPTS-1930	331	371	ARCHIVED	2009-08-23 23:19:32.0
HFIR	HB1	IPTS-1930	331	372	ARCHIVED	2009-08-23 23:19:52.0
HFIR	HB1	IPTS-1930	331	373	ARCHIVED	2009-08-23 23:20:02.0
HFIR	HB1	IPTS-1930	331	374	ARCHIVED	2009-08-23 23:20:19.0
HFIR	HB1	IPTS-1930	331	375	ARCHIVED	2009-08-23 23:20:29.0
HFIR	HB1	IPTS-1930	331	376	ARCHIVED	2009-08-23 23:20:37.0
HFIR	HB1	IPTS-1930	331	377	ARCHIVED	2009-08-23 23:20:46.0

- Enables viewings of the process of creating and cataloguing experimental data (NeXus files)

Data Archive for Facilities

NeXus Utilities

- Enable users to ‘control’ NeXus generation
  - Override Geometry
  - Alter data binning
- NeXus files are histograms
- Event based NeXus coming soon.
- Defining an ‘analysed’ NeXus format.

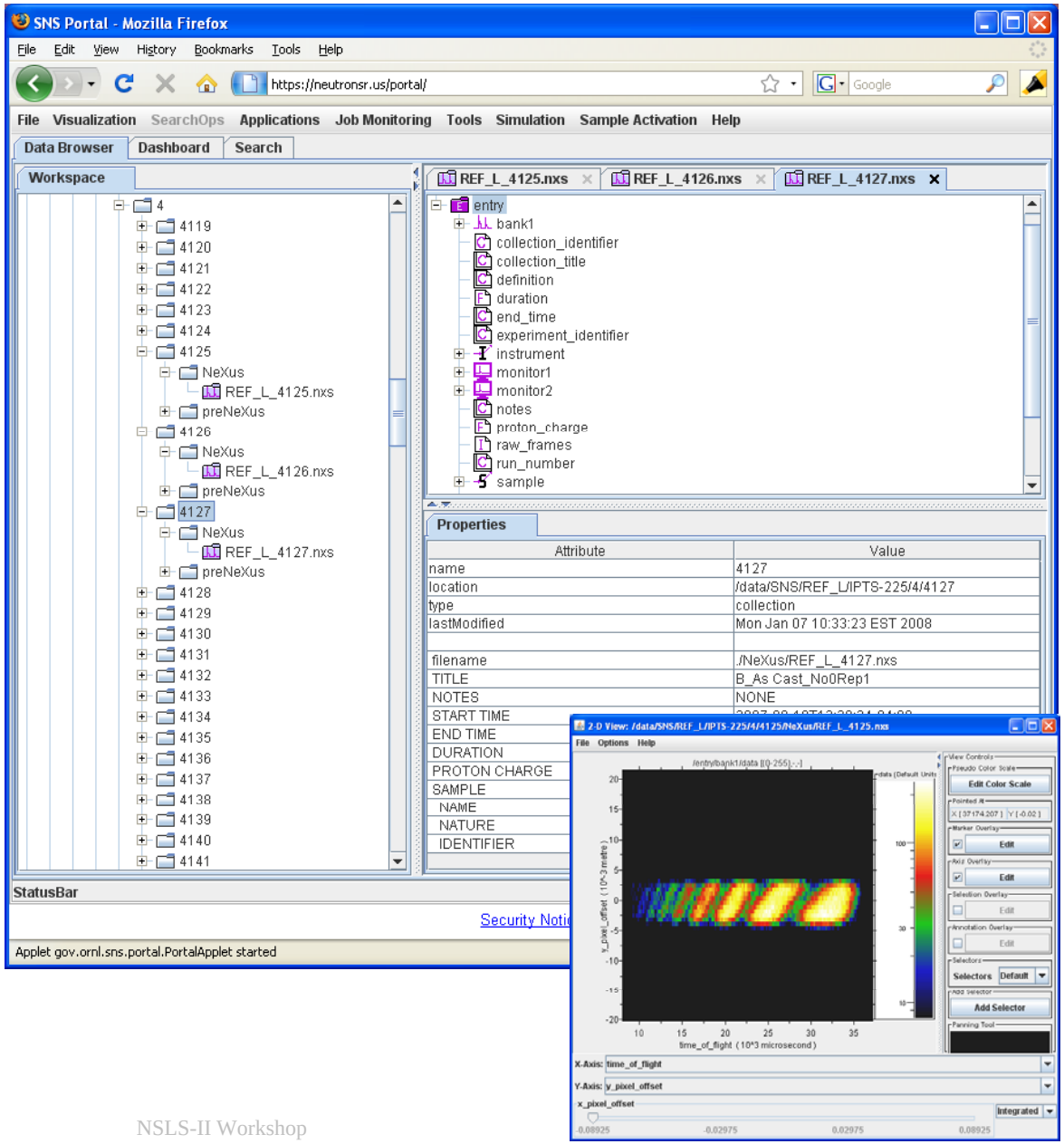


A Look at SNS Data Sizes

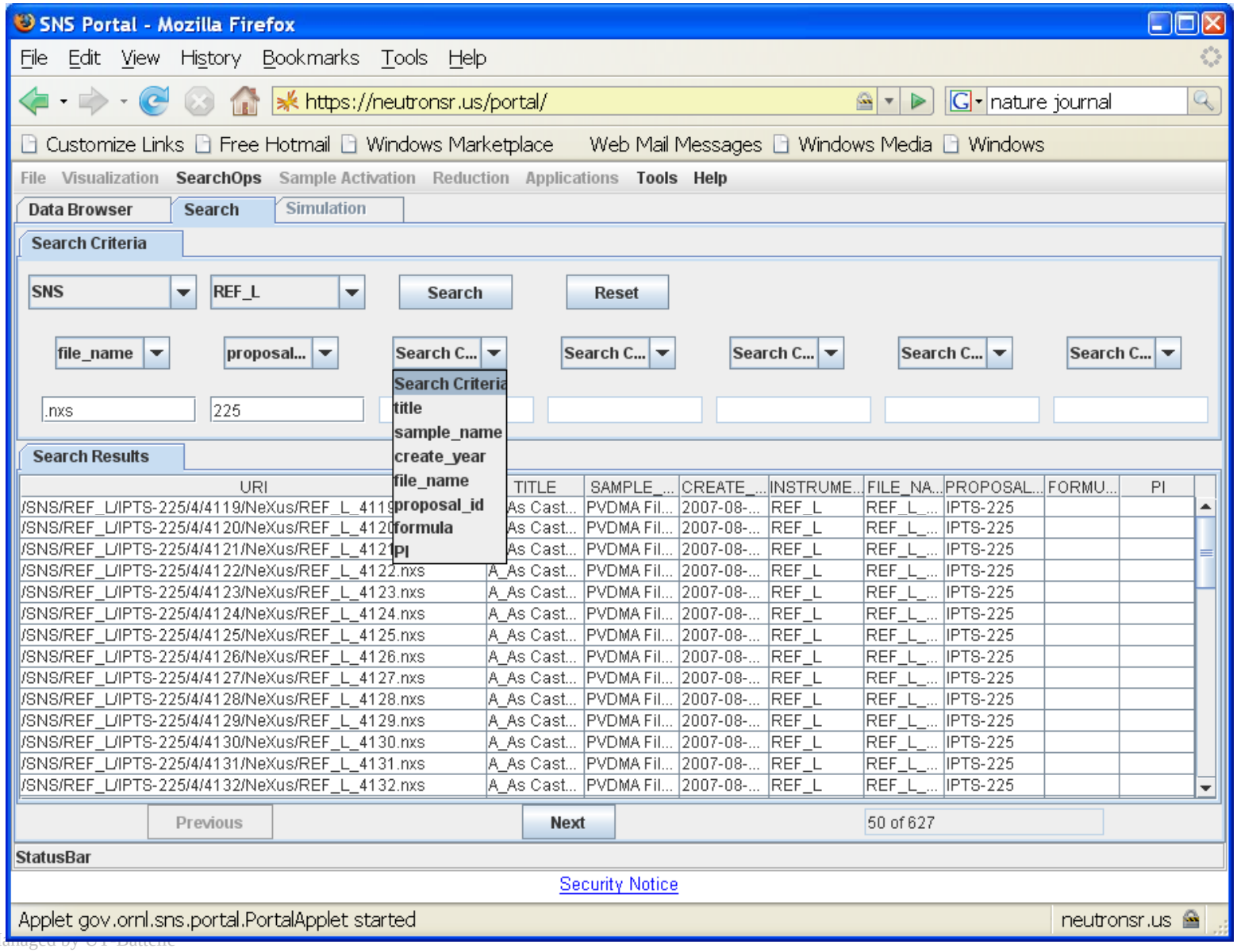
Instrument	Typical Histogram Size	NeXus File Size	Event File Size
Ref_M	149MB	27.2MB	24.8MB
BASIS	136MB	3.5MB	3.89MB
Powgen	2.1GB estimated	2.0MB	30.1MB
ARCS	3.6GB	29.6MB	116.4MB
Sequoia	4.3GB	34.69MB	136.2MB
CNCS	0.8GB	14.8MB	4.3MB
SNAP	7.7GB	83.1MB	118.9MB
TOPAZ	14.9GB estimated	?	?

Data Access/Download for Users (Data Portal)

- Users get an XCAMS “account” (username & password)
- Account gives them access to:
  - Beamline Analysis Computer
  - Central User Disk Space
  - Experimental Data
- Data Portal gives access to
  - User’s ‘Home’ area
  - Raw data - NeXus
  - Metadata browser for NeXus
  - download/upload of files
  - 1D and 2D visualization tools are built-in for NeXus files
- Data Search (ICAT)



Data Search


SNS Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
https://neutronsr.us/portal/
nature journal
Customize Links Free Hotmail Windows Marketplace Web Mail Messages Windows Media Windows
File Visualization SearchOps Sample Activation Reduction Applications Tools Help
Data Browser Search Simulation
Search Criteria
SNS
REF_L
Search
Reset
file_name
proposal...
Search C...
.nxs
225
Search Criteria
title
sample_name
create_year
file_name
proposal_id
formula
pi
Search Results
URI
TITLE
SAMPLE_...
CREATE_...
INSTRUME...
FILE_NA...
PROPOSAL...
FORMU...
PI
/SNS/REF_L/IPTS-225/4/4119/NeXus/REF_L_4119
/SNS/REF_L/IPTS-225/4/4120/NeXus/REF_L_4120
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/SNS/REF_L/IPTS-225/4/4132/NeXus/REF_L_4132.nxs
Previous
Next
50 of 627
StatusBar
Security Notice
Applet gov.ornl.sns.portal.PortalApplet started
neutronsr.us

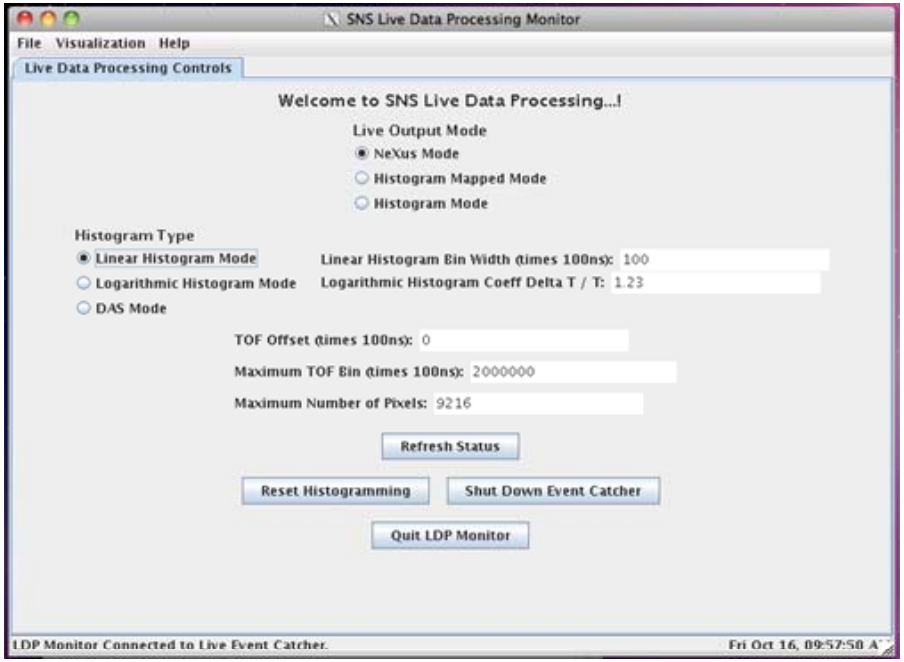
Data Access Requirement

- Strong requirement from users and beamline staff was for command line access to data.
- We defined a storage hierarchy to support hosting data from multiple facilities with multiple beamlines.
- Built infrastructure to support command line access and web portal access
- Used NFS with ACLs to restrict access to directories.
- We are currently rethinking this approach!

Data Policy

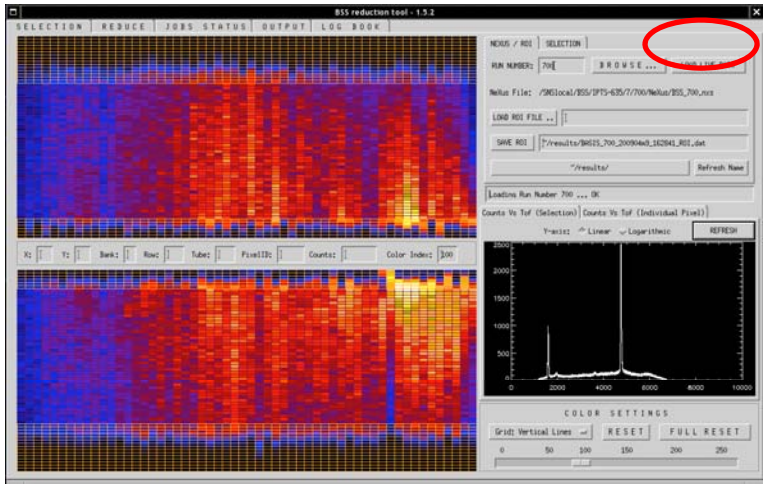
- Went for the simple option…
  - The Principle Investigator owns the data.
  - Users can only see data for experiments they are part of.
  - We permanently archive the data.

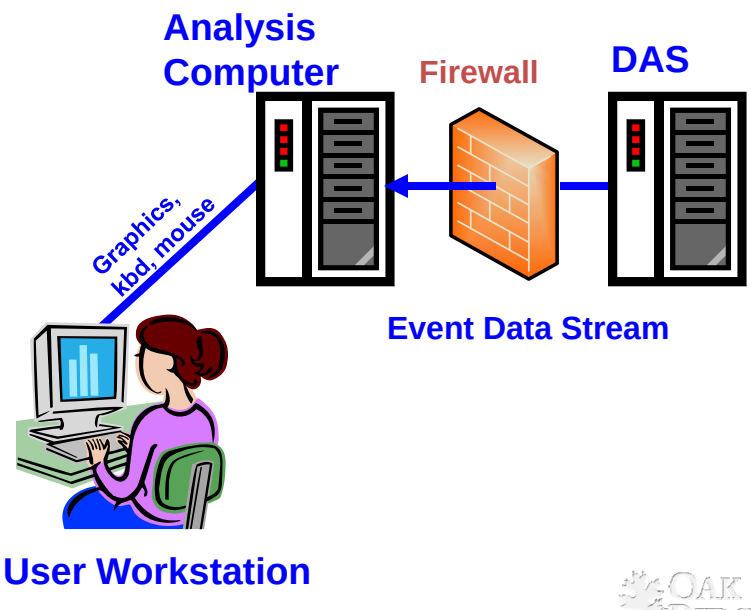
Live Data Streaming



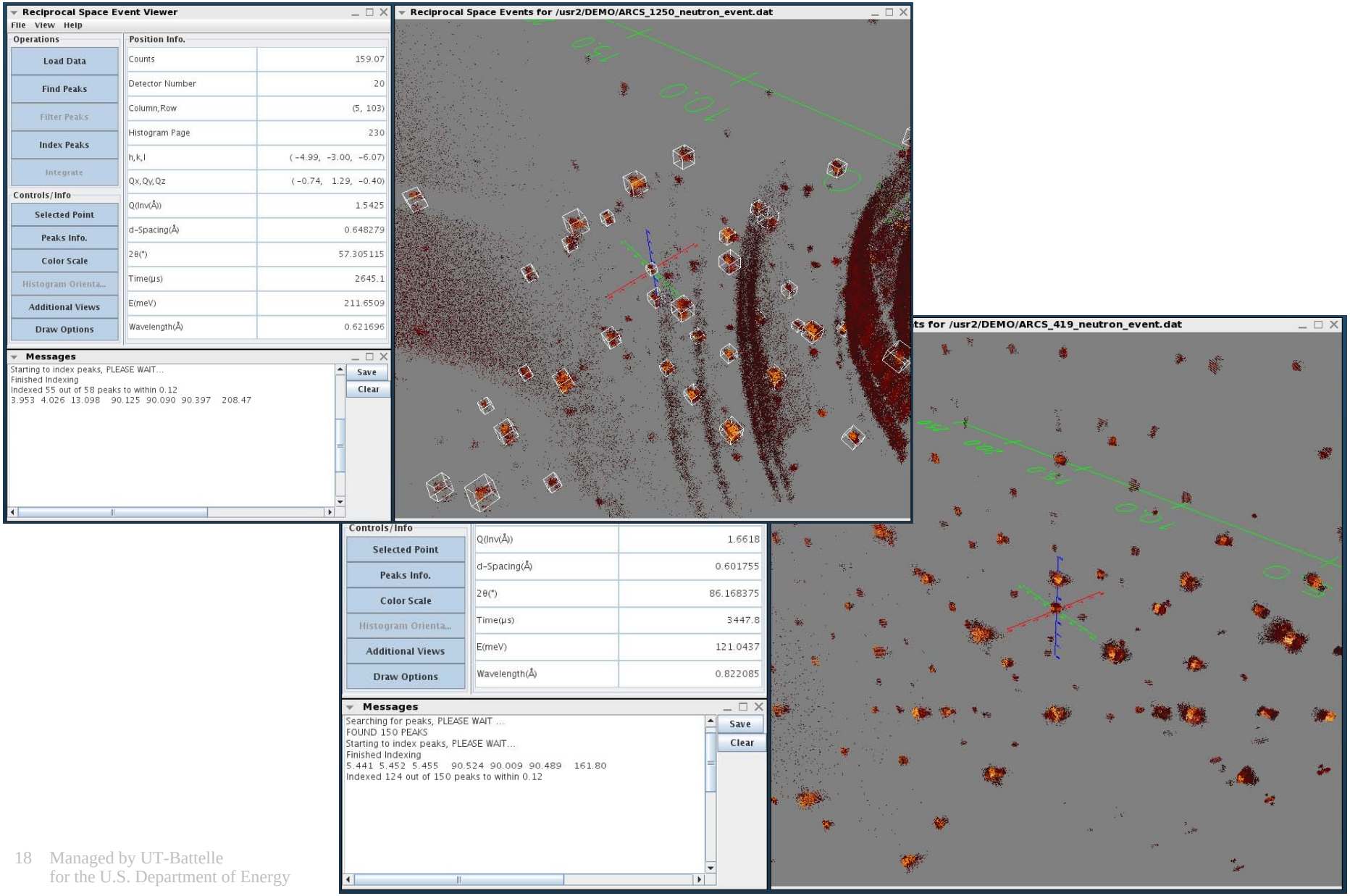
- Events and metadata are streamed from the DAS to the instrument analysis computer.
- Events are continuously processed and temporary NeXus files and event lists are periodically produced.
- Does not produce the data of record for the experiment.
- Can ‘pass through’ events to other programs.

Reduction GUI



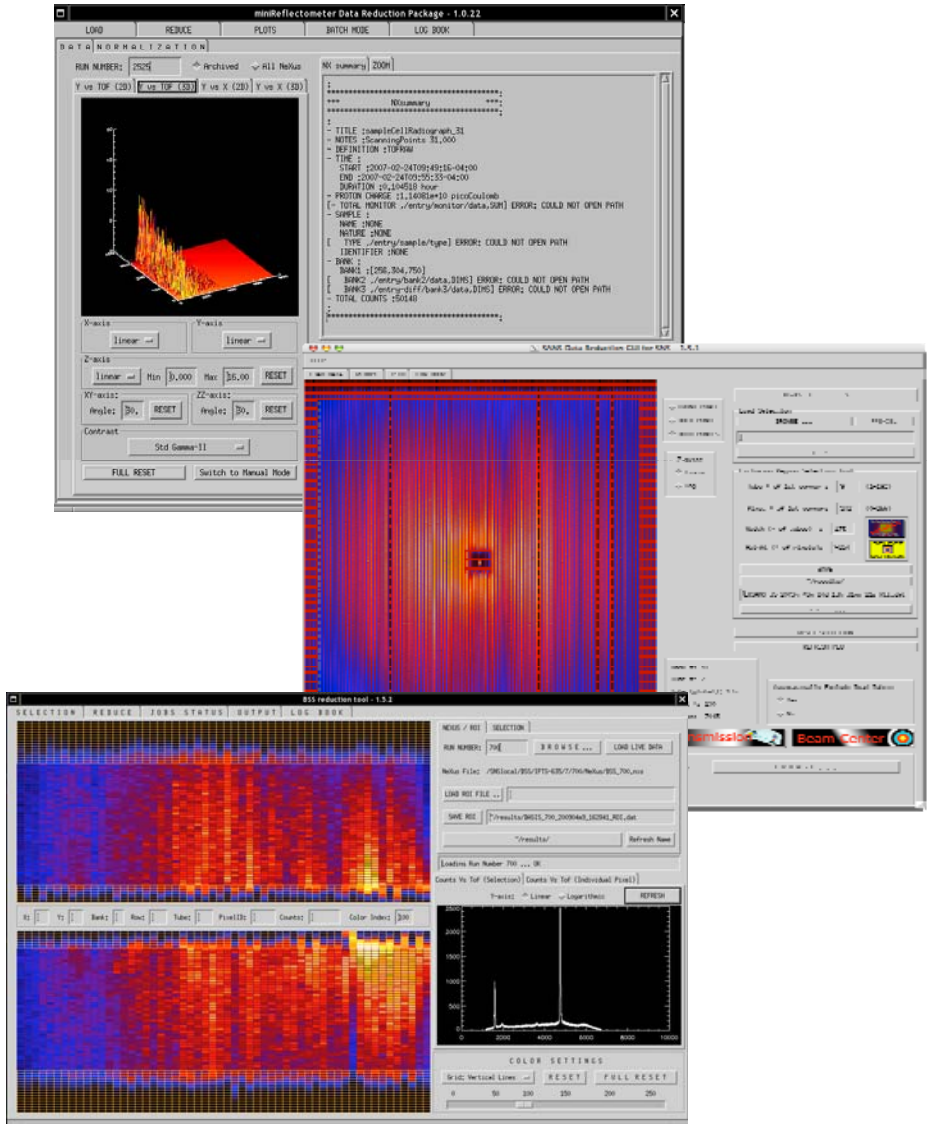


Viewing the live event data (IsawEV)



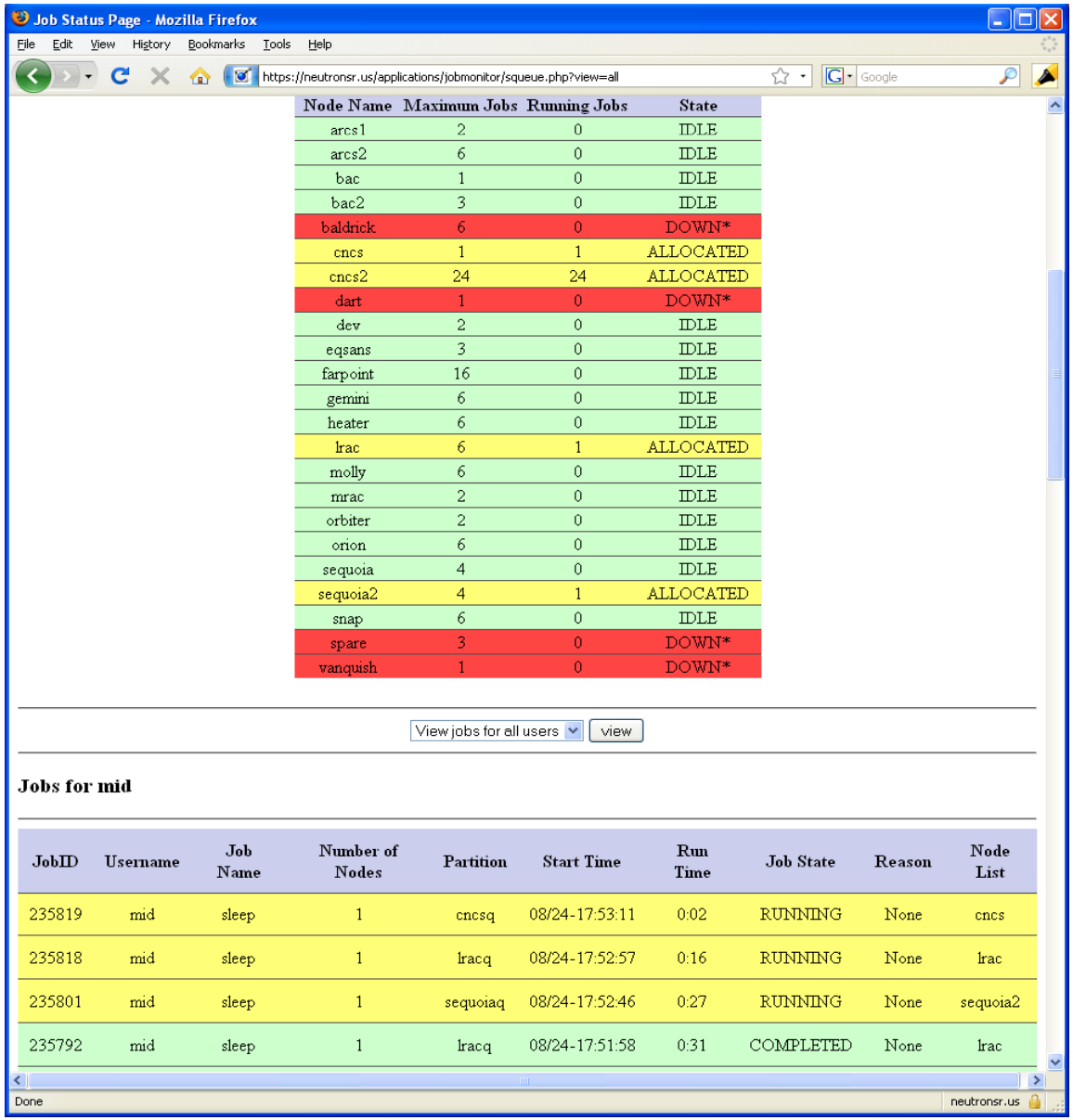
Data Reduction

- C++ Core Algorithms
- Python ‘Glue’
- IDL user GUIs
- Read NeXus files
- Reduction can be split up by detector ‘bank’
- Processed in parallel (SLURM) on analysis machines



Job Monitor

- Users can track the execution status of their jobs



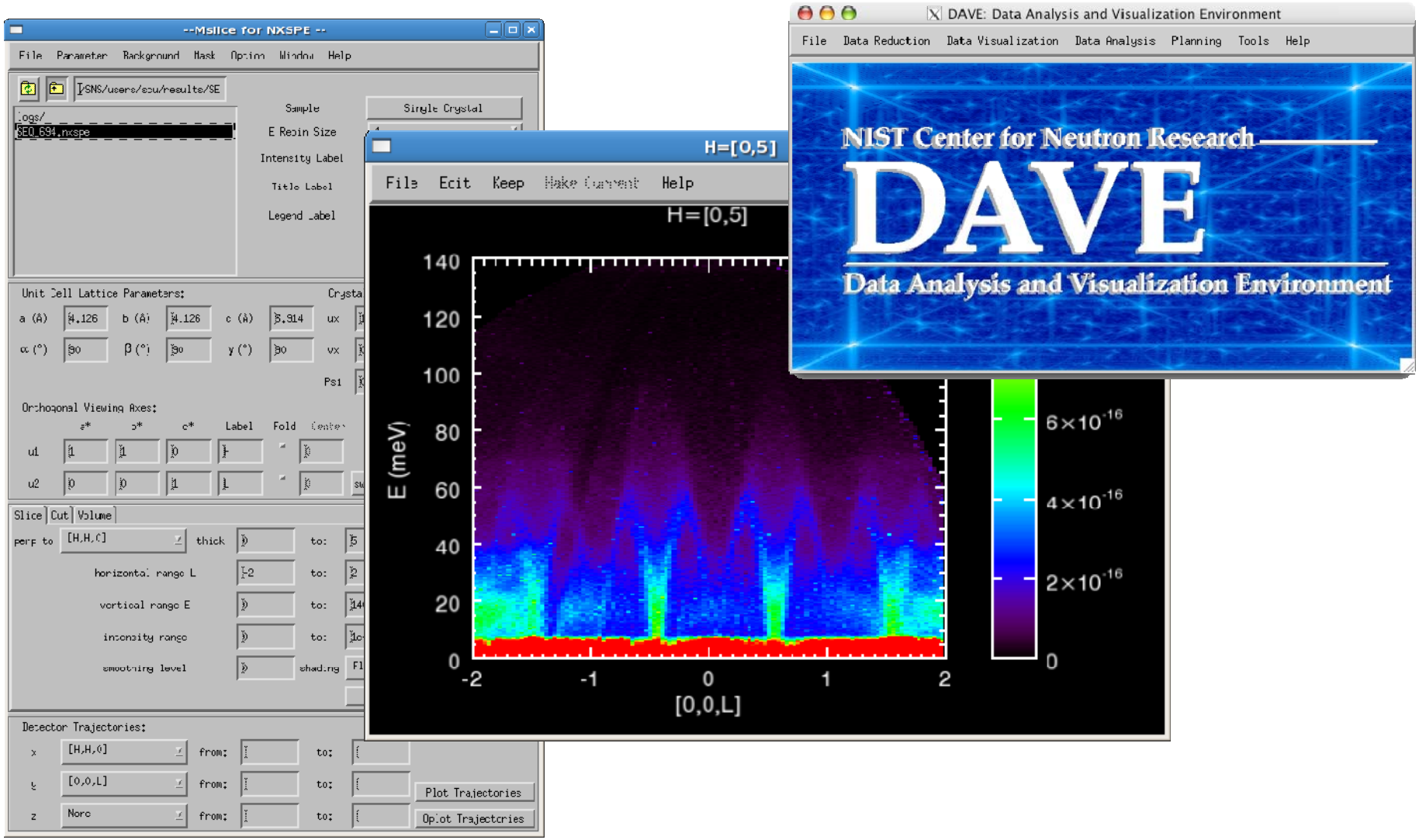
Node Name	Maximum Jobs	Running Jobs	State
arcs1	2	0	IDLE
arcs2	6	0	IDLE
bac	1	0	IDLE
bac2	3	0	IDLE
baldrick	6	0	DOWN*
cncs	1	1	ALLOCATED
cncs2	24	24	ALLOCATED
dart	1	0	DOWN*
dev	2	0	IDLE
eqsans	3	0	IDLE
farpoint	16	0	IDLE
gemini	6	0	IDLE
heater	6	0	IDLE
lrac	6	1	ALLOCATED
molly	6	0	IDLE
mrac	2	0	IDLE
orbiter	2	0	IDLE
orion	6	0	IDLE
sequoia	4	0	IDLE
sequoia2	4	1	ALLOCATED
snap	6	0	IDLE
spare	3	0	DOWN*
vanquish	1	0	DOWN*

JobID	Username	Job Name	Number of Nodes	Partition	Start Time	Run Time	Job State	Reason	Node List
235819	mid	sleep	1	cncsq	08/24-17:53:11	0:02	RUNNING	None	cncs
235818	mid	sleep	1	lracq	08/24-17:52:57	0:16	RUNNING	None	lrac
235801	mid	sleep	1	sequoiaq	08/24-17:52:46	0:27	RUNNING	None	sequoia2
235792	mid	sleep	1	lracq	08/24-17:51:58	0:31	COMPLETED	None	lrac

Infrastructure Hardware

- 32 core, 256 GB RAM Machines (1 or 2 per beamline)
  - Physically located on beamlines
  - 30” Monitor (1 or 2)
- Gigabit Ethernet
- Central Disks served by NFS

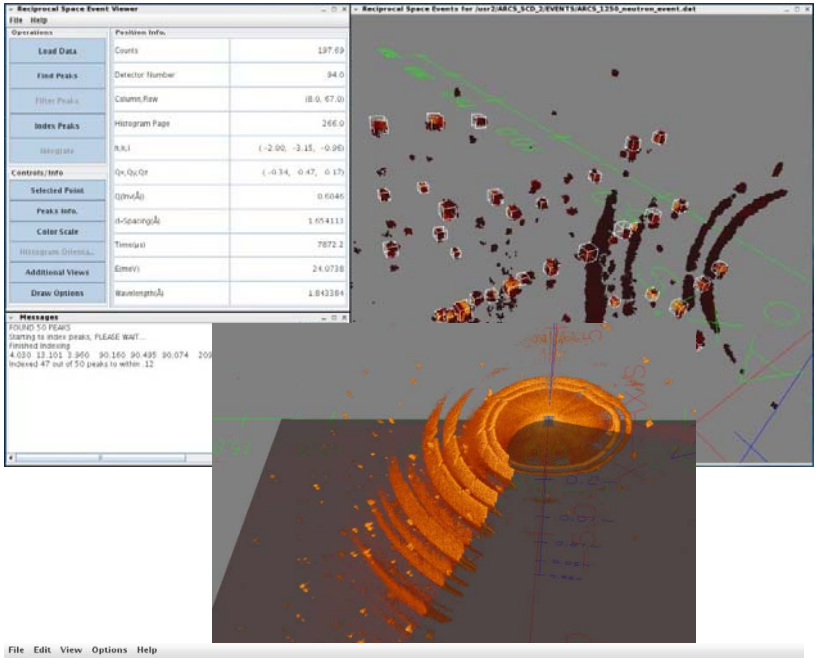
Community Codes – DAVE (NIST)

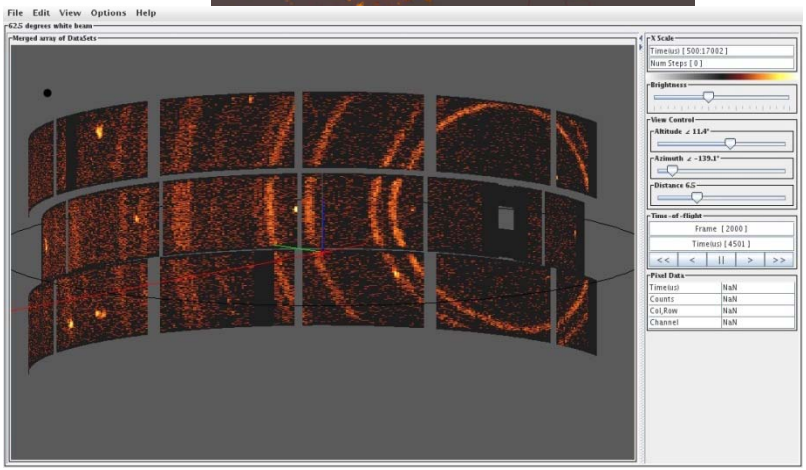


Typical Data Size ~ 1-50 GB

Community Codes - ISAW

- The ISAW application has been extended to support SNS instruments
  - Reduces single crystal and powder diffraction data
  - Can reduce event data to Q-space directly (no corrections)
  - Can perform data reduction in distributed computing mode
  - ISAW has 230K lines of code, 32K SCD specific, 8K for event data processing, and 6K for 3D visualization



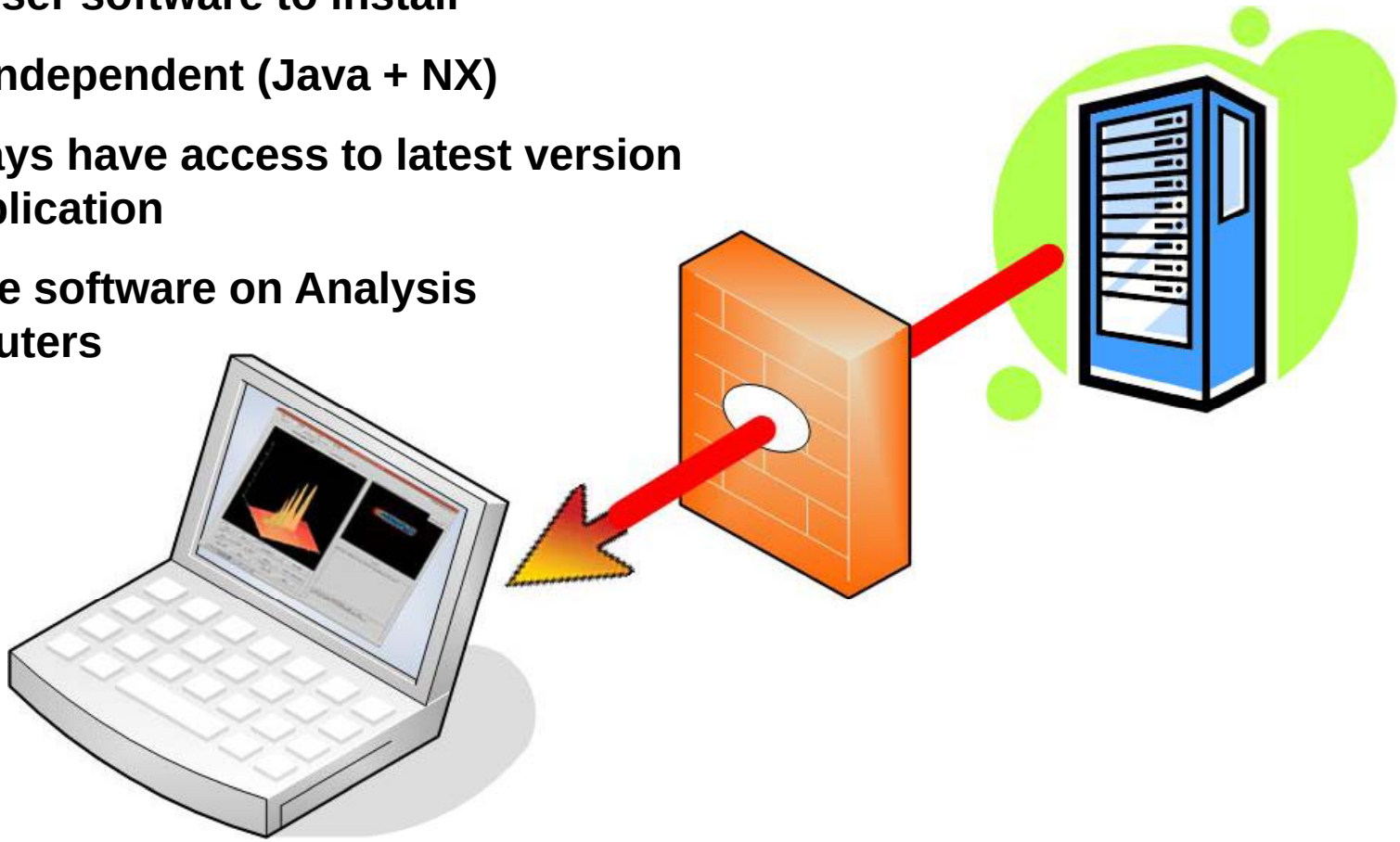


Other Software

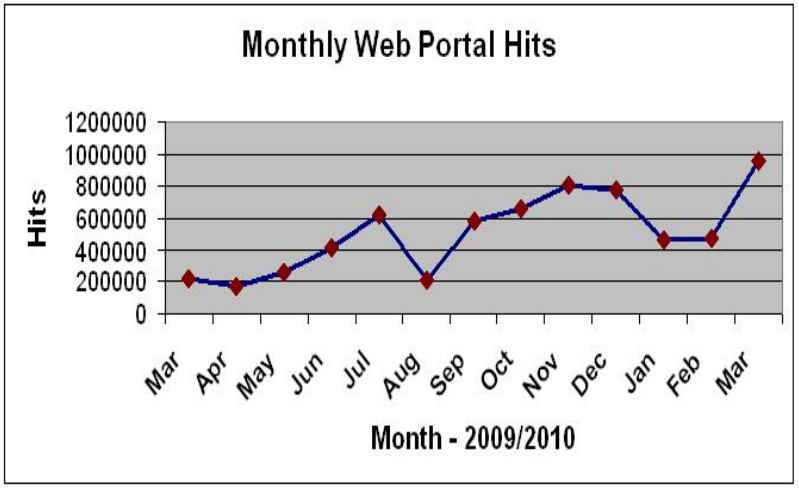
- IDL
- Matlab
- Igor Pro
- SigmaPlot
- Origin

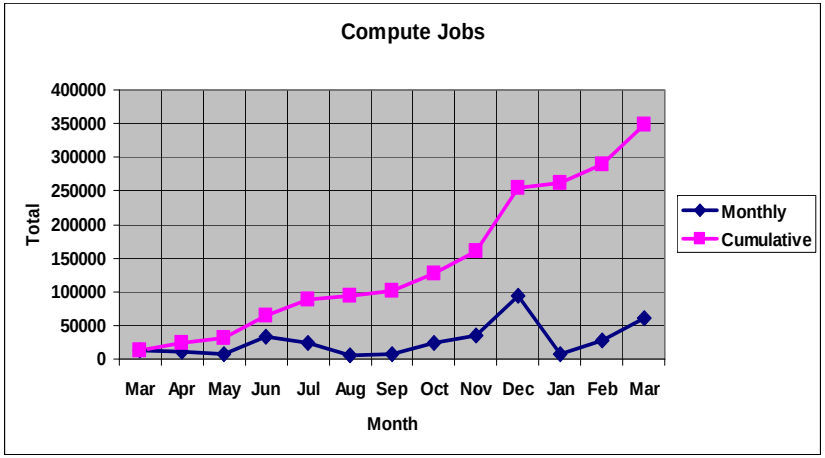
Remote Applications

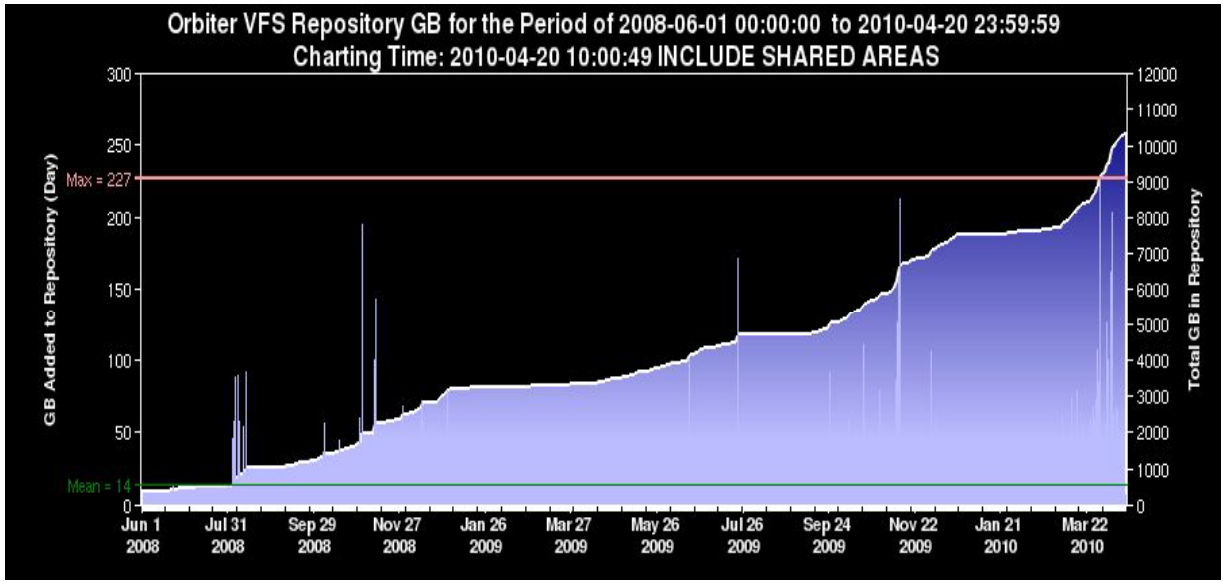
- **Applications hosted remotely and viewed locally**
- **No user software to install**
- **OS independent (Java + NX)**
- **Always have access to latest version of application**
- **Same software on Analysis computers**



Data and Computing Statistics







- 10.3 TB of Experiment Data (to date)
- 4.6 TB in shared areas (reduced data)
- 6.5TB size of user home areas
- 1,516,819 total files cataloged

Assessing from Here…

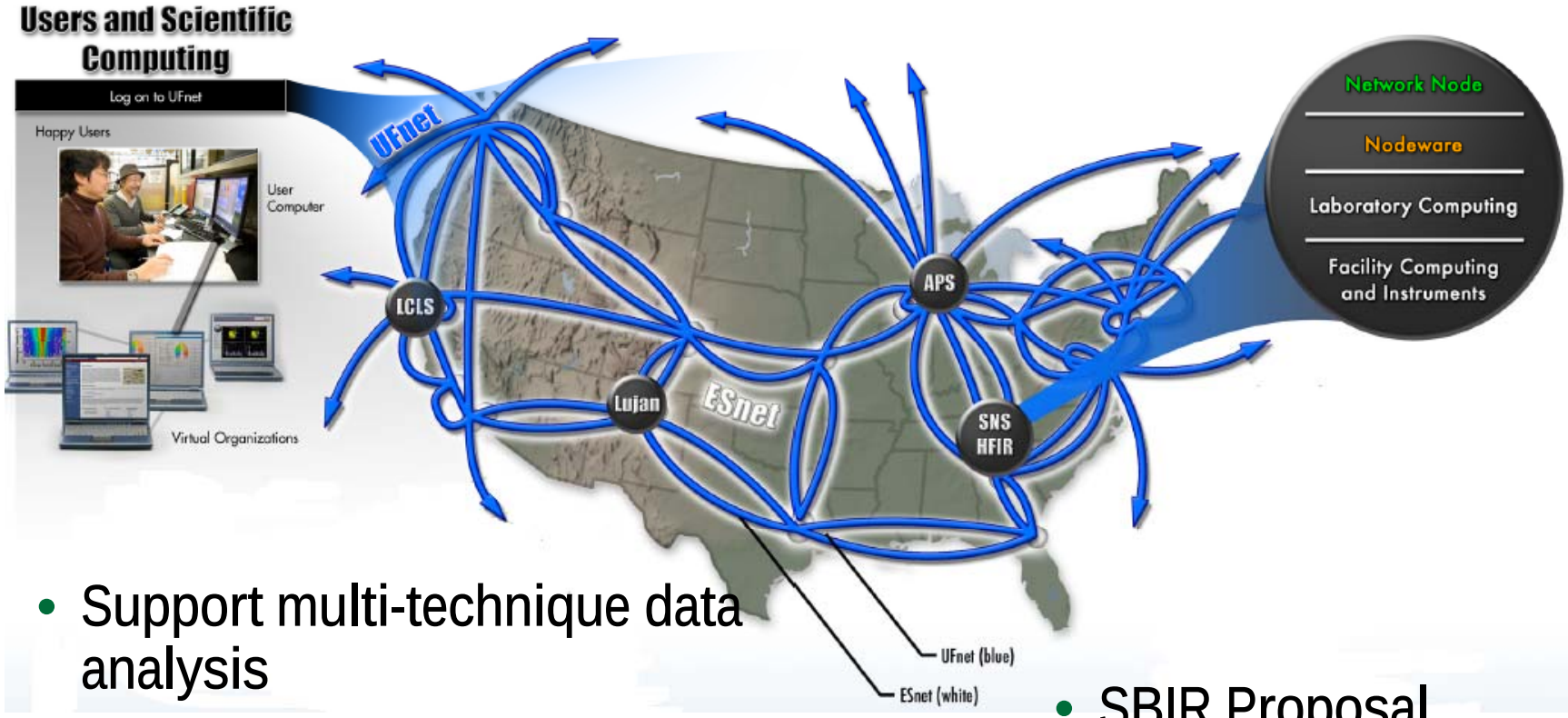
- More visualization tools needed – during and following an experiment
- Community produced analysis tools not always suited towards working with SNS data sizes
- Better integration between experiment and analyses processes
- More ‘commonality’ across science areas
- Higher performance computing requested – this involves computers, disks, and network performance

Collaborations

- Software produced will be Open Source.
  - Required approval from DOE and UT-Battelle/ORNL
  - Required Export Control Approval

- Already working with the authors of ISAW and DAVE.
- Currently forming a software collaboration with ISIS based upon the Mantid Python/C++ framework.
- Currently working with the DANSE team to develop the plan for how to transition DANSE software to ORNL.

Emerging Vision – Interconnected Facilities



- Support multi-technique data analysis
- Thick Client Apps utilizing web services at facilities
- Inter-facility data movement

- SBIR Proposal
  - SNS, HFIR, APS, Lujan, LCLS

Slide courtesy of Steve Miller

Summary

- Data reduction software is available for all operating and commissioning instruments at SNS.
- Near-term software development focus areas are:
  - To provide additional data reduction visualization tools during and following an experiment
  - To improve the performance for running data reduction jobs
- Development scope now includes providing new analysis software in addition to providing data reduction.
- The Scientific Computing Group is working more closely with science teams

Thank you.

Questions ?