

SHUG (SNS HFIR User Group), <http://neutrons.ornl.gov/users/shug/>  
SHUG executive committee minutes.

Teleconference held July 6, 2010.

Attendees:

Executive Committee: Cora Lind, Matthew Stone, Peter Khalifa, Eugenia Kharlampieva, Mark Crawford, Ursula Perez-Salas

Guests: Dean Myles, Ian Anderson, Al Ekkebus, and Emily Liu

Minutes submitted for review July 7, 2010 by M. B. Stone.

#### ACTION ITEMS:

- Need to gather outreach items, ideas and suggestions for Al Ekkebus, please see last paragraph of item 2 below.
  - Need to gather ideas for future teleconferences of how to broaden interactions with the neutron user community. Please see first paragraph of item 1 below.
  - When attending your meetings, please contact Al to request a poster highlighting the ORNL neutron facilities. Also, there may be additional support for your travel if you help in this endeavor.
  - The SHUG executive committee teleconferences are scheduled for the second Tuesday of each month at 1 PM. The next meeting will be Tuesday August 10, 2010.
  - Please review the X-ray equipment anticipated being moved from CNMS to the CLO laboratories (attached), and respond with any further suggestions for this space to the SHUG executive committee secretary at [stonemb@ornl.gov](mailto:stonemb@ornl.gov)
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ATTACHMENTS and WEBSITES of interest from the teleconference:

Website for collaborative research visits with ORNL neutron sciences,  
<http://neutrons.ornl.gov/crv/>

Website for second floor CLO laboratories, <http://neutrons.ornl.gov/facilities/SNS/userlabs.shtml>

Dean Myles's ACNS talk.

Lou Santodonato's ACNS talk.

X-ray equipment anticipated being moved from CNMS to CLO laboratories.

X-ray equipment requested by the condensed matter science center.

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## 1. ORNL/NScD update (Ian Anderson and Dean Myles)

Ian welcomes new committee members and challenges the committee to engage more with the user community. This should be especially geared toward education, outreach, and awareness of new facilities and how to engage additional users, i.e. closer interactions and more feedback. Ian would like to put this on the agenda for future meetings.

Dean presented a session at the ACNS 2010 meeting in Ottawa (see attachments). There are five instruments at SNS coming through the commissioning process. These instruments are SEQUOIA, Powgen, EQ Sans, Vulcan and Topaz. SEQUOIA is currently the furthest along in this process, and is considered to be ready to fully enter the user program. Management would like to include the user community as part of this commissioning process, especially in terms of instrument readiness reviews for each instrument.

The second floor CLO laboratories are ready for occupancy. These laboratories will be both for beamlines and for user operations. NScD management would like to have SHUG survey the community and make further suggestions for laboratory space. There was a good response from the community, and there will be a summary of the anticipated capabilities distributed to the SHUG executive committee.

The splitting of the software group into infrastructure and data management (group leader Steven Miller), and data analysis groups (Interim group leader Mark Hagan) has taken place. The full time position for the data analysis group has been posted.

## 2. National User Facility Organization activities (AI)

NUFO met the first week of June 2010 at Brookhaven. Attendees included individuals from throughout the US and worldwide interested in user facilities. X-ray, neutron, high energy facilities were represented. Industrial outreach discussions were a focus topic. Also Secretary Chu would like to improve site access for department of energy facilities for users. Foreign national access is anticipated to be processed faster than current practice at DOE facilities.

Ian Anderson: The North American neutron facility directors (ORNL, NIST, Chalk River, Lujan) met with the NSSA (Neutron Scattering Society of America) at the ACNS 2010. The question arose "Are there ways to improve communication between these different advocacy groups from the different facilities?" SNUG (Synchrotron and Neutron User Group) is one mechanism to improve this communication. One way to start this dialog is to invite executive members from these different groups to meet at ORNL during Users Week September 13-17<sup>th</sup>.

The JINS building will be ready for occupancy in August 2010.

The guest house is on schedule to open at the end of calendar year 2010.

The national x-ray and neutron school at ORNL has been successfully completed for 2010. 63 attendees were in the school and there were 211 applicants.

Al is looking for suggestions for outreach: workshops at ORNL, workshops at other meetings, should the ORNL neutron booth be sent to specific meetings, what type of user meeting should be held next year? Currently planning on going to AAAS (Washington, D.C.) , the ACS southeast southwest regional meeting (New Orleans, November 30-December 4, 2010), the MRS in San Francisco, the APS march meeting (Dallas, February 2011) and the Bio-international meeting in June.

Please note that EPSCOR funding is able to support travel of users from EPSCOR states. Collaborative Research visits: there is money for faculty or graduate students to come for more extended stays (see website <http://neutrons.ornl.gov/crv/>).

### 3. SHUG election of officers and committee members (Cora)

Matthew Stone was nominated, and agreed to be the SHUG EC secretary

Vice-Chair, this vote will be done by email. Cora will distribute a message requesting for a vote for this officer position.

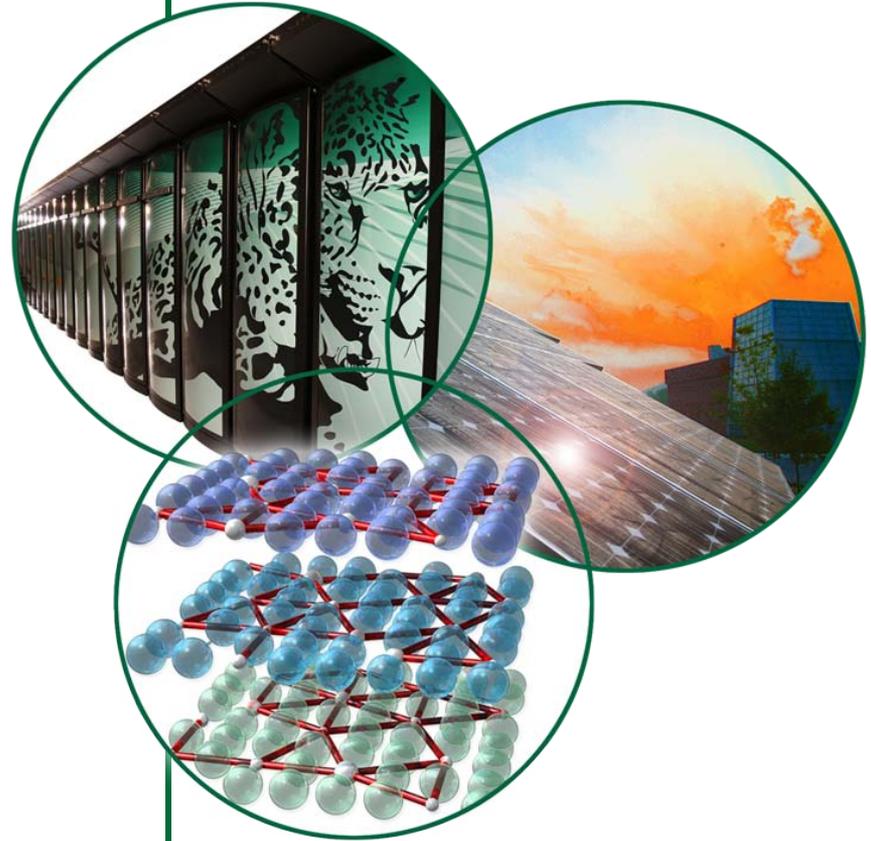
### 4. SHUG meeting at ACNS (Emily)

ACNS 2010 was held the last week of June 2010 in Ottawa Canada. A SNS HFIR User Group session was held on the third day of the meeting. Dean Myles presented information regarding both the SNS and HFIR facilities (attached). Lou Santodonato presented information regarding the sample environment progress at the SNS and HFIR facilities (attached). There were over 80 people in attendance at this session.

# SNS & HFIR User Group

Dean Myles at al..... (Lou)  
Neutron Scattering Sciences Division

ACNS, June, 2010



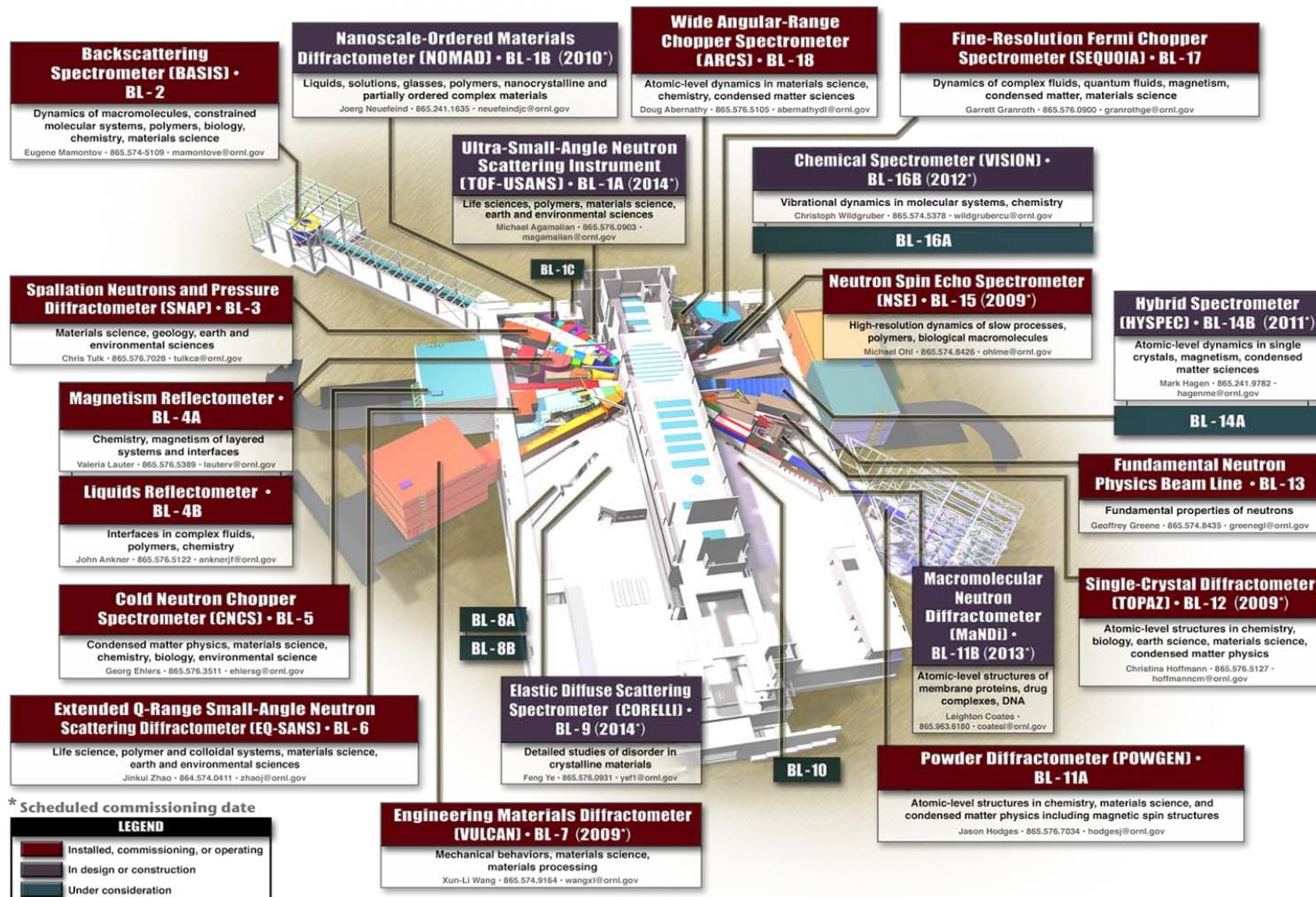
# A world leading science center and user facility for neutron scattering research

- Carry out world class research
- Provide an outstanding User Science Program
- Develop cross cutting signature science programs and partnerships
- Stay at the leading edge of neutron science by developing new capabilities, instruments, and tools



# SNS instruments

13 operating (6 in user program, 7 in commissioning) plus 6 in construction

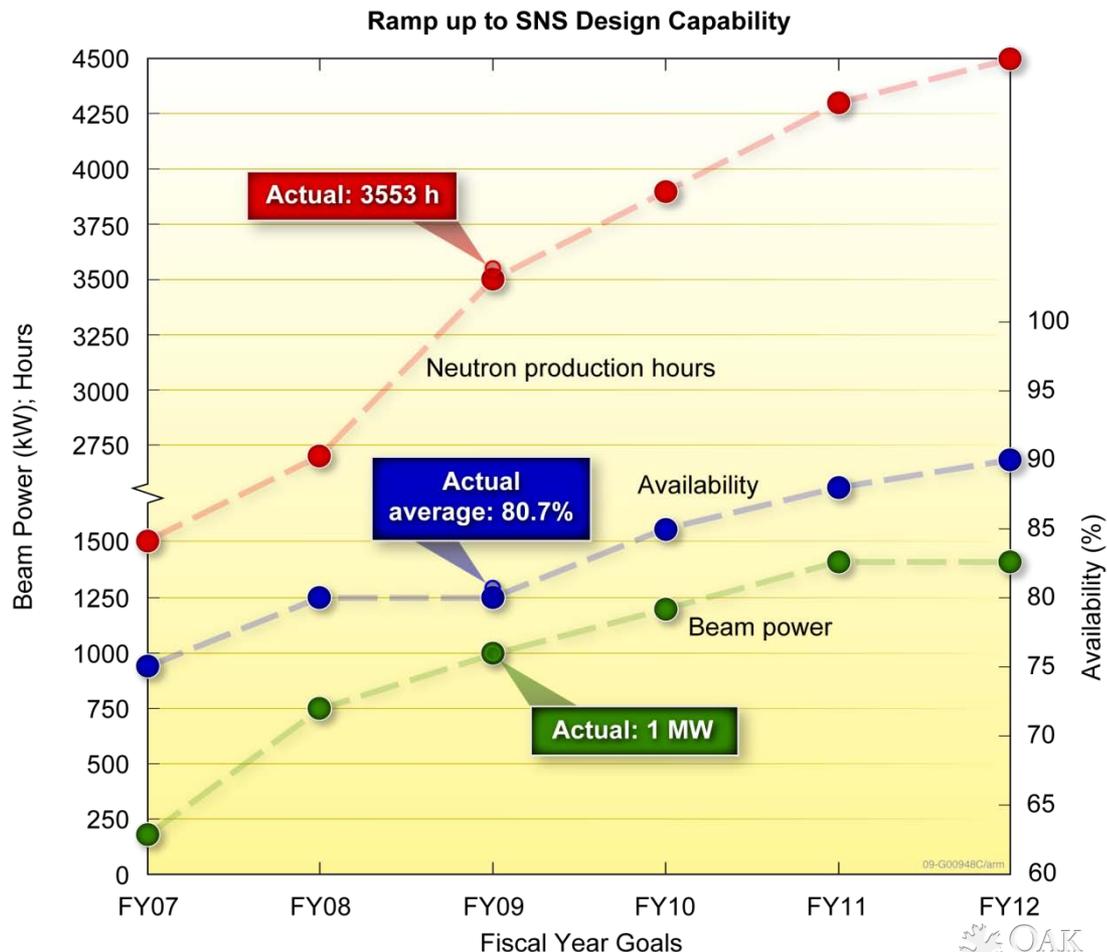


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# SNS Operations: beam power will reach 1.2 MW by 2010 and 1.4 MW by 2011

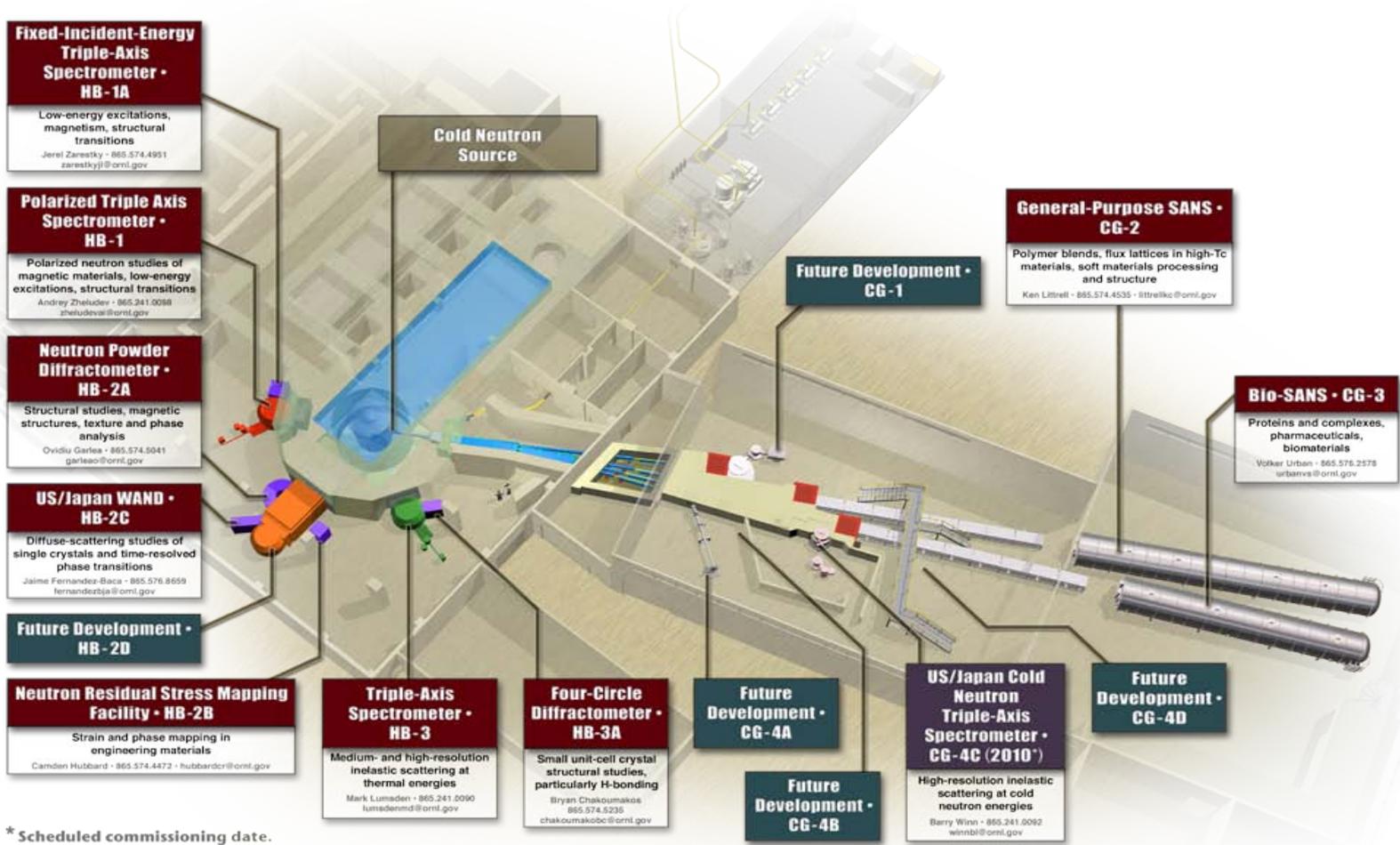
## SNS Operating Statistics (FY 2009)

- Neutron production hours: 3553
- Average availability 80.7%; availability as high as 98%
- Beam power on target: 1 MW
- Proton bunch intensity:  $1.55 \times 10^{14}$  protons per pulse



# HFIR instruments

9 operating, plus 2 in construction and 1 in development

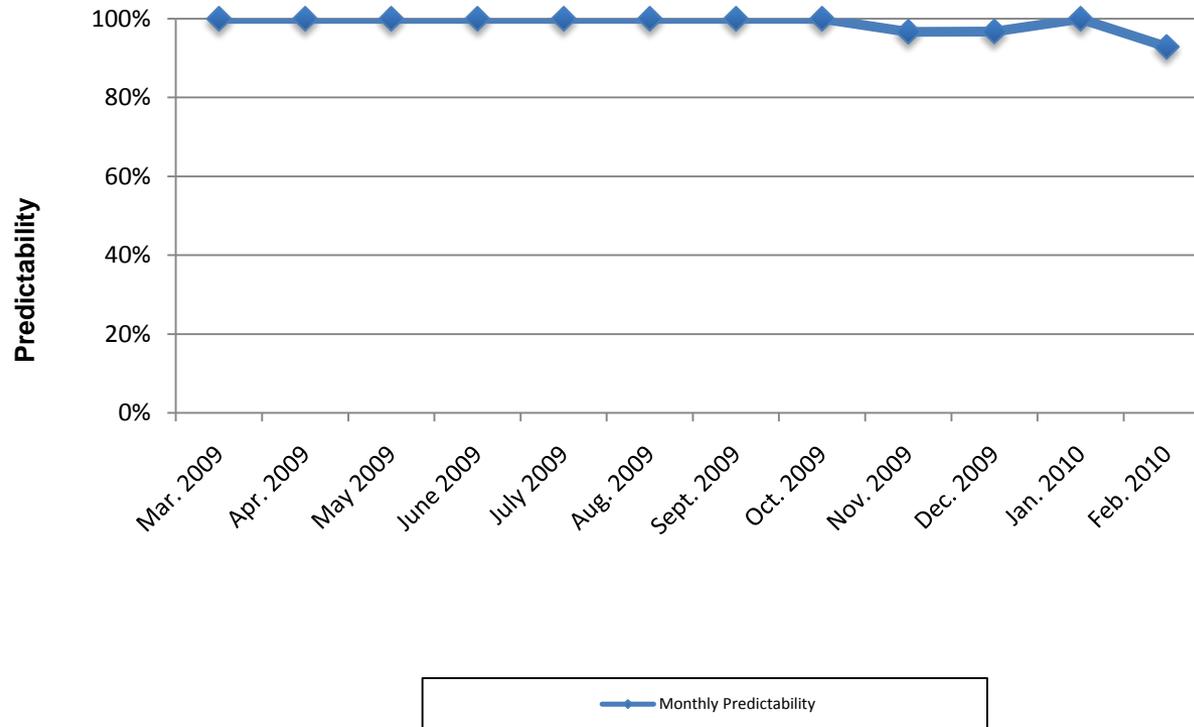


\* Scheduled commissioning date.

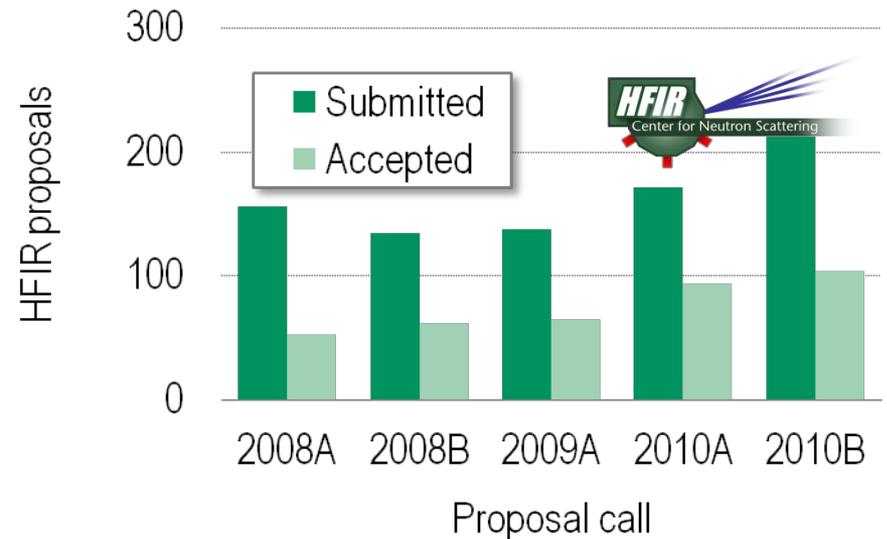
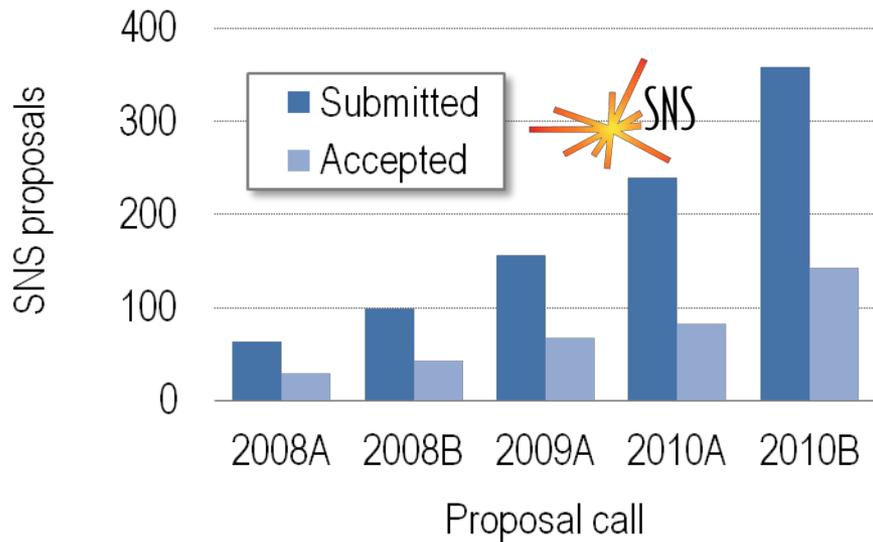
LEGEND	
<span style="display:inline-block; width:15px; height:10px; background-color:red; border:1px solid black;"></span>	Installed, commissioning, or operating
<span style="display:inline-block; width:15px; height:10px; background-color:purple; border:1px solid black;"></span>	In design or construction
<span style="display:inline-block; width:15px; height:10px; background-color:blue; border:1px solid black;"></span>	Under consideration

# HFIR Operations:

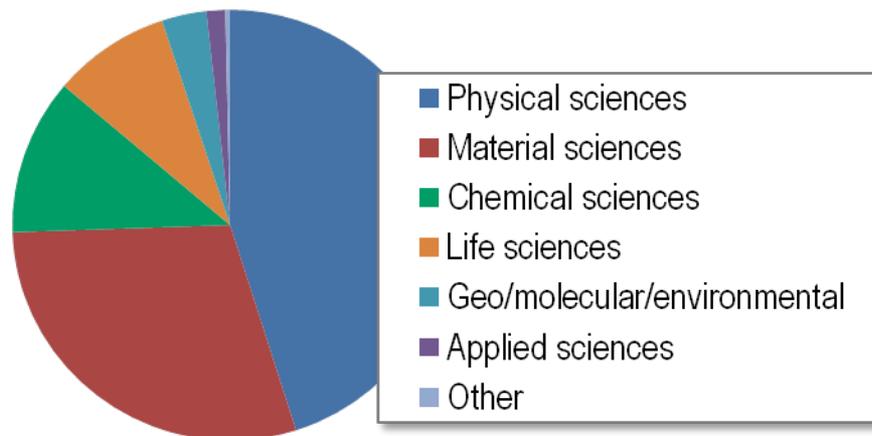
EOC 426 Refueling outage ended in February with cycle 427 starting on February 19th at 0915 on fuel elements 427-I and 426-O. Cycle 427 continued into March accumulating 815.21 MWd in February.



# The user community is growing with the buildup of instruments



Distribution of proposals for 2010B by scientific area



# NSSD staffing: >65 new positions opened

- *Building a strong ORNL team, balanced across beam line, user program and science needs*
- ORNL jobs: <http://jobs.ornl.gov/>
  - Powder diffraction group leader
  - SANS instrument scientist
  - Senior Scientist: energy materials, environmental geosciences, nano-structured materials, and biological systems
  - Scientific computing scientist for SANS and reflectometry
- ORAU positions: <http://www.ornl.gov/orise/edu/ornl/default.htm>
  - Entry-level (5 year) trial instrument scientist positions
  - Postdoctoral fellowships
  - Post-masters instrument associates

# Excellence in Science

## Building critical mass and experience

Science Theme	Focus areas
Condensed Matter Sciences	<ul style="list-style-type: none"> <li>• Correlated electrons</li> <li>• Magnetism</li> <li>• Superconductivity</li> <li>• Phase transitions</li> </ul>
Biological and Biomedical Sciences	<ul style="list-style-type: none"> <li>• Bio-energy and bio-fuels</li> <li>• Bioremediation</li> <li>• Human health</li> <li>• Pharmaceuticals</li> </ul>
Materials Science and Engineering	<ul style="list-style-type: none"> <li>• Advanced ceramics</li> <li>• Super alloys</li> <li>• Composites and nanomaterials</li> <li>• Engineering systems</li> </ul>
Soft Matter Science	<ul style="list-style-type: none"> <li>• Nano-structured materials</li> <li>• Surfactants/colloids/micelles</li> <li>• Biomimetic materials</li> </ul>
Materials Chemistry	<ul style="list-style-type: none"> <li>• Energy materials and storage</li> <li>• Smart materials</li> <li>• Crystal engineering</li> </ul>
Environmental Geosciences	<ul style="list-style-type: none"> <li>• Geosciences</li> <li>• Liquid and amorphous</li> <li>• Materials under extreme environments</li> </ul>



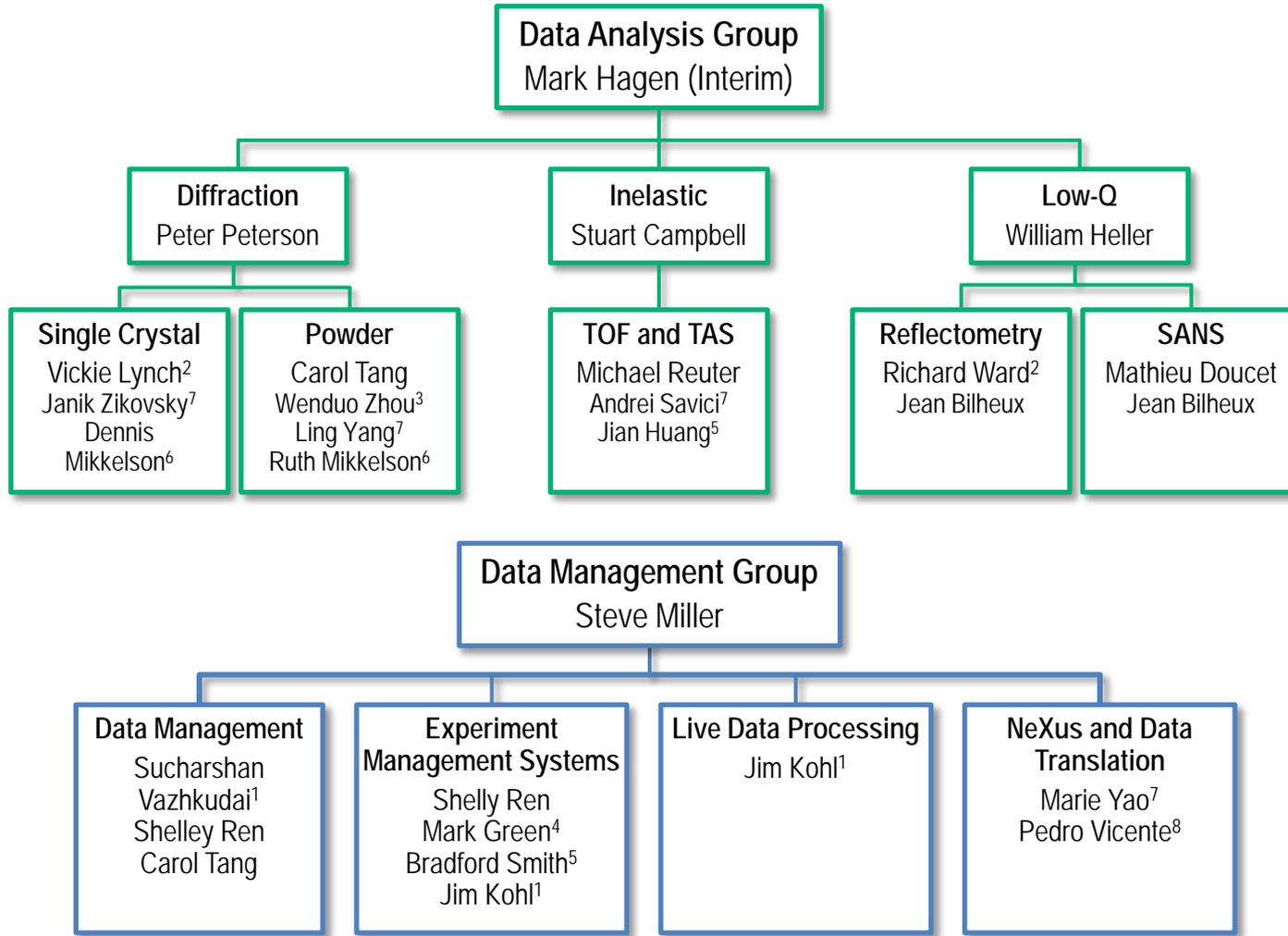
# Delivering excellence in science and operations

## Key enablers

Instrument Software	<ul style="list-style-type: none"><li>• Focused on science structure</li></ul>
Sample Environment	<ul style="list-style-type: none"><li>• Science support and innovation</li></ul>
Instrument Support Groups	<ul style="list-style-type: none"><li>• User surveys consistently rank staff support highly</li></ul>
Science Support Laboratories	<ul style="list-style-type: none"><li>• X-ray characterization suite (with CNMS)</li><li>• Sample synthesis and characterization</li></ul>
Instrument Core User Groups	<ul style="list-style-type: none"><li>• Continual evaluation of operating instrument effectiveness</li><li>• Core user engagement in commissioning new instruments – Extended Commissioning Plan (ECP)</li></ul>
Sabbatical and Visitor Program	<ul style="list-style-type: none"><li>• Faculty sabbaticals and secondments</li><li>• Internships for Students and Post-Docs</li><li>• EPSCoR Travel grants for faculty and students</li></ul>



# Instrument software Focused on science structure



<sup>1</sup> ORNL Computer Science and Mathematics

<sup>2</sup> ORNL Computational Sciences and Engineering

<sup>3</sup> NSSD Data Acquisition and Controls Group

<sup>4</sup> Tech-X Corporation

<sup>5</sup> University of Tennessee, Knoxville

<sup>6</sup> University of Wisconsin, Stout

<sup>7</sup> ORISE

<sup>8</sup> Space Research Inc.

# Instrument software: Focused on science

## Generation 1: Today

- Stabilize the current software situation
- Provide operating instruments with efficient data reduction software
- Ensure that upcoming instruments have reliable reduction software

## Generation II: Next 2 years

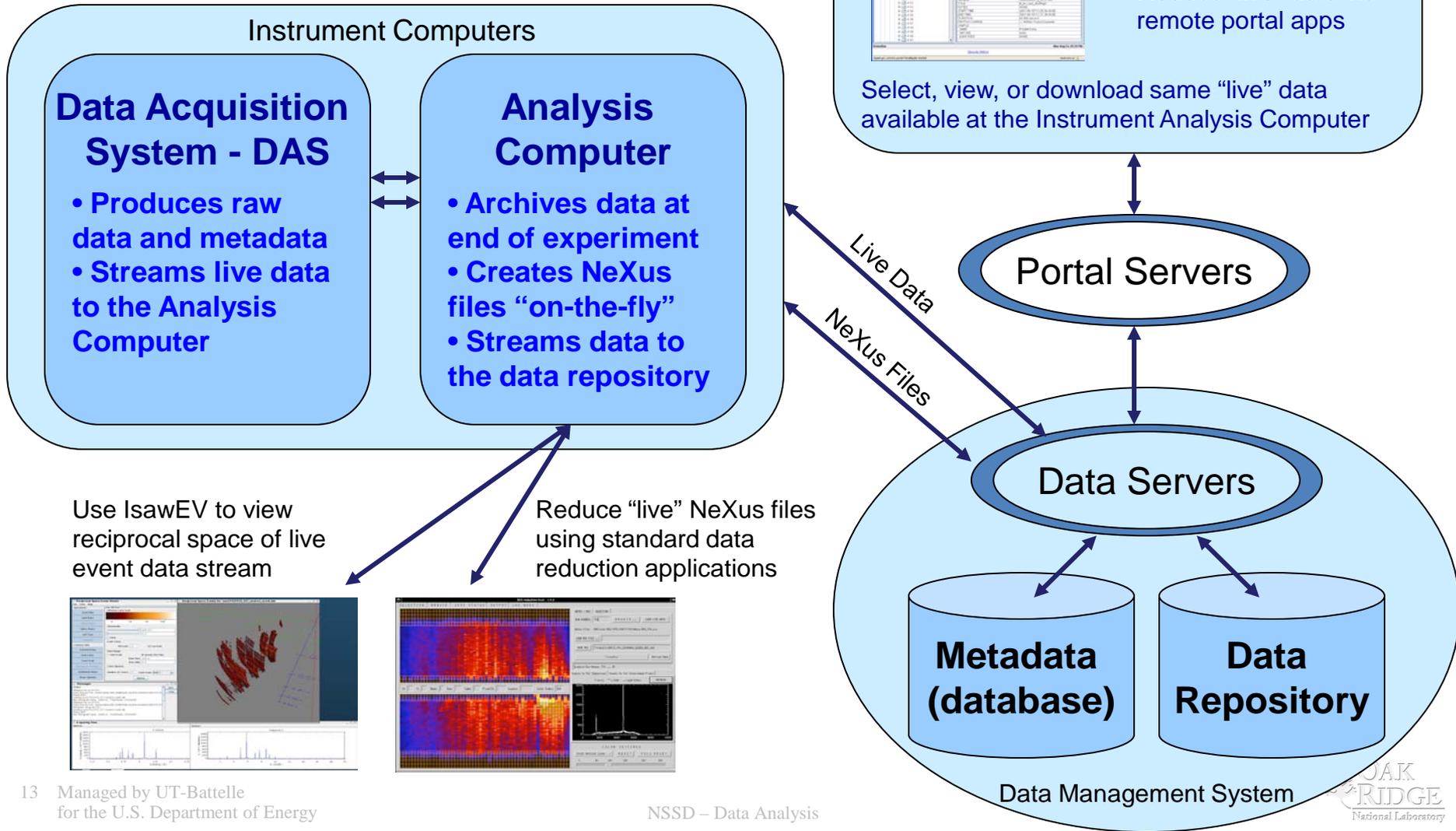
- Create a single high-performance data reduction workbench for all instruments that works at SNS/HFIR and can be distributed to users
- Incorporate Powder and SANS software from DANSE
- Build in automated reduction and parametric/real-time features

## Generation III: Long-term outlook

- Advanced analysis methods utilizing modeling, simulation, DFT, etc.

# Live Data at SNS

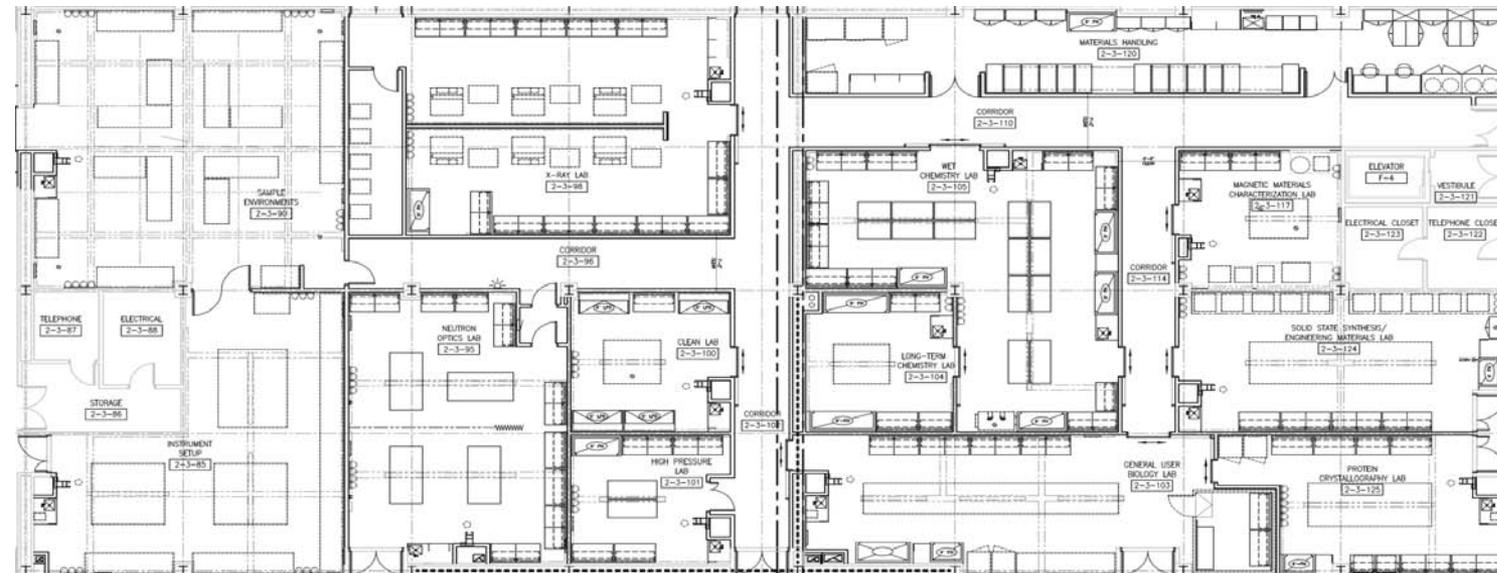
View and process near-real-time data on the Analysis Computers and via the Neutron Science Portal



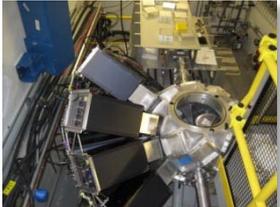
# User Support Laboratories:

User survey: 913 surveys - 170 detailed responses.

- HFIR Cold Guide Hall (Operational)
- SNS Experiment Hall (Operational)
- SNS Central Labs and Offices (will operate in July)
  - Deuterium labeling laboratories with CSMB and CNMS
  - Joint X-ray Characterization Laboratory with CNMS
  - Magnetic Materials Characterization Laboratory with CNMS

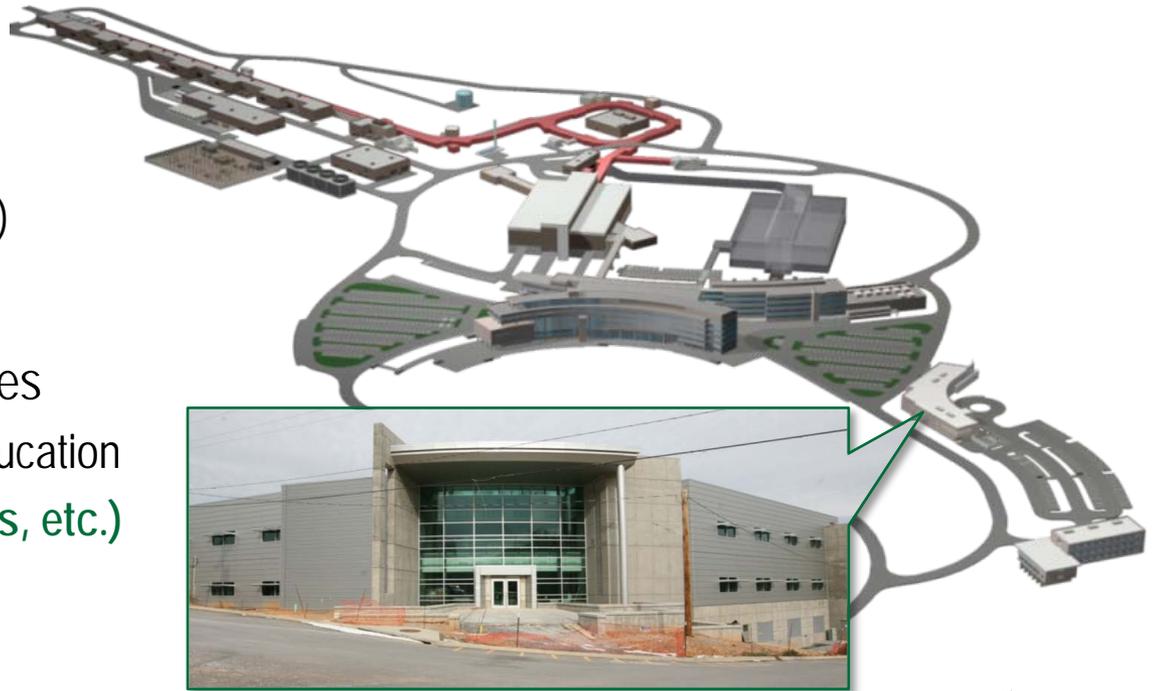


# New instruments – ready for science

	Instrument	CD4 date	ECP end date	Core user (affiliation)
	<b>SEQUOIA (BL 17)</b>	September 2008	IRR for users complete science review TBD	<ul style="list-style-type: none"> <li>• Bruce Gaulin (McMaster University)</li> </ul>
	<b>POWGEN (BL11a)</b>	December 2008	September 2010	<ul style="list-style-type: none"> <li>• Mike Crawford (DuPont)</li> <li>• Angus Wilkinson (Georgia Tech)</li> <li>• Peter Khalifah (Stony Brook University)</li> <li>• Andrew Payzant (ORNL, CNMS)</li> </ul>
	<b>EQ-SANS (BL 6)</b>	December 2008	October 2010	<ul style="list-style-type: none"> <li>• Sow-Hsin Chen (MIT)</li> <li>• Greg Beaucage (University of Cincinnati)</li> <li>• Sheng Dai (ORNL, CNMS)</li> <li>• Besim Ogretman (University of South Carolina)</li> </ul>
	<b>VULCAN (BL 7)</b>	June 2009	December 2010	<ul style="list-style-type: none"> <li>• Tom Holden (Northern Stress Technologies)</li> <li>• Bjorn Clausen (LANL)</li> <li>• Sven Vogel (LANL)</li> <li>• Zhili Feng (ORNL)</li> </ul>
	<b>TOPAZ (BL 12)</b>	August 2009	September 2010	<ul style="list-style-type: none"> <li>• Art Schultz (former IPNS SCD Inst. scientist)</li> <li>• Gary McIntyre (ILL)</li> <li>• Bo Iverson (Aarhus University)</li> <li>• Joe Ng (University of Alabama–Huntsville)</li> </ul>

# Building a vibrant science community and constituency

- SHUG and Instrument Core User Groups:
  - Invested in facility, staff and science
  - Drive leading-edge science – challenge capabilities
  - Demand continual improvement and enhanced capabilities
- Science Review Committees:
  - Spring/Fall, 100 experts on site
- Sabbatical and Visitor Program
  - Science symposia (with Science centers and JINS)
  - Fellowships/sabbaticals
- Joint Institute for Neutron Sciences
  - Partnership for Science and Education
  - **Strategic partnerships (EFRCs, etc.)**
  - Workshops and schools



# Visitor & Collaborative Research Program

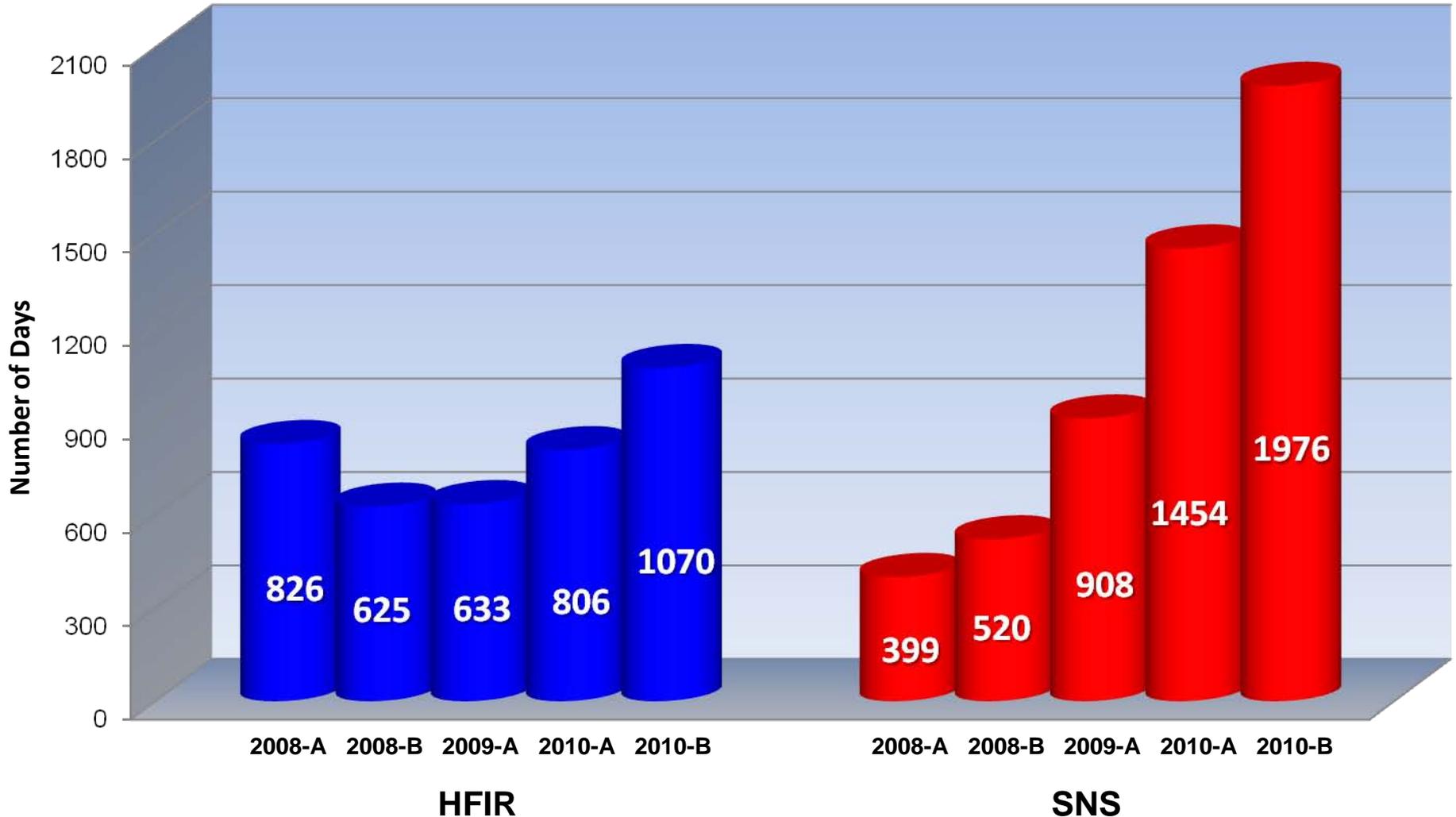
- Sabbatical program
  - Short stay: summer salary -> 12 months
  - Secondments: 1- 5 years
- Collaborative research program
  - (a) Faculty summer sabbaticals up to \$40,000
  - (b) Postdoctoral researchers up to \$30,000 per year
  - (c) Graduate students up to \$20,000 dollars per year
- Instructions at <http://neutrons.ornl.gov/crv/application.shtml>

# EPSCoR travel grants

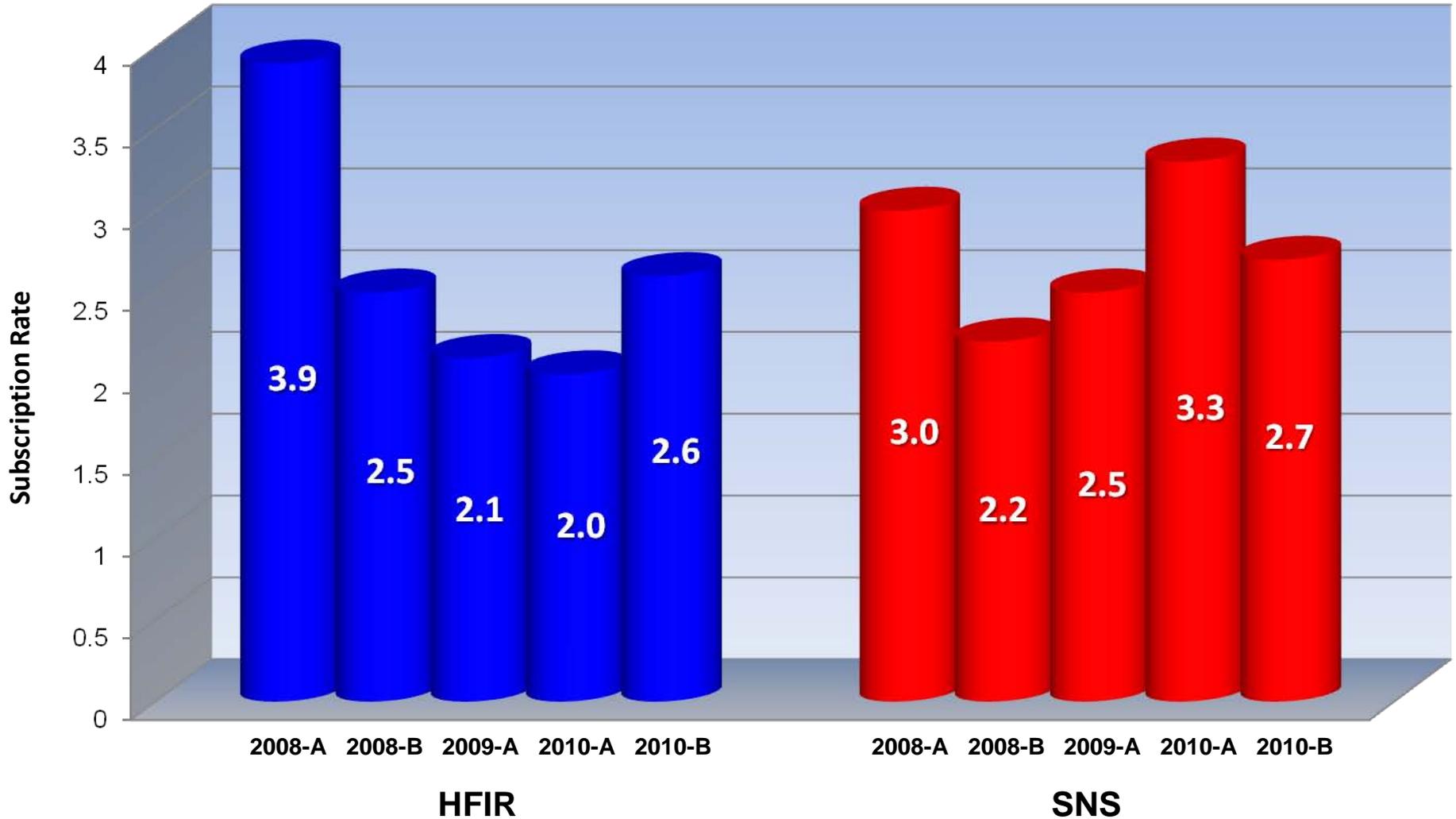
- To carry out experiments at the Spallation Neutron Source and the High Flux Isotope Reactor at Oak Ridge National Laboratory
- For travels to discuss experiments before and after the measurements
- Available through The University of Tennessee for a limited number of faculty and students from EPSCoR institutions
- Contact Hope Moore-Webb, [hmoore2@utk.edu](mailto:hmoore2@utk.edu), 865-974-1407 for details
- EPSCoR funding provided by the U.S. Department of Energy, Office of Basic Energy Sciences

# Questions ?

# General User Proposal Days Requested by Proposal Call



# Subscription Rates by Proposal Call



# Sample Environment Plans and Progress at the SNS & HFIR

SNS HFIR User Group Meeting

American Conference on Neutron Scattering

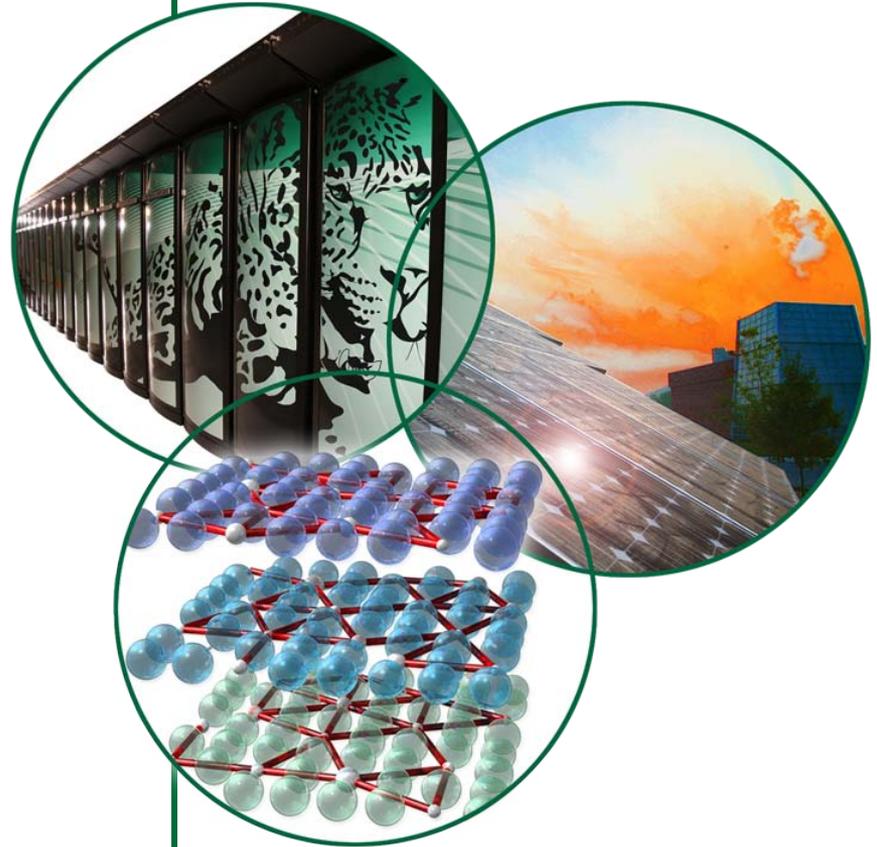
Ottawa, Canada

June 26 – 30, 2010

Lou Santodonato

Sample Environment Group Leader

Neutron Scattering Science Division



# 16 Tesla "Fat Sam" is Operational at SNS



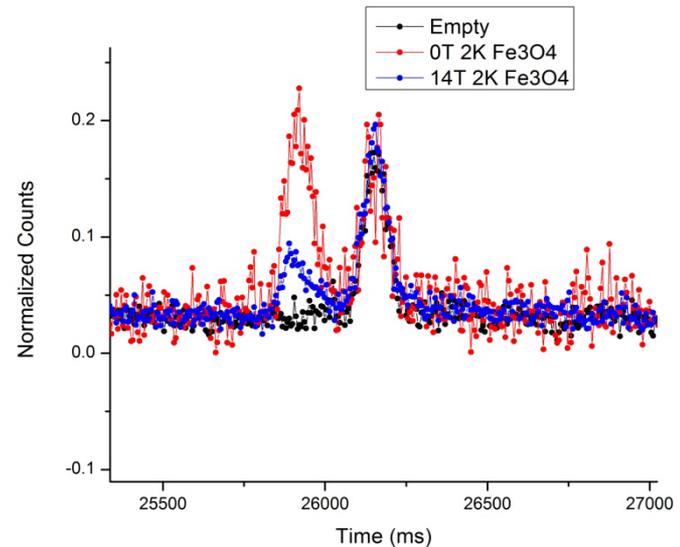
Switzerland  
April 2010

The 16T magnet moved to POWGEN on Monday 06/21/2010. The field was ramped up to 14T on Tuesday.

Data showing the (400) reflection of magnetite at  $T = 25.9\text{ms}$  ( $d = 2.1\text{\AA}$ ) 2K at zero field and 14T. The intensity difference is most likely due to the Preferred orientation of the powder due to the Presence of the field. The reflection next to it is from the magnet and shows no change in intensity.



Running on POWGEN  
June 2010



# Thank You!

- Scientists throughout the community are playing crucial role in improving our sample environment capabilities
  - Feedback
    - SHUG meetings
    - User surveys
    - Sample Environment Steering Committee
      - [Welcoming new members](#)
  - Collaborative development
    - User Partnership for Sample Environment Equipment Development
    - Several projects

# Sample Environment Steering Committee

## ➤ Charge

- Evaluate equipment inventory status
- Recommend resource priorities (purchasing, R&D projects, staffing)
- Help develop Five Year Plan

## ➤ Membership

- SHUG-nominated reps (presently two – should we have more?)
- One NSSD rep for each instrument group
- NSSD Chief Scientist & Deputy Division Director
- ORNL Center for Nanophase Materials Research – one rep
- Chair: Sample Environment Group Leader

## ➤ Reports and Recommendations Made to NSSD Deputy Division Director

## ➤ Meets Monthly at ORNL (external reps join by telecon)

# User Partnership for Sample Environment Equipment Development

- Launched in early 2010
- Mini-proposal form and info available on web
- \$20 k materials budget plus travel support
- First round of proposals was evaluated by Steering Committee in May 2010

## Projects Underway

- **Ultra High pressure Gas Loading Cell (Carnegie Inst., M. Guthrie)**
- **Crystal De-twinning Clamp Cell (Boston College., S. Wilson)**
- **Air Torch Furnace (Univ. Tennessee, P. K. Liaw)**
- **Electrolyte Chamber (Georgia Tech., G. Yushin)**
- **High Temperature Module for VULCAN Load Frame (UCF, R. Vaidyanathan)**
- **Gas Cell for Single Crystal Diffraction Experiments (U. C. Berkeley, J. Long)**
- **100 Bar Automated Gas Loading System (W. Kentucky Univ., E. Kintzel)**

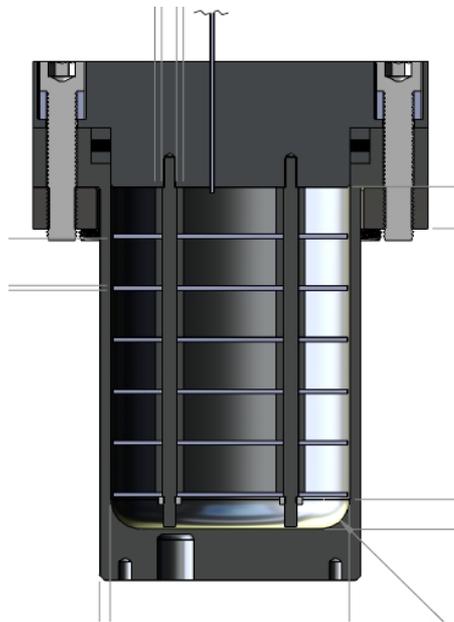
# Examples: Instrument-Integrated Standard Environments

- Rotating bottom-loading CCR with low background heat shields for TOF spectrometers
- Horizontal hot-stage CCR for Reflectometry
- SNAP-customized CCR rig
- Vulcan furnace, baby load frame
- Low-Q air furnace



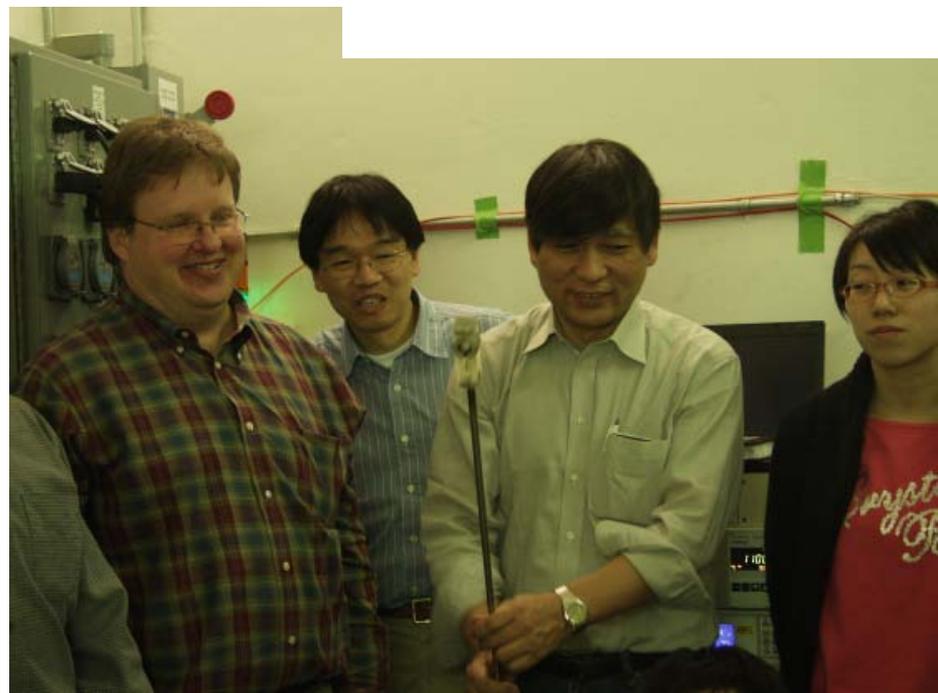
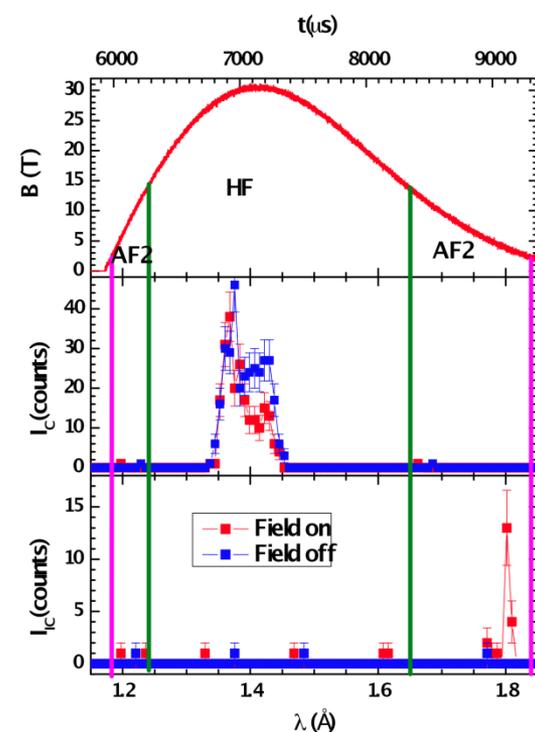
# Examples: Special Environments

- Sample sticks with gas loading, high current, and photo-excitation capability
- Pressure cells
- High capacity dil-fridge & cell for studying quantum liquids and solids



# Examples: Pushing the Limits

- Pulsed magnet collaboration
  - Diffraction at 30 Tesla!
  - Cross-cutting effort throughout NSSD, and international users
  
- High temperature (3000 C) conical nozzle levitator system
  - New arrival!



# So Many Requests!

## How Do We Gather, Prioritize and Track Them?

- **The process is open and online at:**  
<https://neutrons-shared.ornl.gov/sites/Sample%20Environment%20Steering%20Committee/default.aspx>
  - XCAMS login (same as experiment proposal)
  
- **SE Steering Committee plays big role**
  - Is your voice heard here?

# Thanks for Your Attention



X-ray equipment designated to move to the SNS CLO second floor laboratories (please see <http://neutrons.ornl.gov/facilities/SNS/userlabs.shtml>). These will be for external and internal use.

- **X-ray Diffraction**
  - **2-circle x-ray diffraction**  
q-2q X-ray powder diffraction with temperature-controlled sample environment. 77K to 1200K at 1 Bar, 273K to 1200K at 10 Bar. Reactive gasses such as H<sub>2</sub>, CO for varying chemical composition in sample environment.
  - **4-circle x-ray diffraction**  
4-circle plus translation stage, high temperature, in-plane thin film diffraction. Also texture, reflectivity, microdiffraction.
- **X-ray Fluorescence**
  - Bulk, powder, liquids, thin-film. Standardless and standards-based analysis. Mapping and multipoint capable with 50-micrometer resolution.
- SAXS (Anton Paar)

X-ray equipment which was requested internally by a group of NSCD scientists to be placed in these laboratories for external and internal use.

Piece of equipment	cost(x\$1000)	priority (within your subset-local)	Priority (NSSD-global)	Options (that can added/removed)	Cost of options(x\$1000)
Multiwire real time Laue Camera	163.3	1			
Generator for Laue System	45.393	(same as above)			
Smart Apex II single crystal diffractometer	251.8	2		Oxford N-Helix (28K - 300K)	98.75
Oxford cryostat for CNMS x-ray setup (Tmin=11K)	111.5	3			
PANanalytical high resolution powder x-ray	255.15	4		Phoenix cryostat	111.447